POSIVA 2016-03

Safety Evaluation for a KBS-3H Spent Nuclear Fuel Repository at Olkiluoto — Features, Events and Processes

Posiva Oy

May 2017
POSIVA 2016-03

Safety Evaluation for a KBS-3H Spent Nuclear Fuel Repository at Olkiluoto — Features, Events and Processes

Posiva Oy

May 2017

This work has been carried out under KBS-3H System Design project co-funded by Posiva and SKB.
Features, Events and Processes has the objective of presenting the main features, events and processes (FEPs) that are considered to be potentially significant for the long-term safety of a KBS-3H repository for spent nuclear fuel at Olkiluoto. The primary purpose of this report is to support KBS-3H Performance Assessment by ensuring that the evolution of the repository along time take account of all significant FEPs.

The FEPs are described for each relevant subsystem component or barrier (i.e. the spent nuclear fuel, the canister, the buffer and filling components, etc). Indicative parameter values are provided, in some cases, to illustrate the magnitude or rate of a FEP, but it is in the KBS-3H Performance Assessment that a complete set of numerical values that are used to estimate, through calculations, the long-term performance of the repository.

Many of the FEPs are interdependent and, therefore the descriptions also identify the most important direct couplings between the FEPs.
Tämän raportin tavoitteena on kuvata ne ilmiöt, tapahtumat ja prosessit (FEPit), joita pidetään poten­tiaalisesti merkittävinä käytetyn ydinpolttoaineen KBS-3H-tyyppisen loppusijoitustaitoksen pitkäaikaiseturvallisuudelle Olkiluodossa. Raportin pääasiallinen tarkoitus on tukea KBS-3H:n toimintakvy­analyysia (KBS-3H Performance Assessment) varmistamalla, että kaikki merkit­tävät FEPit on otettu huomioon kuvattaessa loppusijoitustilan kehityskulkua ajan myötä.

FEPit on kuvattu erikseen kullekin loppusijoitustärj­jestyelmän komponentille tai vapautumis­esteelle (näitä ovat mm. käytetty ydinpolttoaine, kapseli, puskuri ja täyttökomponentit). Joissain tapauksissa on myös esitetty viitteellisiä parametri­arvoja kuvaamaan prosessin suuruusluokkaa tai nopeutta, mutta lukuarvot, joita käytetään loppusijoitustilan pitkäaikaisen toimintakvyyn analysi­ointiin tarvittavissa laskussa, esitetään kattavasti KBS-3H Performance Assessment -raportissa.

Monet FEPit ovat toisistaan riippuvia ja sen tähden kuvauksissa luetellaan kaikkein tärkeimmät suorat kytkennät niiden välillä.

Avainsanat - Keywords
Ilmiöt, tapahtumat, prosessit, FEPit, Olkiluoto, käytetty ydinpolttoaine, kapseli, puskuri, asennuspakkausen suojakuori, täyttökomponentit, sul­keminen, kallioperä, toimintakvy­analyysi, KBS-3H.
FOREWORD

This report was compiled at Saanio & Riekkola Oy (S&R) by Nuria Marcos, Annika Hagros, Aimo Haatujärvi, Margit Snellman and Pirjo Hellä. Elina Hankiola participated in the final editing of the report. Barbara Pastina and Johannes Suikkanen (Posiva Oy) contributed to the updating of FEPs related to spent fuel and geosphere, respectively, Nick Smart contributed to all titanium components related FEPs. Simca Stroes-Gascoyne updated microbial activity FEP for the components it applies; Anssu Ranta-aho (Teollisuuden Voima Oy) reviewed the update of criticality and Teemu Laurila and Tim Schatz (B+Tech) updated the buffer related FEPs of mechanical erosion and chemical erosion, respectively.

The progress of the report was supervised by the KBS-3H Safety Evaluation Core Group consisting of Margit Snellman (S&R), Lasse Koskinen and Barbara Pastina (Posiva Oy), Jan-Olof Selroos (SKB), Aimo Haatujärvi, Pirjo Hellä, Nuria Marcos, Annika Hagros and Heini Reijonen (S&R) and Paul Smith (SAM Ltd). The members of the Core Group contributed to the report by providing comments during the working process.

The final report review was carried out by Mike Thorne (Mike Thorne and Associates Ltd). The received comments are greatly appreciated.
# TABLE OF CONTENTS

ABSTRACT

TIIVISTELMÄ

ABBREVIATIONS AND DEFINITIONS ................................................................. 5

1 INTRODUCTION .......................................................................................... 9
   1.1 Background ........................................................................................... 9
   1.2 The KBS-3H design alternative ............................................................ 9
   1.3 KBS-3H project phases and overall programme ..................................... 11
   1.4 Regulatory context for the management of spent nuclear fuel ............... 11
   1.5 Safety concept and safety functions ..................................................... 12
   1.6 KBS-3H Safety Case portfolio ............................................................... 17
   1.7 Quality assurance ................................................................................. 19
   1.8 Scope and structure of the present report ............................................. 20

2 THE APPLICATION OF FEPS TO THE SAFETY CASE ......................... 23
   2.1 Identification and screening of FEPS for potential significance ............. 23
   2.2 The classification of FEPS .................................................................. 24
   2.3 Organisation of FEPS and system components ...................................... 25
   2.4 FEPS couplings and interactions between system components ............. 30
      2.4.1 Couplings between individual FEPS ............................................. 30
      2.4.2 Component interactions ............................................................... 30
   2.5 The FEPS description template ............................................................ 32

3 SPENT NUCLEAR FUEL ....................................................................... 35
   3.1 Description .......................................................................................... 35
      3.1.1 Long-term safety and performance .............................................. 39
      3.1.2 Overview of the potentially significant FEPS ............................. 39
   3.2 System evolution FEPS ....................................................................... 45
      3.2.1 Radioactive decay (and in-growth) .............................................. 45
      3.2.2 Heat generation .......................................................................... 48
      3.2.3 Heat transfer .............................................................................. 49
      3.2.4 Structural alteration of the fuel pellets ........................................ 51
      3.2.5 Radiolysis of residual water (in an intact canister) ..................... 54
      3.2.6 Radiolysis of the canister water .................................................. 57
      3.2.7 Corrosion of cladding tubes and metallic fuel assembly parts ....... 59
      3.2.8 Alteration and dissolution of the fuel matrix ............................... 64
      3.2.9 Release of the labile fraction of the inventory .............................. 72
      3.2.10 Production of helium gas .......................................................... 75
      3.2.11 Criticality ................................................................................. 77
   3.3 Migration FEPS .................................................................................. 81
      3.3.1 Aqueous solubility and speciation .............................................. 81
      3.3.2 Precipitation and co-precipitation .............................................. 84
      3.3.3 Sorption .................................................................................... 88
      3.3.4 Diffusion in fuel pellets .............................................................. 89

4 CANISTER ............................................................................................ 93
   4.1 Description .......................................................................................... 93
      4.1.1 Long-term safety and performance .............................................. 95
      4.1.2 Overview of the potentially significant FEPS ............................. 96
   4.2 System evolution FEPS ....................................................................... 102
      4.2.1 Radiation attenuation ................................................................. 102
      4.2.2 Heat transfer ............................................................................. 104
4.2.3 Deformation ................................................................. 107
4.2.4 Thermal expansion of the canister ................................. 112
4.2.5 Corrosion of the copper overpack ................................. 115
4.2.6 Corrosion of the cast iron insert ................................... 128
4.2.7 Stress corrosion cracking .............................................. 133

4.3 Migration FEPs ............................................................... 138
4.3.1 Aqueous solubility and speciation ................................. 139
4.3.2 Precipitation and co-precipitation ................................. 140
4.3.3 Sorption ....................................................................... 141
4.3.4 Diffusion ....................................................................... 143
4.3.5 Advection ...................................................................... 144
4.3.6 Colloid transport ........................................................... 146
4.3.7 Gas transport ................................................................. 148

5 BUFFER ............................................................................. 151
5.1 Description ....................................................................... 151
5.1.1 Long-term safety and performance ................................. 153
5.1.2 Overview of the potentially significant FEPs ................... 154

5.2 System evolution FEPs ....................................................... 159
5.2.1 Heat transfer ................................................................. 159
5.2.2 Water uptake and swelling ............................................ 162
5.2.3 Mechanical erosion ....................................................... 167
5.2.4 Chemical erosion .......................................................... 170
5.2.5 Radiolysis of porewater .................................................. 173
5.2.6 Montmorillonite transformation .................................... 176
5.2.7 Alteration of accessory minerals .................................... 183
5.2.8 Microbial activity ........................................................ 187
5.2.9 Freezing and thawing .................................................... 197
5.2.10 Desiccation, formation of cracks .................................. 200

5.3 Migration FEPs ............................................................... 201
5.3.1 Aqueous solubility and speciation ................................. 201
5.3.2 Precipitation and co-precipitation ................................. 204
5.3.3 Sorption ....................................................................... 206
5.3.4 Diffusion ....................................................................... 210
5.3.5 Advection ...................................................................... 213
5.3.6 Colloid transport ........................................................... 214
5.3.7 Gas transport ................................................................. 217

6 SUPERCONTAINER SHELL AND MINOR TITANIUM COMPONENTS .......... 221
6.1 Description ....................................................................... 221
6.1.1 Long-term safety and performance ................................. 222
6.1.2 Overview of the potentially significant FEPs ................... 222

6.2 System evolution FEPs ....................................................... 224
6.2.1 Corrosion ...................................................................... 224
6.2.2 Deformation ................................................................. 231

6.3 Migration FEPs ............................................................... 234

7 FILLING COMPONENTS ....................................................... 235
7.1 Description ....................................................................... 235
7.1.1 Long-term safety and performance ................................. 235
7.1.2 Overview of the potentially significant FEPs ................... 236

7.2 System evolution FEPs ....................................................... 237
7.2.1 Heat transfer ................................................................. 237
7.2.2 Water uptake and swelling ............................................ 237
7.2.3 Mechanical erosion .............................................................. 237
7.2.4 Chemical erosion ............................................................... 237
7.2.5 Montmorillonite transformation .......................................... 237
7.2.6 Alteration of accessory minerals ........................................ 237
7.2.7 Microbial activity ............................................................... 237
7.2.8 Freezing and thawing ......................................................... 237
7.2.9 Desiccation, formation of cracks ....................................... 238

8 COMPARTMENT AND DRIFT PLUGS ........................................... 239
8.1 Description ............................................................................. 239
8.1.1 Long-term safety and performance .................................... 240
8.1.2 Overview of the potentially significant FEPs ....................... 240
8.2 System evolution FEPs .............................................................. 243
8.2.1 Corrosion ........................................................................... 243
8.2.2 Deformation (of titanium plugs) .......................................... 244
8.2.3 Degradation of the cast concrete for the fastening ring .......... 251
8.3 Migration FEPs ................................................................. 251
8.3.1 Diffusion ............................................................................ 252
8.3.2 Advection ........................................................................... 253
8.3.3 Gas transport ................................................................. 255

9 CLOSURE ...................................................................................... 257
9.1 Description ............................................................................. 257
9.1.1 Long-term safety and performance .................................... 258
9.1.2 Overview of the potentially significant FEPs ....................... 259
9.2 System evolution FEPs .............................................................. 260
9.2.1 Water uptake and swelling ................................................ 261
9.2.2 Mechanical erosion .............................................................. 263
9.2.3 Chemical erosion ............................................................... 265
9.2.4 Montmorillonite transformation .......................................... 268
9.2.5 Alteration of accessory minerals ........................................ 269
9.2.6 Microbial activity ............................................................... 271
9.2.7 Freezing and thawing (in closure backfill) ......................... 273
9.2.8 Chemical degradation (of closure plugs) ......................... 276
9.2.9 Physical degradation (of closure plugs) ............................. 281
9.2.10 Freezing and thawing (in closure plugs) ........................... 284
9.3 Migration FEPs ................................................................. 287
9.3.1 Transport through closure backfill and plugs .................... 287

10 GEOSPHERE ............................................................................... 293
10.1 Description ............................................................................. 293
10.1.1 Long-term safety and performance .................................... 296
10.1.2 Overview of the potentially significant FEPs ....................... 297
10.2 System evolution FEPs .............................................................. 303
10.2.1 Heat transfer ................................................................. 303
10.2.2 Stress redistribution .......................................................... 305
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.2.3</td>
<td>Reactivation-displacement along existing fractures</td>
<td>308</td>
</tr>
<tr>
<td>10.2.4</td>
<td>Rock mass damage</td>
<td>312</td>
</tr>
<tr>
<td>10.2.5</td>
<td>Creep</td>
<td>315</td>
</tr>
<tr>
<td>10.2.6</td>
<td>Erosion and sedimentation in fractures</td>
<td>317</td>
</tr>
<tr>
<td>10.2.7</td>
<td>Rock-water interaction</td>
<td>319</td>
</tr>
<tr>
<td>10.2.8</td>
<td>Methane hydrate formation</td>
<td>324</td>
</tr>
<tr>
<td>10.2.9</td>
<td>Salt exclusion</td>
<td>326</td>
</tr>
<tr>
<td>10.2.10</td>
<td>Microbial activity</td>
<td>329</td>
</tr>
<tr>
<td>10.3</td>
<td>Migration FEPs</td>
<td>332</td>
</tr>
<tr>
<td>10.3.1</td>
<td>Aqueous solubility and speciation</td>
<td>333</td>
</tr>
<tr>
<td>10.3.2</td>
<td>Precipitation and co-precipitation</td>
<td>337</td>
</tr>
<tr>
<td>10.3.3</td>
<td>Sorption</td>
<td>339</td>
</tr>
<tr>
<td>10.3.4</td>
<td>Diffusion and matrix diffusion</td>
<td>341</td>
</tr>
<tr>
<td>10.3.5</td>
<td>Groundwater flow and advective transport</td>
<td>345</td>
</tr>
<tr>
<td>10.3.6</td>
<td>Colloid transport</td>
<td>350</td>
</tr>
<tr>
<td>10.3.7</td>
<td>Gas transport</td>
<td>353</td>
</tr>
</tbody>
</table>
### ABBREVIATIONS AND DEFINITIONS

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>3DEC</td>
<td>A rock mechanics code, a three-dimensional numerical program based on distinct element method for discontinuum modelling.</td>
</tr>
<tr>
<td>Air evacuation</td>
<td>Removing of air from a drift compartment through pipes during artificial watering.</td>
</tr>
<tr>
<td>ANME</td>
<td>ANaerobic MEthanotrophic archaea.</td>
</tr>
<tr>
<td>Artificial watering</td>
<td>Adding water through pipes to drift compartments to facilitate buffer saturation.</td>
</tr>
<tr>
<td>Buffer</td>
<td>Swelling clay material used to surround the canisters in the supercontainers and as distance blocks between the supercontainers.</td>
</tr>
<tr>
<td>BWR</td>
<td>Boiling Water Reactor (see also OL1−2).</td>
</tr>
<tr>
<td>CEC</td>
<td>Cation Exchange Capacity.</td>
</tr>
<tr>
<td>Closure</td>
<td>Closure is a structural part of the disposal facility and it includes backfill and plugs in repository accesses, central tunnels, miscellaneous excavations, and investigation holes. Different types of closure components may be used in different parts of the disposal facility. Closure shall complete the isolation of spent nuclear fuel and support the safety functions of the other barriers.</td>
</tr>
<tr>
<td>Compartment plug</td>
<td>A metal plug in the middle of a deposition drift, used for sectioning the drift into two compartments.</td>
</tr>
<tr>
<td>CP</td>
<td>Compartment plug.</td>
</tr>
<tr>
<td>Cu-OF</td>
<td>Oxygen Free, High Conductivity Copper.</td>
</tr>
<tr>
<td>DAWE</td>
<td>Drainage, Artificial Watering and air Evacuation. The KBS-3H reference design alternative.</td>
</tr>
<tr>
<td>Deposition drift</td>
<td>A 100–300 m long horizontal hole with a circular profile, where the supercontainers are emplaced consecutively.</td>
</tr>
<tr>
<td>Deposition niche</td>
<td>A space excavated between the two parallel central tunnels hosting the deposition equipment used for the two opposite drifts.</td>
</tr>
<tr>
<td>DIC</td>
<td>Dissolved Inorganic Carbon.</td>
</tr>
<tr>
<td>Disposal facility</td>
<td>An entirety comprising the rooms for the disposal of the waste packages and the adjoining underground and above-ground auxiliary facilities.</td>
</tr>
<tr>
<td>Disposal system</td>
<td>Repository system + surface environment.</td>
</tr>
<tr>
<td>Distance blocks</td>
<td>Bentonite blocks between the supercontainers. The role of the distance blocks is to provide separation answering up to hydraulic and thermal requirements.</td>
</tr>
<tr>
<td>DP</td>
<td>Drift plug.</td>
</tr>
<tr>
<td>Term</td>
<td>Definition</td>
</tr>
<tr>
<td>--------------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>Drift plug</td>
<td>A metal plug to seal the whole deposition drift.</td>
</tr>
<tr>
<td>EBS</td>
<td>Engineered Barrier System. Includes (in KBS-3H) the following components: canister, buffer, filling components, plugs and closure.</td>
</tr>
<tr>
<td>EBW</td>
<td>Electron Beam Welding.</td>
</tr>
<tr>
<td>EdZ</td>
<td>Excavation disturbed Zone; section of the rock where less intensive excavation-induced changes occur that are potentially reversible.</td>
</tr>
<tr>
<td>EDZ</td>
<td>Excavation Damaged Zone; section of the rock that is irreversibly damaged by the excavation of underground openings.</td>
</tr>
<tr>
<td>Eh</td>
<td>Redox potential.</td>
</tr>
<tr>
<td>EPR</td>
<td>European Pressurised water Reactor (trade name for the pressurised water reactor used at OL3).</td>
</tr>
<tr>
<td>FEP</td>
<td>Feature, Event or Process (or as plural FEPs: Features, Events and Processes).</td>
</tr>
<tr>
<td>Filling block</td>
<td>A filling component that is emplaced at drift locations where supercontainer sections cannot be positioned because inflow is higher than the positioning criterion.</td>
</tr>
<tr>
<td>Filling component</td>
<td>A clay component in a deposition drift needed at locations where supercontainers and distance blocks cannot be emplaced.</td>
</tr>
<tr>
<td>Fracod&lt;sup&gt;2D&lt;/sup&gt;</td>
<td>A fracture mechanics code based on the Displacement Discontinuity Method (DDM) that has been used for predicting potential for spalling.</td>
</tr>
<tr>
<td>FSW</td>
<td>Friction Stir Welding.</td>
</tr>
<tr>
<td>HRL</td>
<td>Hard Rock Laboratory (at Äspö).</td>
</tr>
<tr>
<td>HVDC</td>
<td>High Voltage Direct Current.</td>
</tr>
<tr>
<td>Initial state</td>
<td>The state when direct control over a specific part of the system ceases and only limited information can be obtained on the subsequent development of conditions in that part of the system or its near-field. For surface environment, initial state is defined as the present conditions.</td>
</tr>
<tr>
<td>KBS</td>
<td>(Kärnbränslesäkerhet). The method for implementing the spent nuclear fuel disposal concept based on multiple barriers (as required in Sweden and in Finland). KBS-1, KBS-2 and KBS-3 are variations of this method.</td>
</tr>
<tr>
<td>KBS-3</td>
<td>An abbreviation of kärnbränslesäkerhet (nuclear fuel safety) version 3. The KBS-3 method for</td>
</tr>
</tbody>
</table>
implementing the spent nuclear fuel disposal concept based on multiple barriers.

KBS-3H
(Kärnbränslesäkerhet 3-Horisontell). Design alternative of the KBS-3 method in which several spent nuclear fuel canisters are emplaced horizontally in each deposition drift.

KBS-3V
(Kärnbränslesäkerhet 3-Vertikal). The reference design alternative of the KBS-3 method, in which the spent nuclear fuel canisters are emplaced in individual vertical deposition holes.

\( K_d \)
Distribution coefficient.

KR
(Deep) drill hole (in Finnish: KairanReikä).

LDF
Layout-Determining Feature.

LET
Linear Energy Transfer.

LLW
Low Level (radioactive) Waste.

LO1−2
Loviisa reactors 1 and 2; pressurised water reactors of type VVER-440.

LOT
The long-term test of buffer material (at Äspö).

Low-pH concrete
A concrete with a pH of the leachate < 10, with a short period of initially higher pH of the leachate, about 11.

MIC
Microbiologically Influenced Corrosion.

MICADO
Model Uncertainty for the Mechanism of Dissolution of Spent Fuel in Nuclear Waste Repository.

MX-80
Commercial name of a high-grade sodium bentonite from Wyoming, U.S., with a montmorillonite content of 75–90 %.

NDA
Nuclear Decommissioning Authority.

NF-PRO
The Near Field Processes research project (EC funded project).

OL1−2
Olkiluoto 1 and 2 reactors. Boiling water reactors.

OL3

OL-KR
Olkiluoto (deep) drill hole.

ONKALO
Underground rock characterisation facility at Olkiluoto, Finland.

OPC
Ordinary Portland Cement.

PLFA
Phospholipid Fatty Acid.

POSE
Posiva’s Olkiluoto Spalling Experiment.

PRECCI
Programme de Recherches sur l’Evolution à long-terme des Colis de Combustibles Irradiés.

PWR
Pressurised Water Reactor.
RD&D: Research, Development & Demonstration (or Research, technical Development and Design).

RSC: Rock Suitability Classification.

RTD: Research, Technical development and Design (acronym RD&D is also used).

SCC: Stress Corrosion Cracking.

SKB: Swedish Nuclear Fuel and Waste Management Company.

SRB: Sulphate-Reducing Bacteria.

STUK: Finnish Radiation and Nuclear Safety Authority.

Supercontainer: Assembly consisting of a canister surrounded by bentonite clay and a perforated titanium shell.

Supercontainer section: A drift section containing one supercontainer and two halves of distance block, one half on both sides of the supercontainer.

SURE: Sulphate REduction experiment (in ONKALO).

TDS: Total Dissolved Solids.


THMCB: Thermo-Hydraulic-Mechanical-Chemical-Biological.

Transition block: The part of the filling component “transition zone” that is made of solid clay blocks.

Transition zone: A filling component needed next to a plug in a deposition drift. Composed of a transition block and clay pellets.

TURVA-2012: Posiva’s safety case supporting the construction licence application submitted in 2012 for the Olkiluoto spent nuclear fuel encapsulation plant and disposal facility (KBS-3V) at Olkiluoto. The name TURVA is Finnish for safety.

VVER-440: Pressurised water reactor type at Loviisa (see also LO1–2).

YVL: STUK’s (see STUK) regulatory guide series for nuclear facilities.
1 INTRODUCTION

1.1 Background

On assignment by its owners, Fortum Power and Heat Oy and Teollisuuden Voima Oyj, Posiva Oy will manage the disposal of spent nuclear fuel from the Loviisa and Olkiluoto nuclear power plants. At Loviisa, two pressurised water reactors (VVER-440) are in operation (LO1 and LO2); at Olkiluoto, two boiling water reactors are operating (OL1 and OL2) and one pressurised water reactor (OL3) is under construction. Plans also exist for a fourth nuclear power unit (OL4) at Olkiluoto, although they are currently not being put forward. At both sites there are facilities available for interim storage of the spent nuclear fuel before disposal.

In 2001, the Parliament of Finland endorsed a Decision-in-Principle (DiP) whereby the spent nuclear fuel generated during the operational lives of the operating Loviisa and Olkiluoto reactors will be disposed in a geological repository at Olkiluoto. This first DiP allowed for the disposal of a maximum amount of spent nuclear fuel corresponding to 6500 tonnes of uranium (tU) from the four operating reactors. Subsequently, additional DiPs were issued in 2002 and 2010 allowing extension of the repository (up to 9000 tU) to also accommodate spent nuclear fuel from the operations of the OL3 reactor and the planned OL4 reactor. In 2012, Posiva submitted a construction licence application for a disposal facility at Olkiluoto, supported by a safety case, TURVA-2012 (summarised in Posiva 2012a). In November 2015, the construction licence was granted. The safety case was based on the KBS-3V design alternative with vertical deposition holes. The horizontal design alternative KBS-3H has been studied for more than 15 years (see Section 1.3) due to its several advantages, e.g. a significantly smaller volume of excavation needed for the repository.

1.2 The KBS-3H design alternative

The 2001 DiP states that disposal of spent nuclear fuel shall take place in a geological repository at the Olkiluoto site, developed according to the KBS-3 method. In the KBS-3 method, spent nuclear fuel encapsulated in water-tight and gas-tight sealed copper canisters with a mechanical-load-bearing insert is emplaced deep underground in a geological repository constructed in the bedrock. According to the DiP, the repository shall be located at a minimum depth of 400 m.

In the KBS-3H design alternative, canisters are emplaced horizontally in deposition drifts with a maximum length of 300 m (Figure 1-1). Unlike the KBS-3V design (reference design), the KBS-3H variant utilises a prefabricated installation package called a supercontainer, which is assembled in an industrial process at the canister reloading station before disposal. The supercontainer consists of a perforated metallic shell with a copper canister installed inside it, surrounded by compacted bentonite (Figure 1-2). Bentonite is also used in distance blocks between the supercontainers. Together, the distance blocks and the bentonite originally inside the supercontainers are termed the buffer.
Figure 1-1. Schematic drawing of the KBS-3V reference design (to the left) and the KBS-3H alternative (to the right). Courtesy of SKB, Illustrator: Jan Rojmar.

Figure 1-2. Detailed illustration of the KBS-3H supercontainer (based on Posiva 2012b, Figure 2-1). The diameter of the supercontainer is 1761 mm (length depends on fuel type).
The DAwE (Drainage, Artificial Watering and air Evacuation) design has recently been selected as the reference design for KBS-3H. The artificial watering used in the DAwE design guarantees that a certain amount of water is accessible for initial buffer swelling (Posiva 2013a).

1.3 KBS-3H project phases and overall programme

The development of the KBS-3H design alternative has been carried out mainly as a joint project between SKB and Posiva. Some tasks, especially related to site-specific issues, such as e.g. layout adaptation at Olkiluoto, have been carried out by Posiva alone.

In 2001, Posiva and SKB decided jointly to carry out a Research, Development & Demonstration (RD&D) programme for a KBS-3 repository with horizontal emplacement (SKB 2001). This programme has provided a basis for the development of the KBS-3H design.

During 2002–2003, the development of KBS-3H was initiated with the Feasibility study phase, which dealt mainly with technical matters such as rock excavation techniques, the handling of deposition equipment and the design of the supercontainer. The main conclusion from this project phase was that the design is technically feasible and would meet the requirements for long-term safety (SKB 2004).

The Demonstration phase in 2004–2007 was planned on the basis of the understanding developed up to 2003 and the issues identified that needed to be resolved to further demonstrate the feasibility of the KBS-3H design. Thus, the overall objectives for this project phase were to use practical trials to demonstrate that the horizontal deposition alternative was technically feasible and that it fulfilled the same long-term safety requirements as the reference design KBS-3V (Posiva 2008, 2013a).

The Demonstration phase was followed by the Complementary studies of horizontal emplacement KBS-3H, 2008–2010 (Posiva 2013a), including critical issues on design and material selection, and plans for the current KBS-3H System Design (2011–2016) phase. The objective of the System Design phase is to develop a system design level of KBS-3H and to accomplish a long-term safety evaluation for Olkiluoto (see Section 1.6), which has been used as the reference site for long-term safety activities.

1.4 Regulatory context for the management of spent nuclear fuel

According to the law, the Finnish Ministry of Employment and the Economy (TEM; previously the Ministry of Trade and Industry, KTM) decides on the principles to be followed in waste management of spent nuclear fuel and other nuclear waste types.

The schedule for disposal of spent nuclear fuel was established in the KTM’s Decision 9/815/2003. According to that Decision, the parties under the nuclear waste management obligation shall, either separately, together or through Posiva Oy, prepare to present all reports and plans required to obtain a construction licence based on the KBS-3 method for a disposal facility for spent nuclear fuel as stated in the Nuclear Energy Decree by the end of 2012. The disposal facility is expected to become operational around the year 2020.
The legislation concerning nuclear energy was updated in 2008. As part of the legislative reform, a number of the relevant Government Decisions were replaced with Government Decrees (GDs). The Decrees entered into force on 1st December 2008. The Government Decision (478/1999) regarding the safety of disposal of spent nuclear fuel, which applied specifically to the disposal facility, was replaced by the Government Decree 736/2008, issued 27 November 2008.

The detailed long-term safety requirements for spent nuclear fuel disposal are given in the Finnish Radiation and Nuclear Safety Authority’s (STUK) recently published YVL Guide D.5 (STUK 2014a), dated 15.11.2013, and are applied to the KBS-3H safety evaluation. It should be noted that, in the 3V-specific TURVA-2012 safety case, the Draft 4 version of the Guide D.5, dated 17.3.2011, was used, causing slight differences compared with the KBS-3H safety evaluation. These differences are discussed in Section 2.3 of the Design Basis – KBS-3H report.

Other YVL Guides pertaining to the disposal of spent nuclear fuel include: Guide YVL D.1, dealing with regulatory control on nuclear safeguards, D.2 dealing with the transport of nuclear materials and nuclear waste, D.3 dealing with handling and storage of nuclear fuel and D.4 dealing with predisposal management of low and intermediate level nuclear waste (also relevant for spent fuel disposal if the same disposal facility is used) and decommissioning of a nuclear facility. These have been taken into account as appropriate and the proposed conceptual design for KBS-3H is compliant with them.

### 1.5 Safety concept and safety functions

The long-term safety principles of Posiva’s planned repository system have been updated in order to apply to the KBS-3H design alternative. The 3H-specific long-term safety principles (VAHA Level 2) are:

1. The spent fuel elements shall be disposed of in a repository located deep in the Olkiluoto bedrock. The release of radionuclides shall be prevented with a multi-barrier disposal system consisting of a system of engineered barriers (EBS) and host rock such that the system effectively isolates the radionuclides from the living environment.

2. The engineered barrier system of KBS-3H consists of
   a) the canister to contain the radionuclides as long as they could cause significant harm to the environment
   b) the buffer, which is initially in the supercontainers (surrounding the canister) and in the distance blocks between the supercontainers, to protect the canisters as long as containment of radionuclides is needed
   c) the filling components, i.e. the filling blocks to separate possible transmissive fractures from the canisters and buffer, and the transition zones related to the plugs
   d) the compartment plugs to divide the drift into two compartments, and the drift plugs to keep all components in the drift in place until the adjacent central tunnel is backfilled and saturated
   e) the closure, i.e. the backfill and sealing structures to decouple the repository from the surface environment.
3. The host rock and depth of the repository shall be selected in such a way as to make it possible for the EBS to fulfil the functions of containment and isolation described above.

4. Should any of the canisters start leaking, the repository system as a whole shall hinder or retard the releases of radionuclides to the biosphere to the level required by the long-term safety criteria.

It should be noted that the supercontainer is not defined as a barrier, because its main components, the canister and the buffer, are barriers themselves. The only additional component of the supercontainer is the supercontainer shell, which is needed for the proper emplacement of the canister and buffer during the operational phase and does not have any safety function. By definition, it is thus not a barrier.

The safety concept, as depicted in Figure 1-3, is a conceptual description of how these principles are applied together to achieve safe disposal of spent nuclear fuel in the conditions of the Olkiluoto site. Due to the long-term hazard of the spent nuclear fuel, it has to be isolated from the surface environment over a long period of time. The KBS-3 method provides long-term isolation and containment of spent nuclear fuel and its associated radionuclides by a system of multiple barriers, both engineered and natural, and by ensuring a sufficient depth of disposal (the key safety features of the system in Figure 1-2). All of these barriers have their roles in establishing the required long-term safety of the repository system. These roles constitute the safety functions of the barriers (see Table 1-1). The surface environment is not assigned any safety functions; instead it is considered as the object of the protection provided by the repository system.

Most radionuclides in the spent nuclear fuel are embedded in a ceramic matrix (UO$_2$) that itself is resistant to dissolution in the expected repository conditions. The slow release of radionuclides from the spent nuclear fuel matrix in the event of canister failure is part of Posiva’s safety concept. Moreover, the near-field conditions should contribute to maintaining the low solubility of the matrix.

The safety functions for each barrier in the KBS-3H system are presented in Table 1-1. In the safety evaluation documentation, the spent nuclear fuel, EBS and the host rock are jointly termed the repository system, whereas the term disposal system is used when the repository system and the surface environment are both considered (see Figure 1-4).
Figure 1-3. Outline of the safety concept for a KBS-3 type repository for spent nuclear fuel in a crystalline bedrock (adapted from Posiva 2003). Pillars and blocks shown in dark cyan colour indicate the primary safety features and properties of the disposal system. Yellow pillars and blocks indicate the secondary safety features that may become important in the event of a radionuclide release from a canister.
Table 1-1. Summary of safety functions assigned to the barriers (EBS components and host rock) in Posiva’s KBS-3H repository concept.

<table>
<thead>
<tr>
<th>Barrier</th>
<th>Safety functions (KBS-3H)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Canister</td>
<td>• Ensure a prolonged period of containment of the spent nuclear fuel. This safety function rests first and foremost on the mechanical strength of the canister’s cast iron insert and the corrosion resistance of the copper surrounding it.</td>
</tr>
<tr>
<td>Buffer</td>
<td>• Contribute to mechanical, geochemical and hydrogeological conditions that are predictable and favourable to the canister.</td>
</tr>
<tr>
<td></td>
<td>• Protect canisters from external processes that could compromise the safety function of complete containment of the spent fuel and associated radionuclides.</td>
</tr>
<tr>
<td></td>
<td>• Limit and retard radionuclide releases in the event of canister failure. In addition, the buffer in the distance blocks shall</td>
</tr>
<tr>
<td></td>
<td>• Hydraulically and thermally separate the supercontainers from each other.</td>
</tr>
<tr>
<td>Filling components</td>
<td>• Contribute to favourable and predictable mechanical, geochemical and hydrogeological conditions for the buffer and canisters.</td>
</tr>
<tr>
<td></td>
<td>• Limit and retard radionuclide releases in the possible event of canister failure. In addition, the filling blocks (at inflow locations) shall</td>
</tr>
<tr>
<td></td>
<td>• Separate possible transmissive fractures intersecting the drift from the canisters and buffer.</td>
</tr>
<tr>
<td>Compartment plugs and drift plugs</td>
<td>• Contribute to favourable and predictable mechanical, geochemical and hydrogeological conditions for the filling components, buffer and canisters by keeping the drift components in place.</td>
</tr>
<tr>
<td>Closure</td>
<td>• Prevent the underground openings from compromising the long-term isolation of the repository from the surface environment and normal habitats for humans, plants and animals.</td>
</tr>
<tr>
<td></td>
<td>• Contribute to favourable and predictable geochemical and hydrogeological conditions for the other engineered barriers by preventing the formation of significant water conductive flow paths through the openings.</td>
</tr>
<tr>
<td></td>
<td>• Limit and retard inflow to and release of harmful substances from the repository.</td>
</tr>
<tr>
<td>Host rock</td>
<td>• Isolate the spent fuel repository from the surface environment and normal habitats for humans, plants and animals and limit the possibility of human intrusion, and isolate from changing conditions at the ground surface.</td>
</tr>
<tr>
<td></td>
<td>• Provide favourable and predictable mechanical, geochemical and hydrogeological conditions for the engineered barriers.</td>
</tr>
<tr>
<td></td>
<td>• Limit the transport and retard the migration of harmful substances that could be released from the repository.</td>
</tr>
</tbody>
</table>
Figure 1-4. The components of the disposal system for KBS-3H.
1.6 KBS-3H Safety Case portfolio

The purpose of the studies underpinning the safety case for KBS-3H is to achieve the required level of knowledge that will allow an assessment to be made of whether the horizontal concept is at least as safe as the vertical concept. The Olkiluoto-specific safety evaluation for KBS-3H is planned to be compiled in a report portfolio in the same manner as the safety case for KBS-3V, which is summarised in Posiva (2012a). The complete portfolio will consist of the reports shown in Figure 1-5. In the current project phase ending in spring 2017, the following reports are being produced:

- Design Basis – KBS-3H
- Features, Events and Processes – KBS-3H
- Description of the Disposal System – KBS-3H
- Production Lines – KBS-3H, see detailed listing of planned reports below
- Performance Assessment – KBS-3H.

If a decision is made to compile a complete safety case for KBS-3H at a later stage, all documents in Figure 1-5 will be produced. This also means that updates of the reports made in the first phase ending in spring 2017 may need to be produced.

As shown in the figure, some of the 3V-related reports in the TURVA-2012 portfolio would need to be modified and updated to make them applicable to 3H, whereas some of the other reports are common to 3V and 3H. The reports shown in yellow are specific to KBS-3H, whereas the reports shown in green would need to be modified and updated to be in accordance with the 3H approach. The reports shown in blue are the same as those in the TURVA-2012 safety case produced for the KBS-3V approach (Posiva 2013b).

Naturally, the present state and past evolution of the bedrock and the biosphere of the disposal site are the same as those for the 3V approach. These are not to be updated for the present safety evaluation, even if newer data might be available, as it is outside the scope of this project to re-write the Site Description (Posiva 2013c) and Biosphere Description (Posiva 2013d) reports. The safety analysis reports are, however, be updated as necessary, and the results of safety analyses for the KBS-3H and KBS-3V approaches will then be comparable on the basis of geosphere/biosphere releases. A Complementary Considerations report is not produced for KBS-3H, as a Complementary Evaluations report with a similar scope (Neall et al. 2007) was produced for the KBS-3H safety assessment in 2007. Moreover, a more recent Complementary Considerations report (Posiva 2012c) applies to both KBS-3V and KBS-3H. Necessary updates regarding complementary considerations for KBS-3H are presented in connection with the Performance Assessment – KBS-3H report.
Alongside the performance analyses (to be reported in *Performance Assessment − KBS-3H*) related to the deposition drift, production line reports are produced for the KBS-3H alternative. They are used as the basis for determining the initial state for the safety assessment. In all, five production line reports are produced, one of them an overarching report “Repository Production”. The four more specific production line reports are:

- Buffer and filling components
- KBS-3H underground openings
- Plugs (compartment and drift plugs)
- Supercontainer.
The production line reports focus on the 3H-specific features. Regarding the common areas (3V and 3H), brief summaries are given and otherwise reference is made to the 3V reports (Posiva 2013b).

If there are any 3H-specific updates to the requirements on the canister, these will be included in the overarching Repository Production report. The Closure Production Line report (Sievänen et al. 2012) compiled for KBS-3V is generally valid also for KBS-3H, but some changes exist and these are also discussed in the Repository Production report. Backfill of the deposition tunnels does not apply to the KBS-3H design, which is why this production line report is excluded from the KBS-3H work. The KBS-3H-specific plugs are included in a new report called the Plug Production Line report (Posiva 2013a, Section 9.1.2).

To allow the safety of the two design alternatives (KBS-3V and KBS-H) to be compared, data and analyses used in TURVA-2012 (see Posiva 2012a) are also used in the KBS-3H portfolio reports whenever they are (i) applicable to KBS-3H as well and (ii) still considered to be correct. Significant parts of the safety case are, however, different, and when the changes are due to the specific properties of the KBS-3H alternative, this has been indicated by showing the term “KBS-3H” in bold in the paragraph that is specific to 3H. The KBS-3H safety case considers the feedback received from the authorities, i.e. STUK and the Swedish Radiation Safety Authority (SSM), on the previous KBS-3H-specific safety assessment, summarised in Smith et al. (2007). Feedback received so far from STUK on the TURVA-2012 safety case is also taken into account, as far as it applies to 3H as well.

1.7 Quality assurance

Posiva’s management system defines general quality objectives and forms the foundation for the quality management of safety case activities. Special attention is paid to the management of the processes that are applied to produce the safety case and its foundations. The purpose of this enhanced process control is to provide full traceability and transparency of the data, assumptions, modelling and calculations. The KBS-3H safety case, if completed, will address the need to be fully compliant with all aspects of the regulatory requirements (Government Decrees and YVL Guides, see Section 1.4).

Even though the approach is based on management according to the standard ISO 9001:2008, a graded approach proposed for nuclear facilities is being adopted, i.e. the primary emphasis is on the quality control of the safety case, particularly for those activities that have a direct bearing on long-term safety, whereas standard quality measures may be applied in the supporting work. This means in practise that all KBS-3H safety case reports are subjected to tighter quality demands than reporting related to activities which do not have a direct bearing on long-term safety, but the KBS-3H safety case needs input from Posiva’s and SKB’s own RTD activities and other research which fulfils general quality standards. Documentation of the supporting activities providing input to the KBS-3H safety case is required to follow the guidelines given by the KBS-3H safety case and include, for example, discussion on the quality of and uncertainties related to the models and data used in these supporting analyses.
Another task of the KBS-3H safety case is to define performance targets for the EBS and target properties for the host rock, the former in co-operation with the EBS work and the latter in co-operation with the Rock Suitability Classification project. These are presented in the Design Basis – KBS-3H report.

Quality assurance and quality control measures related to the production and operation of the repository are discussed in detail in the KBS-3H production line reports (Canister; Buffer and Filling Components; Plugs; Supercontainer; Closure; and Underground Openings).

1.8 Scope and structure of the present report

This report identifies and describes those features, events and processes (FEPs) that are considered to be potentially significant to the long-term safety and performance of a KBS-3H repository. This report explicitly addresses FEPs relevant to the KBS-3H design alternative, including also those FEPs that are common to both KBS-3V and KBS-3H.

As described in Chapter 2, the primary purpose of this report is to support the formulation of radionuclide release scenarios and the performance assessment for KBS-3H by ensuring that the scenarios are comprehensive and take explicit or implicit account of all significant FEPs.

The report has been structured to describe FEPs according to the main components of the disposal system in which they occur:

Chapter 3 FEPs relevant to the spent nuclear fuel
Chapter 4 FEPs relevant to the canister
Chapter 5 FEPs relevant to the buffer
Chapter 6 FEPs relevant to the supercontainer shell
Chapter 7 FEPs relevant to the filling components
Chapter 8 FEPs relevant to the compartment and drift plugs
Chapter 9 FEPs relevant to the closure backfill and plugs at repository depth
Chapter 10 FEPs relevant to the geosphere

To avoid repetition, the FEP descriptions relevant to the surface environment and external to the disposal system are not included in this report; instead, the reader is referred to Posiva (2012d). The exceptions are the FEP names and numbers in the coupling of FEPs, which include those relating to the surface environment. In principle, the geosphere (Chapter 10) is also the same for 3V and 3H, but some updates related to new information on microbial activity and rock mechanics of the deposition drifts have been included, as well as revising the text with other minor changes, mainly related to the 3H repository geometry.

Each individual FEP is described using a standard template, with the exception of the filling components (Chapter 7), where the templates are not filled in order to avoid repetition. The aim of the template is to summarise the nature of each FEP, set out the conditions under which it may occur and discuss the uncertainties in process understanding. The potential couplings between FEPs are also identified, but the analysis of the significance of these couplings will be dealt with in the performance assessment for KSB-3H.
This report is a KBS-3H-specific revision of the TURVA-2012 FEP report (Posiva 2012d) and an update of the previous KBS-3H Process Report (Gribi et al. 2007). This revised report takes account of review comments from STUK on the previous KBS-3H Process Report and new knowledge from the Complementary Study phase of the KBS-3H project (Posiva 2013a) as well as Posiva’s research programme (Posiva 2013b). These inputs have resulted in minor changes to the list of FEPs considered for the near-field components and geosphere, with some renaming, aggregation and disaggregation of individual entries. One of the main differences with respect to the previous KBS-3H Process Report is that the material of the supercontainer shell and of the plugs in the deposition drift has been changed from steel to titanium, which is why the importance of steel-related processes has decreased from the previous version.

In addition to this report, Posiva is developing an electronic FEP Database that will summarise the information contained in this report, and which will be updated over time as new information becomes available.

References


2 THE APPLICATION OF FEPS TO THE SAFETY CASE

2.1 Identification and screening of FEPS for potential significance

The identification and screening of FEPS in Posiva’s safety case(s) development is done in a structured manner using expert judgement. An initial long list of FEPS was derived from the previous Process Reports for KBS-3V, the NEA International FEP list (NEA 1999) plus its supporting project database (NEA 2006), together with various other relevant safety cases. The identified FEPS on the long list were then screened to determine their potential significance against the following qualitative criteria:

- relevance to the KBS-3 type repository design for spent nuclear fuel disposal;
- relevance to the present-day Olkiluoto site characteristics and likely future site characteristics evolving in response to climatic changes and other external factors;
- relevance to the national regulatory requirements and guidelines;
- previous experience in FEP screening and safety case development (see Posiva 2014a);
- knowledge and information gaps identified during the course of Posiva’s and SKB’s ongoing RTD programmes;
- the outcomes from previous safety cases for, and performance assessments of, the KBS-3 type repository design;
- expert knowledge and awareness of other developing national and international RTD and safety case programmes; and
- feedback from the regulatory agency (STUK) on previous safety case reports and Posiva’s RTD programme.

Examples of FEPS that were excluded during the screening process are the following.

- *Spent nuclear fuel degradation due to high-pH waters (pH > 10)*: this FEP was excluded because expert judgement indicates that it is unlikely that significant quantities of high-pH leachate, generated by the chemical degradation of cementitious materials, will migrate through the buffer and come into contact with the spent nuclear fuel. Reaction between bentonite and high-pH waters is addressed, however, because parts of the buffer [5.2.6] may come into contact with cementitious leachates.

- *Deliberate human intrusion*: this FEP was excluded because it is assumed that, if an intrusion was done deliberately, appropriate measures would be taken to protect people and the environment.

This report, therefore, contains descriptions only of those FEPS that passed screening and are considered potentially significant for the long-term safety of the disposal facility.

When identifying the potentially significant FEPS, expert judgement was also applied when deciding how to address coupled processes. For example, ‘water uptake by bentonite’ and ‘swelling of bentonite’ are two separate but connected processes. In this report, these two processes are addressed in a single FEP description [5.2.2] because they are so closely related that it is appropriate to address them as a single process.
In other cases, closely connected processes have been described separately when it has been recognised that they may need to be addressed differently in the development of scenarios and in the performance assessment models. For example, ‘radioactive decay’ and ‘radiogenic heat generation’ are clearly very closely related processes but each has its own FEP description in this report [3.2.1 and 3.2.2].

Since the resulting FEP list (Posiva 2012d) has been compiled with KBS-3V in mind, in this work the FEP list and FEP descriptions were updated in the following way:

- the previous Posiva Process Report produced specifically for KBS-3H (Gribi et al. 2007) was revisited and relevant issues incorporated into this report;
- the FEP screening files compiled for TURVA-2012 (Posiva 2014a), based on NEA’s FEP database (NEA 2006), were revisited to check if there are KBS-3H relevant FEPs among those screened out based on the repository design (screening criterion R4 - “The FEP is not relevant for the KBS-3V type repository design for spent nuclear fuel disposal”; see Posiva 2014a, Section 2.3.2) and no such FEPs were identified;
- FEPs were added or descriptions updated based on the developments and changes in the KBS-3H design (e.g. related to the new supercontainer shell material titanium) since the previous KBS-3H Process Report (Gribi et al. 2007). The design assumed in this safety case is set out in Description of the Disposal System – KBS-3H (Posiva 2016a);
- FEP descriptions were updated based on other developments since the most recent FEP report (Posiva 2012d), for example the new canister welding method (friction stir welding) is assumed.

The individual FEP descriptions include the numerical reference to processes in the previous KBS-3H Process Report (Gribi et al. 2007), for traceability.

### 2.2 The classification of FEPs

Although it is common practice to discuss ‘features, events and processes,’ most FEP lists (including the NEA’s International FEP list) do not, in fact, explicitly distinguish between these three types of factors and broadly treat them all similarly. When processing FEPs in the safety case, however, and deciding how they are to be accounted for in the assessment process, it is sometimes important to make a distinction between different classes of FEPs. Within the KBS-3H safety case, the following distinctions and definitions are used.

- **Feature:** a component of the disposal system, or a parameter or characteristic that influences the behaviour of the component, such as temperature (e.g. of groundwater).
- **Process:** a mechanism that causes a progressive change to the waste or disposal system that may have an impact over a short to long period of time. Processes may be beneficial or non-beneficial with regard to safety performance depending on their extent in time and space. Examples include radionuclide sorption and swelling of bentonite clay.
- **Event:** a mechanism that causes a rapid change to the waste or disposal system over a relatively short period of time. This may be internal or external to the disposal system. Examples include reactivation-displacements along existing fractures (i.e. rock shear) due to an earthquake or inadvertent human intrusion.
Events can influence both features and processes, whereas features and processes can influence each other.

The initial state of the repository is described by a set of features that are dependent on the repository design and characteristics of the site. These features are discussed in Posiva (2016a).

The sets of features that describe the future states of the repository are the result of the operation of processes and the occurrence of events (Figure 2-1). It follows that features may be time dependent (and subject to uncertainty) and so have been sometimes referred to as ‘variables’ as was the case previously (Gribi et al. 2007).

In the safety case, the primary focus is largely on assessing the actions and consequences of processes that control the long-term safety and performance of the repository. This is why the previous versions of this report were called ‘Process Reports’.

\[\text{Figure 2-1. The main influences between features (F), events (E) and processes (P).}\]

In this report and in Posiva’s developing FEP database, the FEPs are further categorised as evolution-related FEPs (i.e. those that mostly affect the physical state of the disposal system) or migration-related FEPs (i.e. those that mostly affect the transport of radionuclides). There is not always a clear-cut separation, and some FEPs are categorised as both evolution and migration-related, but this simple distinction is useful to ensure that all relevant migration-related FEPs are considered when developing the transport models applied in the analyses of the release and transport of radionuclides. The behaviour of the disposal system in response to evolution-related FEPs is checked against safety functions and performance targets as part of the performance assessment.

2.3 Organisation of FEPs and system components

The FEPs have been organised according to the main components of the disposal system in which they occur, and this is reflected in the structure of the following chapters of this report.
The list of FEPs that have been described in this report using a specific FEP description template is given in Table 2-1 below. In addition to these, there is a set of features related to each component of the disposal system, and these have been listed in the respective chapters but have not been specifically described in this report.

Table 2-1. The list of FEPs described in this report.

<table>
<thead>
<tr>
<th>FEP number</th>
<th>FEP name</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>FEPs in the spent nuclear fuel:</strong></td>
<td></td>
</tr>
<tr>
<td>3.2.1</td>
<td>Radioactive decay (and in-growth)</td>
</tr>
<tr>
<td>3.2.2</td>
<td>Heat generation</td>
</tr>
<tr>
<td>3.2.3</td>
<td>Heat transfer</td>
</tr>
<tr>
<td>3.2.4</td>
<td>Structural alteration of the fuel pellets</td>
</tr>
<tr>
<td>3.2.5</td>
<td>Radiolysis of residual water (in an intact canister)</td>
</tr>
<tr>
<td>3.2.6</td>
<td>Radiolysis of the canister water</td>
</tr>
<tr>
<td>3.2.7</td>
<td>Corrosion of cladding tubes and metallic parts of the fuel assembly</td>
</tr>
<tr>
<td>3.2.8</td>
<td>Alteration and dissolution of the fuel matrix</td>
</tr>
<tr>
<td>3.2.9</td>
<td>Release of the labile fraction of the inventory</td>
</tr>
<tr>
<td>3.2.10</td>
<td>Production of helium gas</td>
</tr>
<tr>
<td>3.2.11</td>
<td>Criticality</td>
</tr>
<tr>
<td>3.3.1</td>
<td>Aqueous solubility and speciation</td>
</tr>
<tr>
<td>3.3.2</td>
<td>Precipitation and co-precipitation</td>
</tr>
<tr>
<td>3.3.3</td>
<td>Sorption</td>
</tr>
<tr>
<td>3.3.4</td>
<td>Diffusion in fuel pellets</td>
</tr>
<tr>
<td><strong>FEPs in the canister:</strong></td>
<td></td>
</tr>
<tr>
<td>4.2.1</td>
<td>Radiation attenuation</td>
</tr>
<tr>
<td>4.2.2</td>
<td>Heat transfer</td>
</tr>
<tr>
<td>4.2.3</td>
<td>Deformation</td>
</tr>
<tr>
<td>4.2.4</td>
<td>Thermal expansion of the canister</td>
</tr>
<tr>
<td>4.2.5</td>
<td>Corrosion of the copper overpack</td>
</tr>
<tr>
<td>4.2.6</td>
<td>Corrosion of the cast iron insert</td>
</tr>
<tr>
<td>4.2.7</td>
<td>Stress corrosion cracking</td>
</tr>
<tr>
<td>4.3.1</td>
<td>Aqueous solubility and speciation</td>
</tr>
<tr>
<td>4.3.2</td>
<td>Precipitation and co-precipitation</td>
</tr>
<tr>
<td>4.3.3</td>
<td>Sorption</td>
</tr>
<tr>
<td>4.3.4</td>
<td>Diffusion</td>
</tr>
<tr>
<td>4.3.5</td>
<td>Advection</td>
</tr>
<tr>
<td>4.3.6</td>
<td>Colloid transport</td>
</tr>
<tr>
<td>4.3.7</td>
<td>Gas transport</td>
</tr>
<tr>
<td><strong>FEPs in the buffer:</strong></td>
<td></td>
</tr>
<tr>
<td>5.2.1</td>
<td>Heat transfer</td>
</tr>
<tr>
<td>5.2.2</td>
<td>Water uptake and swelling</td>
</tr>
<tr>
<td>5.2.3</td>
<td>Mechanical erosion</td>
</tr>
<tr>
<td>5.2.4</td>
<td>Chemical erosion</td>
</tr>
<tr>
<td>5.2.5</td>
<td>Radiolysis of porewater</td>
</tr>
<tr>
<td>FEP number</td>
<td>FEP name</td>
</tr>
<tr>
<td>------------</td>
<td>----------------------------------------------</td>
</tr>
<tr>
<td>5.2.6</td>
<td>Montmorillonite transformation</td>
</tr>
<tr>
<td>5.2.7</td>
<td>Alteration of accessory minerals</td>
</tr>
<tr>
<td>5.2.8</td>
<td>Microbial activity</td>
</tr>
<tr>
<td>5.2.9</td>
<td>Freezing and thawing</td>
</tr>
<tr>
<td>5.2.10</td>
<td>Desiccation, formation of cracks</td>
</tr>
<tr>
<td>5.3.1</td>
<td>Aqueous solubility and speciation</td>
</tr>
<tr>
<td>5.3.2</td>
<td>Precipitation and co-precipitation</td>
</tr>
<tr>
<td>5.3.3</td>
<td>Sorption</td>
</tr>
<tr>
<td>5.3.4</td>
<td>Diffusion</td>
</tr>
<tr>
<td>5.3.5</td>
<td>Advection</td>
</tr>
<tr>
<td>5.3.6</td>
<td>Colloid transport</td>
</tr>
<tr>
<td>5.3.7</td>
<td>Gas transport</td>
</tr>
</tbody>
</table>

**FEPs in the supercontainer shell and minor titanium components:**

<table>
<thead>
<tr>
<th>FEP number</th>
<th>FEP name</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.2.1</td>
<td>Corrosion</td>
</tr>
<tr>
<td>6.2.2</td>
<td>Deformation</td>
</tr>
</tbody>
</table>

**FEPs in the filling components:**

<table>
<thead>
<tr>
<th>FEP number</th>
<th>FEP name</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.2.1</td>
<td>Heat transfer</td>
</tr>
<tr>
<td>7.2.2</td>
<td>Water uptake and swelling</td>
</tr>
<tr>
<td>7.2.3</td>
<td>Mechanical erosion</td>
</tr>
<tr>
<td>7.2.4</td>
<td>Chemical erosion</td>
</tr>
<tr>
<td>7.2.5</td>
<td>Montmorillonite transformation</td>
</tr>
<tr>
<td>7.2.6</td>
<td>Alteration of accessory minerals</td>
</tr>
<tr>
<td>7.2.7</td>
<td>Microbial activity</td>
</tr>
<tr>
<td>7.2.8</td>
<td>Freezing and thawing</td>
</tr>
<tr>
<td>7.3.1</td>
<td>Aqueous solubility and speciation</td>
</tr>
<tr>
<td>7.3.2</td>
<td>Precipitation and co-precipitation</td>
</tr>
<tr>
<td>7.3.3</td>
<td>Sorption</td>
</tr>
<tr>
<td>7.3.4</td>
<td>Diffusion</td>
</tr>
<tr>
<td>7.3.5</td>
<td>Advection</td>
</tr>
<tr>
<td>7.3.6</td>
<td>Colloid transport</td>
</tr>
<tr>
<td>7.3.7</td>
<td>Gas transport</td>
</tr>
</tbody>
</table>

**FEPs in the compartment and drift plugs:**

<table>
<thead>
<tr>
<th>FEP number</th>
<th>FEP name</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.2.1</td>
<td>Corrosion</td>
</tr>
<tr>
<td>8.2.2</td>
<td>Deformation</td>
</tr>
<tr>
<td>8.2.3</td>
<td>Degradation of the cast concrete of the fastening ring</td>
</tr>
<tr>
<td>8.3.1</td>
<td>Diffusion</td>
</tr>
<tr>
<td>8.3.2</td>
<td>Advection</td>
</tr>
<tr>
<td>8.3.3</td>
<td>Gas transport</td>
</tr>
</tbody>
</table>

**FEPs in the closure**

<table>
<thead>
<tr>
<th>FEP number</th>
<th>FEP name</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.2.1</td>
<td>Water uptake and swelling</td>
</tr>
<tr>
<td>9.2.2</td>
<td>Mechanical erosion</td>
</tr>
<tr>
<td>9.2.3</td>
<td>Chemical erosion</td>
</tr>
<tr>
<td>9.2.4</td>
<td>Montmorillonite transformation</td>
</tr>
<tr>
<td>9.2.5</td>
<td>Alteration of accessory minerals</td>
</tr>
<tr>
<td>FEP number</td>
<td>FEP name</td>
</tr>
<tr>
<td>------------</td>
<td>----------------------------------------------</td>
</tr>
<tr>
<td>9.2.6</td>
<td>Microbial activity</td>
</tr>
<tr>
<td>9.2.7</td>
<td>Freezing and thawing</td>
</tr>
<tr>
<td>9.2.8</td>
<td>Chemical degradation (of closure plugs)</td>
</tr>
<tr>
<td>9.2.9</td>
<td>Physical degradation (of closure plugs)</td>
</tr>
<tr>
<td>9.2.10</td>
<td>Freezing and thawing (in closure plugs)</td>
</tr>
<tr>
<td>9.3.1</td>
<td>Transport through closure backfill and plugs</td>
</tr>
</tbody>
</table>

*FEPs in the geosphere:*

<table>
<thead>
<tr>
<th>FEP number</th>
<th>FEP name</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.2.1</td>
<td>Heat transfer</td>
</tr>
<tr>
<td>10.2.2</td>
<td>Stress redistribution</td>
</tr>
<tr>
<td>10.2.3</td>
<td>Reactivation-displacement along existing fractures</td>
</tr>
<tr>
<td>10.2.4</td>
<td>Rock mass damage</td>
</tr>
<tr>
<td>10.2.5</td>
<td>Creep</td>
</tr>
<tr>
<td>10.2.6</td>
<td>Erosion and sedimentation in fractures</td>
</tr>
<tr>
<td>10.2.7</td>
<td>Rock-water interaction</td>
</tr>
<tr>
<td>10.2.8</td>
<td>Methane hydrate formation</td>
</tr>
<tr>
<td>10.2.9</td>
<td>Salt exclusion</td>
</tr>
<tr>
<td>10.2.10</td>
<td>Microbial activity</td>
</tr>
<tr>
<td>10.3.1</td>
<td>Aqueous solubility and speciation</td>
</tr>
<tr>
<td>10.3.2</td>
<td>Precipitation and co-precipitation</td>
</tr>
<tr>
<td>10.3.3</td>
<td>Sorption</td>
</tr>
<tr>
<td>10.3.4</td>
<td>Diffusion and matrix diffusion</td>
</tr>
<tr>
<td>10.3.5</td>
<td>Groundwater flow and advective transport</td>
</tr>
<tr>
<td>10.3.6</td>
<td>Colloid transport</td>
</tr>
<tr>
<td>10.3.7</td>
<td>Gas transport</td>
</tr>
</tbody>
</table>

The entire disposal system with its main components can be represented in a matrix format, as is shown in Table 2-2. The structure of this matrix reflects the order in which FEPs are described in this report, starting with FEPs relevant to spent nuclear fuel (Chapter 3) and ending with the FEPs relevant to the surface environment and external FEPs, which are described in Posiva (2012d).
Table 2-2. The high-level matrix of system components associated with the FEPs described in later sections of this report.
Each main component of the repository system can be further divided into sub-components. For example, the canister is comprised of four separate parts:

- the cast iron insert,
- the copper overpack,
- the void spaces within the canister that are initially gas or air filled, and
- the water in the canister.

### 2.4 FEP couplings and interactions between system components

#### 2.4.1 Couplings between individual FEPs

Due to the complex and dynamic nature of the disposal system, many of the FEPs described in this report are coupled with each other through various thermal, hydraulic, mechanical, chemical and biological (THMCB) mechanisms. For example, within the buffer, the transfer of heat [5.2.1] will affect the rate of water uptake and swelling during resaturation [5.2.2] and this, in turn, can affect such things as microbial activity [5.2.8] and the rates of gas transport through the buffer [5.3.7].

The potential couplings between FEPs are identified and listed in each FEP description, and are also summarised in a table close to the beginning of each chapter for the respective disposal system component (e.g. Table 3-3).

The consequences of the potential couplings between FEPs are not, however, assessed or described in this report, but will be dealt with in *Performance Assessment − KBS-3H* (Posiva 2016b), where appropriate.

#### 2.4.2 Component interactions

The different components of the disposal system can interact with each other through the action of certain FEPs. Many of these interactions are obvious and inevitable, such as heat transfer through the canister [4.2.2], which will cause heat transfer to occur in the surrounding buffer [5.2.1]. Other interactions are less obvious, and their occurrence and consequence is dependent on certain other FEPs and their rates. For example, groundwater flow and advective transport in the geosphere [10.3.5] may lead to chemical erosion of swelling clays in the buffer [5.2.4] depending on, amongst other things, the groundwater composition and flow rate in the hydraulically active fractures.

It is possible to summarise the potential interactions between system components and sub-components using the interaction matrix format. An interaction matrix (Hudson 1992, see also e.g. Haapanen et al. 2009) is a compact approach to systematically describe features and their interactions or other relationships between them. The general principles of the interaction matrix are presented as an example in Table 2-3. The same system can be represented with a box-and-arrow diagram, as shown on the right side of Table 2-3, but for large systems with many interactions, the matrix presentation is usually clearer and more compact. The system is divided into components that are listed along the leading diagonal of the matrix, referred to as diagonal elements below. FEPs (mostly processes but sometimes
events) that relate the diagonal elements are entered in the off-diagonal elements. The matrix is read in a clockwise sense so that FEPs by which Component 1 affects Component 2 are located in the crossing of the row of the component of the origin and the column of the receiving component (the off-diagonal element denoted A in Table 2-3). Correspondingly, FEPs by which Component 2 affects Component 1 are located in the crossing of the row of the component of the origin and the column of the receiving component (the off-diagonal element denoted B in Table 2-3). It is important to ensure that the effects of FEPs are direct and are not mediated by interactions via a third component (diagonal element).

In this report, the features shown on the leading diagonal elements of the interaction matrix correspond to components and sub-components of the disposal system. For the interactions between them, in the off-diagonal elements in the matrix, FEPs are presented. An interaction matrix is provided at the beginning of each chapter, where appropriate (e.g. for Chapters 6, 8 and 9 no matrix is provided since the processes affecting the supercontainer shell, titanium plugs and closure are internal to the components. The consequences of these processes are, however, accounted for in the process description of other components: e.g. the corrosion products of titanium are accounted for in Section 5.2.6). All external features, events and processes are included in the interaction matrices for the system components, since external FEPs overarch and influence the entire disposal system either directly or indirectly.

Table 2-3. Conceptual illustration of the interaction matrix. The diagonal elements 1, 2 and 3 are system components. The off-diagonal elements (white boxes) are populated with zero, one or more FEPs. The arrows illustrate e.g. how Component 1 affects Component 2 via FEP A, how Component 2 affects Component 1 via FEP B and how Component 2 affects Component 3 via FEP C. On the right, a similar system is represented by a box-and-arrow diagram.
2.5 The FEP description template

The aim of the FEP descriptions is to provide a concise summary of the current understanding of each FEP and its associated uncertainties, and to set out when and where it may occur in the disposal system, how it is coupled to other FEPs, and the likely consequences of its operation. The descriptions are not intended to define how the FEP is treated in the KBS-3H safety case. The FEP description templates have the following components:

*Name and number:* a name and a unique number are given to each FEP. The same names and numbers have been also to Posiva’s FEP database.

*Type:* indicates whether the FEP is a feature, process or event.

*Class:* indicates whether the FEP is system evolution related or migration related, or both.

*General description:* this is a concise description of the FEP and its potential consequences for system evolution and safety of a KBS-3H repository, covering:

- current fundamental scientific understanding,
- any relevant properties, conditions and constraints that affect its operation,
- the likely temporal and spatial variability of its operation,
- the conditions under which it may be expected to occur at Olkiluoto, and
- when in the evolution of the disposal system it is expected to occur.

Reference is made to evidence for the FEP from R&D studies in the field or laboratory. Where possible, quantities are given to illustrate the ‘magnitude’ of the FEP (e.g. process rates) but these are not intended to define the actual parameter values or ranges used in the safety case: these will be defined in Posiva (2016b).

*Uncertainties in the understanding of the FEP:* this is a short discussion about any uncertainties and their management in conceptual understanding and gaps in knowledge, but generally not about uncertainties in data or modelling approaches. These will be defined in Posiva (2016b).

*Couplings to other FEPs:* this section lists which other FEPs potentially affect, or are affected by, the FEP being described. The details of how the FEP (especially FEPs from Chapter 3 to Chapter 10) interacts with other FEPs, and under what conditions and with what consequences, will be discussed in Posiva (2016b).

*References and bibliography:* provides a small number of key references to the main scientific literature and any relevant Posiva reports, particularly any recent summary reports on the FEP. This is not intended to be a comprehensive bibliography, but is a ‘signpost’ to the relevant literature for readers that require further information. The list, therefore, includes both the references given in the text plus other literature not explicitly mentioned in the FEP description.
The FEP description texts are partly based on Posiva (2012d), as many processes are similar regardless of the repository design (KBS-3V or KBS-3H). Whenever the text has been modified due to the characteristics of the KBS-3H design, the term “**KBS-3H**” (in bold) is mentioned in the paragraph that has been modified.

**References**


Posiva 2016b. Safety evaluation for a KBS-3H spent nuclear fuel repository at Olkiluoto – Performance Assessment. Eurajoki, Finland: Posiva Oy. POSIVA 2016-02 (in prep.).
3 SPENT NUCLEAR FUEL

3.1 Description

At the time of discharge from the reactor, spent nuclear fuel contains, in addition to UO₂ in the pellet matrix, fission products and actinides, as well as activation products formed in the cladding and other metallic parts of the fuel assembly. Most of the fission products and actinides/lanthanides are retained in the fuel matrix. However, some of the fission products can be volatile at reactor operating temperatures, and migrate during reactor operation to the fuel/cladding gap or to within cracks in the fuel pellets. Other fission products can migrate to grain boundaries, and reside there in fission gas bubbles, or separate into solid phases such as metallic epsilon (ε) particles (Mo, Ru, Rh, Pd, Tc).

Therefore, the ‘spent nuclear fuel’ can be divided into a number of physical sub-components:

- the spent nuclear fuel matrix itself, which is in the form of fuel pellets of UO₂ (uranium dioxide) containing actinides, fission products, and nuclides generated by decay and in-growth;
- the gaps (such as cracks in the fuel pellets and between the pellet and the cladding), which contain the most volatile and mobile fraction of the radionuclide inventory (referred to as the labile fraction);
- the zirconium alloy cladding tubes, which contain the fuel pellets within individual fuel rods, together with the other zirconium alloy components in the fuel assembly (e.g. end caps); and
- the other metallic structural parts of the fuel assembly, such as upper and lower tie-plates, spacer grid, channel nose piece etc., which are fabricated from stainless steel, nickel-based alloys or iron-based alloys.

If the canister fails after its emplacement in the repository, groundwater will penetrate the canister and corrode the insert and the cladding, and will eventually interact with the spent nuclear fuel. This water in the canister is referred to as canister water to indicate groundwater that will first equilibrate with the bentonite buffer and later with the corrosion products from the cast iron insert. In addition, secondary alteration products may subsequently form on the surface of the spent nuclear fuel due to reaction with the canister water.

Different designs and geometries of fuel assemblies (Figure 3-1) are used in each of the reactor types operating in Finland, and these are described in a separate report (Anttila 2005). The currently operating reactors at Olkiluoto (OL1 and OL2) are boiling water reactors (BWR), the Loviisa reactors (LO1 and LO2) are Russian designed-pressurised water reactors (VVER-440) and the third reactor in construction at Olkiluoto (OL3) is a Pressurised Water Reactor (PWR). The number of fuel assemblies of each type is summarised in Table 3-1. The currently cautious estimated total amount of fuel assumed in the safety evaluation is 6500 tU, which will be disposed of in approximately 3325 canisters.
Table 3-1. Details of forecast fuel accumulations at the OL and LO plant units. Values in parentheses are preliminary estimates made in 2011. From Raiko et al. (2012).

<table>
<thead>
<tr>
<th></th>
<th>OL1–2</th>
<th>OL3</th>
<th>LO1–2</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Planned operating life (a)</td>
<td>60</td>
<td>60</td>
<td>50</td>
<td>-</td>
</tr>
<tr>
<td>Predicted number of assemblies</td>
<td>14,034</td>
<td>3816</td>
<td>7752</td>
<td>25,602</td>
</tr>
<tr>
<td>Average discharge burn-up of all assemblies (MWd/kgU)</td>
<td>39.5</td>
<td>45.0</td>
<td>40.6</td>
<td>41.7</td>
</tr>
<tr>
<td>Numbers of canisters</td>
<td>1170</td>
<td>954</td>
<td>646</td>
<td>2770</td>
</tr>
<tr>
<td>Predicted tonnage (tU)</td>
<td>2460</td>
<td>2030</td>
<td>950</td>
<td>5440</td>
</tr>
<tr>
<td>Dimensioning number of canisters</td>
<td>1400</td>
<td>1175</td>
<td>750</td>
<td>3325</td>
</tr>
<tr>
<td>Dimensioning tonnage (tU)</td>
<td>2950</td>
<td>2500</td>
<td>1050</td>
<td>6500</td>
</tr>
</tbody>
</table>

Once removed from the reactors, spent nuclear fuel assemblies are stored and actively cooled to disperse their decay heat. The Olkiluoto and the Loviisa nuclear power plants (reactors OL1–2 and LO1–2) began operations between 1977 and 1980, and the spent nuclear fuel generated at them is stored underwater at the plant sites in water ponds. The spent nuclear fuel from the Loviisa power plant was returned to Russia up until 1996, after which time it has been stored at Loviisa pending disposal. The OL3 reactor is currently being constructed.

Once the initial decay heat has dissipated, it is planned to encapsulate the fuel assemblies in canisters prior to disposal in the repository. The design of the canisters is described in Chapter 4. The minimum cooling time for spent nuclear fuel assemblies is about 30 years, for fuel with a typical burn-up of 40 MWd/kgU, as shown in Figure 3-2. The average cooling time until encapsulation will however, be longer (about 50 years) because no encapsulation of spent nuclear fuel has yet taken place and the first reactors were brought into use in the late 70s.
The initial state of the spent nuclear fuel at the time of disposal is defined by the characteristics of the fuel (fuel type, structure, enrichment distribution, amount of burnable poison etc.) and its operational history. Nearly all other parameters can be obtained to the required degree of accuracy by calculations, such as the radionuclide inventory (including the radionuclide distribution in the fuel assembly), radiation intensity, decay heat, mechanical stresses in the fuel rods, as well as gas composition inside the fuel rods. Average irradiation history and geometrical parameters are used to carry out radionuclide inventory calculations. Obaidurrahman & Gupta (2013) carried out a comparative assessment of the total core inventory using core average parameters and space-dependent single point calculations. They showed that using core average parameters to estimate the radionuclide inventory provides conservative values in spite of the known dependence of radionuclide inventory on power and burnup. This is likely due to arithmetic averaging for the different conditions of the fuel rods in the core.

After fuel discharge from the reactor, the radionuclide inventory will continue to evolve during cooling in the spent fuel pool due to radioactive decay and in-growth. Figure 3-3 shows the typical reduction in activity over time. Anttila (2005) calculated the initial radionuclide inventory at the time of discharge and at 8 cooling times. The average fuel characteristics have changed since 2005 only because of a limited increase in the average discharge burn-up; hence, the radionuclide inventories and fuel characteristics are still adequately described in Anttila (2005).
Figure 3-3. Spent nuclear fuels from the three different reactor types, and their activity over time after unloading from the reactor. The enrichment for each fuel type is 4.0 %. The burn-up is 40 MWd/kgU for each type apart from OL3 (“EPR”) fuel which is 60 MWd/kgU (yellow curve), showing the impact of the higher burn-up (Anttila 2005).

Some of the fuel rods may contain some water (referred to as ‘residual water’) at the time of encapsulation. These are fuel rods that have leaked during reactor operation and therefore they contain aerated cooling pool water. Based on over 30 years of operational experience at the Olkiluoto nuclear power plant, there have been about 58 failed rods for OL1–OL2 and LO1–LO2 combined (Rossi & Suolanen 2012, Section 5.1). It is estimated that there will be an additional 73 leaking fuel rods from OL1–OL2, LO1–LO2 and OL3 throughout the encapsulation time (Rossi & Suolanen 2012, Section 5.1). This corresponds to approximately 131 leaking fuel rods to encapsulate over the operational lifetime of the repository. To date, no fuel failure during the normal operation of interim storage pools has been reported. The oldest fuel in Finland has been stored under water for over 30 years. It is thus expected that no additional leaking fuel rods will be produced before encapsulation. So far all OL1–OL2 failed rods have been removed from the bundles prior to cooling and are stored in hermetically sealed capsules. The final plan for handling these capsules has not yet been drafted. The failed rods in LO1–LO2 have not been removed from the fuel bundles. The plan is to dispose of these bundles as they are.

The residual water volume in a leaking fuel rod is estimated based on the plenum (i.e. the gas volume of an intact rod). For design and long-term safety assessment purposes, it is pessimistically assumed that the plenum in a fuel rod is 50 cm³ and it is assumed that there are 12 failed fuel rods in each canister (this would correspond to a total of 39,900 failed rods for 3325 canisters at Olkiluoto). Thus, the amount of residual water used in long-term safety related calculations for all canister types is 600 g. The actual amount of residual water in a canister is expected to be much less. First, the expected number of leaking fuel rods is over two orders of magnitude lower than the assumed number. Second, the plenum for OL1–OL3 and LO1–LO2 fuel rods is less than 50 cm³. And last, prior to encapsulation, the fuel assemblies will be dried in a drying unit using a combination of spent fuel residual
heat and low pressure vacuum. The void spaces in the canister will then be purged with argon to displace water and water vapour (Raiko 2013). Thus, the atmosphere inside the canister in the presence of leaking fuel rods will be a mixture of argon, air and water vapour. It is pessimistically assumed that the atmosphere in the canisters will be composed of humid air (maximum 10 %) and argon gas (minimum 90 %).

3.1.1 Long-term safety and performance

The spent nuclear fuel matrix is considered an engineered barrier based on the new YVL D.5 Guide (STUK 2014). The intrinsically slow release of radionuclides from the UO₂ matrix is part of Posiva’s safety concept and it is taken into account in the radionuclide release and transport model as well as its low solubility in groundwater. The fuel pellets and the fuel assembly are expected to remain inert until the canister is breached and groundwater penetrates into the void space. Upon contact with groundwater, radionuclide release rates will be limited by a number of secondary characteristics, including:

- slow corrosion of the inert zirconium alloy cladding tubes;
- very slow dissolution rates of the UO₂ fuel matrix;
- low solubility of most radionuclide species; and
- slow rates of water movement into and out of the canister.

The labile fraction of the radionuclide inventory that will have migrated to the gaps, cracks and grain boundaries of the fuel is assumed to be released immediately at the time of canister failure.

3.1.2 Overview of the potentially significant FEPs

There are a number of processes and events that are considered to be potentially significant for the long-term safety performance of the spent nuclear fuel that relate to system evolution and to the migration of radionuclides and other substances.

Processes and events related to system evolution are:

3.2.1 Radioactive decay (and in-growth)
3.2.2 Heat generation
3.2.3 Heat transfer
3.2.4 Structural alteration of the fuel pellets
3.2.5 Radiolysis of residual water (in an intact canister)
3.2.6 Radiolysis of the canister water
3.2.7 Corrosion of cladding tubes and metallic parts of the fuel assembly
3.2.8 Alteration and dissolution of the fuel matrix
3.2.9 Release of the labile fraction of the inventory
3.2.10 Production of helium gas
3.2.11 Criticality
Processes related to the migration of radionuclides and other substances are:

3.3.1 Aqueous solubility and speciation
3.3.2 Precipitation and co-precipitation
3.3.3 Sorption
3.3.4 Diffusion in fuel pellets

Other migration processes such as advection, colloid transport and gas transport cannot occur within the spent nuclear fuel matrix itself, but can occur elsewhere in the repository system, including the void spaces in the canister, and so these processes are discussed in other sections of this report, where they are relevant.

These processes and events are each potentially affected by a number of features of the repository system that can influence the occurrence, rate, activity and potential couplings between the processes. These features relate either to aspects of the design of the repository or to parameters (characteristics) of the spent nuclear fuel that might be time-dependent during the repository lifetime. The most significant features are:

- Radionuclide inventory
- Temperature
- Pressure
- Fuel geometry
- Mechanical stresses
- Material composition
- Water composition
- Gas composition.

The possible influences of these features on the processes and events considered to be significant for the long-term safety of the spent nuclear fuel are described in each FEP description, and are summarised in Table 3-2.

Many of the processes occurring within the spent nuclear fuel are interdependent and directly coupled to each other. For example, structural alteration of the fuel pellets [3.2.4] will directly affect the release of the labile fraction of the inventory [3.2.9]. The direct couplings are listed in each FEP description, and are summarised in the matrix shown in Table 3-3.

Similarly, due to the complex interactions between the various parts of the disposal system, the evolution of the spent nuclear fuel can influence (or be influenced by) processes occurring in other parts of the system through interactions between various processes. For example, heat transfer in the spent nuclear fuel [3.2.3] will drive heat transfer in the canister [4.2.2]. An example of a possible interaction between the spent nuclear fuel and the surface environment is given by the inadvertent human intrusion event [see 10.2.5 in Posiva 2012d], which involves drilling from the Earth’s surface into the spent nuclear fuel. The interactions between the spent fuel and other components of the disposal system are summarised in Table 3-4.
References


Table 3-2. Possible influences of features of the disposal system on the processes and events considered to be potentially significant (if they occur) for the long-term performance of the spent nuclear fuel (marked with Y). These influences and couplings are discussed in more detail in each FEP description.

<table>
<thead>
<tr>
<th>Processes and events related to system evolution:</th>
<th>Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.2.1 Radioactive decay (and in-growth)</td>
<td>Y</td>
</tr>
<tr>
<td>3.2.2 Heat generation</td>
<td>Y</td>
</tr>
<tr>
<td>3.2.3 Heat transfer</td>
<td>Y</td>
</tr>
<tr>
<td>3.2.4 Structural alteration of the fuel pellets</td>
<td>Y</td>
</tr>
<tr>
<td>3.2.5 Radiolysis of residual water (in an intact canister)</td>
<td>Y</td>
</tr>
<tr>
<td>3.2.6 Radiolysis of the canister water</td>
<td>Y</td>
</tr>
<tr>
<td>3.2.7 Corrosion of cladding tubes and metallic parts of the fuel assembly</td>
<td>Y</td>
</tr>
<tr>
<td>3.2.8 Alteration and dissolution of the fuel matrix</td>
<td>Y</td>
</tr>
<tr>
<td>3.2.9 Release of the labile fraction of the inventory</td>
<td>Y</td>
</tr>
<tr>
<td>3.2.10 Production of helium gas</td>
<td>Y</td>
</tr>
<tr>
<td>3.2.11 Criticality</td>
<td>Y</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Processes related to the migration of radionuclides and other substances:</th>
<th>Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.3.1 Aqueous solubility and speciation</td>
<td>Y</td>
</tr>
<tr>
<td>3.3.2 Precipitation and co-precipitation</td>
<td>Y</td>
</tr>
<tr>
<td>3.3.3 Sorption</td>
<td>Y</td>
</tr>
<tr>
<td>3.3.4 Diffusion in fuel pellets</td>
<td>Y</td>
</tr>
</tbody>
</table>
Table 3-3. Possible couplings between FEPs within the spent nuclear fuel considered significant for the long-term performance of the disposal system. The numbers on the leading diagonal refer to the FEPs listed in Section 3.1.2. As an example of how to read this table, the blue coloured square means that “Structural alteration of the fuel pellets” [3.2.4] directly affects “Release of the labile fraction of the inventory” [3.2.9].

<table>
<thead>
<tr>
<th></th>
<th>3.2.1</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>3.2.1</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>3.2.2</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.2.3</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>3.2.4</td>
<td></td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.2.5</td>
<td></td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.2.6</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.2.7</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.2.8</td>
<td></td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>3.2.9</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.3.1</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.3.2</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.3.3</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.3.4</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 3-4. Interaction matrix for the spent nuclear fuel. FEPs in italics are addressed in other chapters. A short name for some of the FEPs is used in the table: IRF (Release of the labile fraction of the inventory), Precipitation (Precipitation and co-precipitation).

<table>
<thead>
<tr>
<th>Solid fuel matrix</th>
<th>Structural alteration of the fuel pellets</th>
<th>Alteration &amp; dissolution of the fuel matrix; Radiolysis of residual water (in an intact canister)</th>
<th>Sorption</th>
<th>Sorption</th>
<th>Alteration &amp; dissolution of the fuel matrix; Heat transfer; Radiation attenuation; IRF</th>
<th>Radiolysis of porewater</th>
<th>Exposure from radiation sources</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gaps</td>
<td>Release of the labile fraction of the inventory</td>
<td>Gas transport</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Water</td>
<td>Gas transport</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Water</td>
<td>Diffusion Precipitation and co-precipitation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Cladding and other Zircaloy-based materials</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Other metal parts</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Other metal parts</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Advection Diffusion</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Canister</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Buffer</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Surface environment</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Inadvertent human intrusion</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>External</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
3.2 System evolution FEPs

Various radiation, thermal, chemical and mechanical processes (and their couplings) will affect the evolution of the fuel pellets, the cladding tubes, and other parts of the fuel assembly within the canister. In turn, these processes can affect the stability of the spent nuclear fuel and lead to release of radionuclides, and the migration of radionuclides and other substances through and from the fuel to the water within the canister (Section 3.3). The following descriptions summarise each of these processes and the effects of the different variables on them.

Whenever the FEP description is affected by the specific characteristics of the KBS-3H design, the term “KBS-3H” (in bold) is included in the text.

<table>
<thead>
<tr>
<th>3.2.1 Radioactive decay (and in-growth)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Type:</strong> Process</td>
</tr>
<tr>
<td><strong>Alternative names:</strong> Radioactive decay</td>
</tr>
</tbody>
</table>

**General description:**

Radioactive decay is a fundamental process that affects all radioactive (unstable) nuclides. During decay, an unstable ‘parent’ nuclide undergoes spontaneous transformation releasing radiant energy and particles, causing the formation of a new ‘daughter’ nuclide. The daughter is often (but not always) a nuclide of a different element to the parent, in which case the decay process is called transmutation. The radioactive decay and transmutation process will continue until a nuclide is formed that has a stable nucleus and is not radioactive.

The rate at which radioactive decay occurs is nuclide specific and is defined by the half-life for the particular nuclide. The half-life is independent of all other physicochemical parameters (such as redox, temperature, pressure etc.). If the half-life of the daughter nuclide is longer than that of the parent, or the daughter is stable, it will accumulate over time and this process is called in-growth. The half-lives for most radionuclides are known with a high degree of certainty (DDEP 2011).

As a consequence of radioactive decay and in-growth, the radionuclide content (inventory) of the waste will change over time, both in the spent nuclear fuel and in any other parts of the repository to which radionuclides have migrated. Due to the inherent predictability of radioactive decay, the time-dependent change in inventory can be accurately calculated.

Radioactive decay and in-growth will cause α, β, γ and neutron radiation, and will be accompanied by radiogenic heat generation [3.2.2]. The radiation emitted is the primary reason why such care has to be taken for the disposal of spent nuclear fuel but, over time, the potential hazard posed by the fuel will reduce as a consequence of decay. After around 100,000 years, the fuel will have a radiotoxicity content broadly
comparable to that of a natural uranium ore, although the radionuclide nature and activity inventory will be different (Pastina & Hellä 2006).

The bulk rate of decay in the spent nuclear fuel (Bq/kg) and the resulting radiation fields are dependent on the initial radionuclide content which, in turn, depends on the burn-up history of the fuel in the reactor and the storage time before disposal. The decay power estimates for spent nuclear fuel planned to be disposed in the repository were updated in 2005 taking into account new maximum allowable burn-up and operational conditions in the Finnish nuclear power plants (Anttila 2005).

The decay radiation will interact with the materials in the fuel and the canister cavity. The α and β radiation has limited penetration and most of this radiation remains in, and is attenuated by, the fuel itself. The γ and neutron radiation has greater penetration and can reach and be attenuated by the canister [4.2.1]. Alpha decay also produces helium gas, which could, in principle, affect the mechanical stability of the fuel matrix [3.2.4].

Soon after disposal, the decay of short-lived radionuclides such as Cs-137 and Sr-90 will dominate the radiation field. These nuclides have half-lives of around 30 years and, consequently, will decay to insignificant amounts long before the copper canister is expected to fail in around 100,000 years. The radionuclides of most concern for repository safety are the longer-lived nuclides and their daughters (e.g. Th-229, Th-230, Ra-226) that will be present in the spent nuclear fuel after canister failure and, thus, may migrate away from the near field towards the accessible environment.

Radioactive substances are common in nature (e.g. uranium occurrences) and have been studied as analogues to the behaviour of spent nuclear fuel, although no natural materials contain measurable amounts of the short-lived fission products found in spent nuclear fuel (Miller et al. 2000).

Radioactive decay and in-growth is influenced only by the following feature of the repository system. 

– Initial radionuclide inventory: because the inventory at the time of disposal controls the time-dependent evolution of the radionuclide content during repository evolution.

**Uncertainties in the understanding of the FEP:**

There are no uncertainties in the understanding of radioactive decay and the in-growth of daughter products. Uncertainties relate to the input data used to calculate the inventory evolution as a function of time. Radioactive decay as a function of time can be calculated with great accuracy when the initial radionuclide content is known. This depends on the fuel characteristics and irradiation history, which are recorded and known with sufficient precision for long-term safety purposes. The total uncertainty in the calculated actinide inventories is estimated to be about 20 % and the total uncertainty in fission product inventories is about 12 % (Håkansson 1999, p. 18).

The half-lives of the relevant radionuclides are generally known with good accuracy. The international Decay Data Evaluation Project has the objective of reviewing and updating decay data (DDEP 2011). The most significant recent change concerns the half life of Se-79 which has been updated to $3.27\times10^5$ years. For other radionuclides, the evaluations published by the Decay Data Evaluation Project will be used when available. Uncertainties concerning the inventory at deposition and the half-lives have been further discussed in Posiva (2013e).
**Couplings to other FEPs:**

Radioactive decay and in-growth is directly affected by the following FEP:
- Criticality (if it were to occur) [3.2.11]

Radioactive decay and in-growth directly affects the radionuclide inventory in all repository compartments plus the following FEPs:
- Heat generation [3.2.2]
- Radiolysis of residual water (in an intact canister) [3.2.5]
- Radiolysis of the canister water [3.2.6]
- Release of the labile fraction of the inventory [3.2.9]
- Production of helium gas [3.2.10]
- Criticality (if it were to occur) [3.2.11]
- Aqueous solubility and speciation [3.3.1]
- Precipitation and co-precipitation [3.3.2]
- Sorption [3.3.3]
- Diffusion in fuel pellets [3.3.4]
- Radiation attenuation (by the copper canister) [4.2.1]
- Radiolysis of porewater [5.2.5]

**References:**


DDEP (Decay Data Evaluation Project) 2011. Laboratoire national Henri Becquerel recommended data. Available at: [http://www.nucleide.org/DDEP.htm](http://www.nucleide.org/DDEP.htm)


### 3.2.2 Heat generation

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th>Process</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Class:</strong></td>
<td>System evolution</td>
</tr>
<tr>
<td><strong>Alternative names:</strong></td>
<td>Radiation attenuation/heat generation, Radiogenic heat generation</td>
</tr>
<tr>
<td><strong>Section in 2007-09:</strong></td>
<td>2.3</td>
</tr>
</tbody>
</table>

#### General description:

Radioactive decay of nuclides such as Co-60, Sr-90, Cs-137, Am-241, Pu-239 and Pu-240 will generate heat in the spent nuclear fuel. Most of the heat generated is due to attenuation of radiation by the fuel matrix and by the metallic components of the fuel assembly. This attenuation occurs locally in the fuel assembly for the alpha and beta radiation, but is more widely distributed throughout the canister for the gamma and neutron radiation.

Heat generation from radiation attenuation is a function of the decay rate and the composition of the fuel assembly materials. Heat generation by attenuation will be dominated by short-lived beta and gamma emitters such as Cs-137 (Ba-137m) and Sr-90 (Y-90). These nuclides will have decayed to insignificant amounts within around 1000 years and, consequently, longer-term heat generation will be due entirely to long-lived alpha emitters (e.g. Am-241, Pu-239, Pu-240), which generate less decay heat.

The rate of heat generation due to decay and attenuation, and the resulting temperature in the spent nuclear fuel has been calculated (Ikonen 2006). The peak temperature in the fuel will be around 200 °C and will occur shortly after disposal, corresponding to the highest rate of decay. This calculation applies to the KBS-3H repository as well, although the peak temperature of the fuel may slightly vary due to the different heat dissipation from the canister into the rock (see FEP 3.2.3).

Heat generated in the spent nuclear fuel will be transferred to the canister by different thermal processes [3.2.3], depending on whether the canister remains intact or has failed.

Overall, heat generation in the spent nuclear fuel is influenced by the following features of the repository system.

- Radionuclide inventory: this is the principal control on the rate of radiogenic heat generation over time.
- Material composition: the composition of the spent nuclear fuel controls its thermal conductivity and heat generation due to attenuation.

#### Uncertainties in the understanding of the FEP:

In general, the uncertainties associated with radiogenic heat generation in the spent nuclear fuel are low because the fuel characteristics are well known and the heat generation processes are readily modelled using thermal codes. The actual heat output from each fuel assembly is planned to be measured and verified prior to encapsulation, which will further reduce parameter uncertainty.
**Couplings to other FEPs:**
Heat generation in the spent nuclear fuel is directly affected by the following FEPs:
- Radioactive decay (and in-growth) [3.2.1]
- Criticality (if it were to occur) [3.2.11]
- Radiation attenuation (in the copper canister) [4.2.1]

Heat generation in the spent nuclear fuel directly affects the following FEPs:
- Heat transfer [3.2.3]
- Structural alteration of the fuel pellets [3.2.4]

**References:**

---

### 3.2.3 Heat transfer

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th>Process</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Class:</strong></td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:**
Heat transport

**Section in 2007-09:**
2.4

**General description:**

Thermal processes in the fuel/cavity in the canister do not depend on the specific conditions in **KBS-3H** (identical fuel and canister as in KBS-3V). Differences arise only due to the specific geometry and conditions outside the canister. As concluded by Ikonen (2003) and Ikonen & Raiko (2015), based on model studies, the overall thermal evolution in KBS-3V and 3H are very similar. Furthermore, the analysis of the thermal evolution during the operational phase (Ikonen 2005) demonstrated that the maximal temperature is only marginally affected by the rate of canister emplacement (Gribi et al. 2007, Section 2.4).

Heat generated in the spent nuclear fuel by decay and attenuation of radiation [3.2.2] will be transferred between the subcomponents of the spent nuclear fuel and the fuel assembly, and to the canister by a variety of processes, depending on whether the canister remains intact or has failed.

In an intact canister, heat will be transferred across the annulus between the fuel and the cladding tubes largely by thermal radiation. Between and across metallic components of the fuel assembly and the cast iron insert by a combination of thermal radiation and conduction, depending on the gas composition and pressure in the cavity and the radiation properties of the metal surfaces (emissivity).

After canister failure, heat transfer may also take place by advection and convection of any water that penetrates into the cavity of the canister.

The temperature at any given time in the spent nuclear fuel will be controlled by the heat balance between heat generation within the fuel (input) and the transfer of heat (output) across the canister [4.2.2] to the bentonite buffer [5.2.1]. The temperature of
The spent nuclear fuel is important because the rates of many processes that directly affect it are temperature dependent, such as alteration and dissolution [3.2.8].

The rates of heat transfer in the spent nuclear fuel, cavity and canister metal have been calculated (Ikonen 2006). Within the fuel pellets, conductive heat transfer will dominate and will limit the maximum temperature in the spent nuclear fuel to between 200 °C and 250 °C provided that the copper canister is intact and that the outer surface temperature of the canister does not exceed 100 °C. This calculation is independent of the type of repository, thus is also valid for **KBS-3H**. For the distribution of temperatures in the near field of a KBS-3H repository see Ikonen & Raiko (2015).

If water is present in the void spaces of the canister (either as spent nuclear fuel cooling pool water in perforated cladding tubes or due to early canister failure), the overall thermal conductivity across the canister will be significantly increased, and the temperature of the fuel will be lower than in the case of a dry canister.

Overall, heat transfer in the spent nuclear fuel is influenced by the following features of the repository system.

− Radionuclide inventory: the principal control on the rate of radiogenic heat generation.
− Fuel geometry: in particular, the spacing of the fuel and the geometry of the void spaces between the fuel and cladding, across which heat is transferred primarily by radiation.
− Material composition: the composition of the spent nuclear fuel controls its thermal conductivity and heat generation due to attenuation.

**Uncertainties in the understanding of the FEP:**

In general, the uncertainties associated with radiogenic heat transfer in the fuel and cavity of the copper canister are low because the fuel characteristics are well known and the heat transfer processes are readily modelled using thermal codes. The actual heat output from each fuel assembly is planned to be measured and verified prior to encapsulation, which will further reduce parameter uncertainty.

**Couplings to other FEPs:**

Heat transfer in the spent nuclear fuel is directly affected by the following FEPs:

− Heat generation [3.2.2]

Heat transfer in the spent nuclear fuel directly affects the following FEPs:

− Structural alteration of the fuel pellets [3.2.4]
− Radiolysis of residual water (in an intact canister) [3.2.5]
− Radiolysis of the canister water [3.2.6]
− Corrosion of the cladding tubes and metallic parts of the fuel assembly [3.2.7]
− Alteration and dissolution of the fuel matrix [3.2.8]
− Release of the labile fraction of the inventory [3.2.9]
− Aqueous solubility and speciation [3.3.1]
− Precipitation and co-precipitation [3.3.2]
− Diffusion in fuel pellets [3.3.4]
− Heat transfer (in the canister) [4.2.2]


3.2.4 Structural alteration of the fuel pellets

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:** Structural evolution of fuel matrix  
**Section in 2007-09:** 2.6

**General description:**

Temperature changes and different thermal gradients in the fuel during reactor operations (particularly during power ramping up and ramping down periods) can affect the integrity of the fuel pellets. These temperature gradients lead to fracturing of the pellets and to an increase in their specific surface area (Figure 3-4). The temperature and pressure in the repository will be much lower than in the reactor and they are unlikely to cause any further structural alteration.

The microstructure and density of the pellets are also affected by the radiation field they experienced while in the reactor. Due to an accumulation of fission products and thermal fracturing, the diameter of spent nuclear fuel pellets is greater than that of fresh, unirradiated pellets and the density correspondingly less. The microstructure of an irradiated fuel pellet at burn-up higher than about 45 MWd/kgU will generally consist of two zones:

- a central zone with radial fractures and homogeneous porosity, and  
- a rim zone with higher porosity and submicrometre-size grains.

The rim zone forms because the fuel at the edge of a pellet undergoes fission at a rate up to three times higher than the mean fission rate of the pellet. This is caused by a successive build-up of fissile plutonium and other actinides due to capture of epithermal neutrons. The burn-up in the rim can be up to three times that in the centre of the pellet (Forsyth 1995). The higher fission rate causes a restructuring of the fuel matrix yielding sub-micrometre grains and a higher porosity (exceeding 10 %). The large pores form sharp angles at the grain boundaries, where crack-tips can be initiation
points for crack growth and fracturing of the ceramic matrix. The rim structure usually forms in fuel that has experienced burn-up greater than 45 MWd/kgU. These changes to the microstructure of the fuel pellets increase their surface area and affect the release of radionuclides from spent nuclear fuel both from the gap and void inventory [3.2.9] and from the matrix [3.2.8].

![Spent nuclear fuel pellet macro and micro structure](image)

Figure 3-4. Spent nuclear fuel pellet macro and micro structure. From Fors (2009, Figure 2.2).

In the repository, alpha decay of actinides contained in the spent nuclear fuel will result in the production of helium (He) atoms within the closed pores in the fuel matrix [3.2.10]. Helium is stable and unreactive; hence, the total amount of helium gas in the fuel elements will increase over time as various radionuclides undergo alpha decay. The effect of helium accumulation on the spent nuclear fuel pellet microstructure and on diffusion processes has been reassessed in light of the results from the NF-PRO and PRECCI projects (Ferry et al. 2005, 2008, 2010, Van Brutzel & Crocombette 2007, Martin et al. 2009).

Although experimental studies using He ion implantation at high temperatures (500 °C and 600 °C) showed flaking of the UO₂ surface (Guilbert et al. 2003), Ferry et al. (2010) showed that calculated values of bubble or pore pressure from He accumulation are much lower than that needed to fracture the UO₂ matrix. These results suggest that helium accumulation in pores as a result of alpha decay is not sufficient to produce micro-cracking of grains in the central zone of irradiated UO₂ fuel for several hundreds of thousand years. This conclusion applies also to the rim area, although the modelling results are more uncertain because of the uncertainties in the fracture geometry in the rim area. In spite of the conservative assumptions of the model, the calculated values of bubble or pore pressure are much lower than critical values derived from UO₂ lattice damage criteria. No structural alteration of the microstructure of the spent UO₂ fuel is thus expected before the breaching of the canister.

When water ultimately contacts the fuel, after failure of the copper canister and the cladding, this could lead to the exposure of a larger surface area of the fuel to water, and affect the availability of fission products for dissolution (SKB 2010). This effect is considered to be short lived, however, because the bulk dissolution rate for the fuel [3.2.8] is expected to be solubility limited and not controlled by the available surface area in the long term.
Structural evolution of the fuel matrix does not depend on the specific conditions in KBS-3H (Gribi et al. 2007, Section 2.6).

Overall, structural alteration of the fuel pellets is influenced by the following features and processes of the repository system.

− Radionuclide inventory: controls the rate of production of helium gas during alpha decay [3.2.10].
− Production of helium (He) atoms in the fuel matrix [3.2.10].

Uncertainties in the understanding of the FEP:

Some uncertainty exists in the helium production rates [3.2.10] in high burn-up fuel and the fraction of the alpha particles that actually contribute to helium pressure build-up. The main modelling uncertainty is the value of the critical bubble pressure, which is based on a fracture stress derived from three-point bending tests on polycrystalline UO₂. The impact of this pressure build-up on cladding integrity is also uncertain. For the rim zone, conservative assumptions have been used for the conceptual model of He bubble formation, pressure build-up and fracture of polycrystalline UO₂ (Ferry et al. 2008, 2010). Due to these conservative assumptions, there is confidence in the conclusion that structural alteration is unlikely.

Couplings to other FEPs:

Structural alteration of the fuel pellets is directly affected by the following FEPs:

− Heat generation [3.2.2]
− Heat transfer [3.2.3]
− Production of helium gas [3.2.10]

Structural alteration of the fuel pellets directly affects the following FEPs:

− Alteration and dissolution of the fuel matrix [3.2.8]
− Release of the labile fraction of the inventory [3.2.9]
− Diffusion in fuel pellets [3.3.4]

References:


3.2.5 Radiolysis of residual water (in an intact canister)

**Type:** Process  
**Class:** System evolution  
**Alternative names:** Water radiolysis; Radiolytic acid production; Nitric acid production  
**Section in 2007-09:** 2.7

**General description:**

As discussed in Section 3.1, the canisters may contain a mixture of water vapour (from residual water introduced with a leaking fuel rod), air and argon. This humid air will be subject to the intense radiation field inside the canister from the spent nuclear fuel, causing radiolysis and the generation of small quantities of nitrogen oxide species and even smaller quantities of hydrogen gas (H₂), oxygen gas (O₂) and hydrogen peroxide (H₂O₂). These radiolysis products will then combine to form either nitric (HNO₃) or nitrous (HNO₂) acids (Henshaw 1994). Continued radiolysis in an atmosphere containing hydrogen and nitrogen compounds can generate ammonia (NH₃).

The actual composition and amount of the radiolysis products that will be formed is controlled by the radiation dose rate and by the composition and amount of the air and water vapour mixture contained in the copper canister. The primary control on the dose rate is the gamma radiation intensity due to Cs-137 and Sr-90 decay. These nuclides have a half-life of approximately 30 years and, consequently, gamma radiolysis declines to negligible levels in less than a thousand years. Radiolysis due to alpha, beta and neutron radiation continues for longer periods but the product yields are significantly smaller than with gamma radiolysis (Jones 1959). Water radiolysis does not depend on the specific conditions in **KBS-3H** (Gribi et al. 2007, Section 2.7).
The mass of residual water in a canister is pessimistically assumed to be 600 g and the atmosphere inside the canister is assumed to be composed of 10% of air and 90% argon (Section 3.1). If the availability of water is assumed to be the limiting factor, then 160 g of nitric acid can be produced based on 600 g of residual water (Henshaw et al. 1990, Henshaw 1994). If the availability of nitrogen is assumed to be the limiting factor, then 450 g of nitric acid can be formed (SKB 2010, Section 2.5.2).

These corrosive radiolysis products that are formed in the copper canister may begin to corrode the fuel assembly [3.2.7] and the exposed internal surfaces of the cast iron insert [4.2.6]. If the insert leaks and the internal surfaces of the copper overpack are subject to tensile stresses, the radiolysis products may also initiate stress corrosion cracking of the canister [4.2.7]. However, most of the vapour is expected to react with the massive cast iron insert before reaching the inner surface of the copper overpack. Additional volatile corrosive agents, such as iodine, are not expected to be released in the canister from a leaking fuel rod since they would have already been released at the time of encapsulation.

If the water vapour is derived from typical cooling pool water that contains boric acid, then some boron could potentially be present on the spent nuclear fuel surfaces. This boron (B-10) could react with fast neutrons to form alpha particles which would locally increase the alpha irradiation. The concentration of boric acid used in the cooling pools is, however, very low and typically 0.2 M, which would mean that there could be a maximum of 7 g of H$_3$BO$_3$ per canister. This is likely to be an overestimate because boric acid is volatile and may be expected to be driven off by the vacuum drying process. The amount of additional alpha radiation due to any residual boric acid is, therefore, negligible.

In summary, the amount of corrosive products from radiolysis of residual water is assumed to be small. Given the small volumes of corrosive substances that are formed, they are likely to be consumed in corrosion reactions with the cast iron insert [4.2.7] considering its large surface areas, and with the cladding, considering its proximity. The consumption of radiolysis products has been estimated to occur within a period of a few years or decades (Henshaw et al. 1990, Henshaw 1994). The consequences for the corrosion of the inner surface of the copper overpack are negligible.

Overall, radiolysis of residual water is influenced by the following features of the repository system.

- Radionuclide inventory: provides controls on the radiation field and, thus, the yield of radiolysis products.
- Temperature: affects the kinetics of radiolytic reactions.
- Fuel geometry: particularly presence of perforations in the fuel pins that would control the amount of residual water in a canister.
- Water and gas compositions: forms the humid air and water vapour mixture and thus controls the yield and nature of the corrosive radiolysis products.
**Uncertainties in the understanding of the FEP:**

The amount of residual air and water is the greatest uncertainty related to this process because it depends on the efficiency of the vacuum drying and argon purging during encapsulation. The current assumption of 600 g of water with 10% air is considered to be very pessimistic based on the observed number of perforated fuel pins in spent nuclear fuel assemblies and the likely efficiency of the purging process (see Section 3.1). Radiolytic yields for nitric oxides are also uncertain but conservative values have been used in the estimate of the amount of nitric acid formed, and thus the extent of corrosion that can occur.

**Couplings to other FEPs:**

Radiolysis of residual water is directly affected by the following FEPs:
- Radioactive decay (and in-growth) [3.2.1]
- Heat transfer [3.2.3]

Radiolysis of residual water directly affects the following FEPs:
- Corrosion of the cladding tubes and metallic parts of the fuel assembly [3.2.7]
- Corrosion of the cast iron insert [4.2.6]
- Stress corrosion cracking (of the canister) [4.2.7]

**References:**


3.2.6 Radiolysis of the canister water

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:**
- Water radiolysis;
- Radiolysis of groundwater

**Section in 2007-09:** 2.7

**General description:**
After failure of the copper canister, water may penetrate into the canister void spaces. There the water will be subject to the radiation field and may be decomposed by radiolysis, leading to the generation of oxidants and free hydrogen gas which can affect the radionuclide release and transport processes from the spent nuclear fuel. This canister water will be derived from groundwater that has first equilibrated with the bentonite buffer and subsequently with the corrosion products of the cast iron insert. Water radiolysis does not depend on the specific conditions in KBS-3H (Gribi et al. 2007, Section 2.7).

Radioactive decay causes α, β, γ and neutron radiation [3.2.1]. The linear energy transfer (LET) and penetration distance differs for each type of radiation and, thus, the radiolytic yields are also controlled by the radiation type. The highest potential yields are associated with gamma radiation, with alpha, beta and neutron radiation of water producing significantly less amounts of radiolysis products (Allen 1961).
Gamma radiation has a relatively long penetration distance and a low LET. The gamma dose rate will, however, become insignificant after around 1000 years because it is mostly due to the radioactive decay of Cs-137, which has a half-life of approximately 30 years. Given that the copper canister is expected to remain intact for approximately 100,000 years, radiolysis of water by gamma radiation inside the canister is of concern only in the early canister failure scenarios. Some minor radiolysis of bentonite porewater outside the canister is possible in the first few hundred years due to the ability of gamma radiation and neutrons to penetrate through the canister wall [5.2.5].

Alpha radiation has a very short penetration distance in water (< 1 mm) and a lower radiolytic yield than gamma radiation, but it will continue for many thousands of years because of the long half-lives of the alpha-emitting actinides (e.g. Pu-238, Pu-239 and Pu-240). As a consequence, some alpha and beta irradiation of water in the canister is possible in the long term after the canister has failed, but in very small quantities. Neutrons have a longer penetration distance, but the dose rate is negligible compared with the gamma radiation (Ranta-aho 2008).

Radiolysis of any water that does enter a failed canister will produce O₂, H₂O₂ and H₂ plus other species depending on the composition of the water, via a number of intermediate reactions involving radicals and ions. The oxidising agents will be consumed by corrosion of the cast iron insert. If, however, their rate of production exceeds the rate of reaction due to the formation of a passivating layer on the iron surfaces [4.2.6], then the local redox conditions inside the canister may become progressively more oxidising as radiolysis continues. If conditions were to become oxidising, then this would affect the rate of corrosion of the fuel assembly [3.2.7] and the spent nuclear fuel dissolution [3.2.8], and the solubility of the radionuclides released to the canister water [3.3.1].
Hydrogen produced during the corrosion of the insert, will maintain reducing conditions inside the canister, counteract the formation of radiolytic products (Pastina et al. 1999) and inhibit the dissolution of the UO₂ matrix [3.2.8]. Experimental studies on radiolysis of water containing small amounts of dissolved H₂ suggest that there is a threshold of dissolved H₂ above which no further measurable oxidant production occurs (Pastina et al. 1999, Pastina & LaVerne 2001). Given that the copper canister is expected to remain intact for approximately 100,000 years, radiolysis of water inside the canister by any process is unlikely to occur until after the inventory has been reduced substantially by radioactive decay. Experimental results show the presence of a threshold in alpha activity of the fuel below which the dissolution of the UO₂ matrix is solubility controlled [3.2.8]. From a radiolytic point of view, this implies that all radiolysis products are recombined back to water and there is no net water decomposition below the threshold alpha dose rate. This threshold in alpha activity was observed by Pastina et al. (1999) in pure water containing different amounts of B-10 and exposed to neutron and gamma radiation in a reactor. The threshold of observed UO₂ dissolution against alpha activity corresponds roughly to a fuel aged 10,000 years [3.2.8]. This implies that radiolysis of canister water becomes negligible after this time period.

Radiolysis of groundwater has been observed and evaluated in a number of natural analogue studies of uranium ore bodies, including at Oklo (Gabon) and Cigar Lake (Canada). These studies suggest that, although radiolysis occurs, redox conditions are affected only very locally to the ore. Consequently, the radiolysis may have only a small-scale influence on radionuclide transport because radiolytic oxidants will be consumed by reaction with iron in the canister and in minerals in the bentonite buffer (Miller et al. 2000). Overall, radiolysis of canister water is influenced by the following features of the repository system.

- Radionuclide inventory: controls the radiation field and, thus, the yield of radiolysis products.
- Temperature: affects the kinetics of radiolytic reactions.
- Fuel geometry: particularly the integrity of the fuel rods affects alpha radiolysis, which can occur if water comes into contact with fuel at the fuel/cladding gap.
- Water composition: is a primary control on the yield of radiolysis products after canister failure.

**Uncertainties in the understanding of the FEP:**

The mechanism of water radiolysis is well understood, but there are some uncertainties regarding the exact nature and yield of the radiolytic products that would be generated in a failed copper canister. These uncertainties are affected by the spatial and temporal variability of the radiation type (alpha, beta, gamma, neutrons) and the composition of the water that might enter the canister, which is, in itself, variable over time. There are few data available for radiolysis of saline solutions that are relevant to the groundwater composition at Olkiluoto. Nonetheless, given that the copper canister is expected to remain intact for a very long period of time, these uncertainties do not affect the overall understanding of the process or the life-time of the canister.
**Couplings to other FEPs:**
Radiolysis of canister water is directly affected by the following FEPs:
- Radioactive decay (and in-growth) [3.2.1]
- Heat generation [3.2.2]
- Heat transfer [3.2.3]
- Corrosion of the copper overpack [4.2.5]
- Corrosion of the cast iron insert [4.2.6]
Radiolysis of canister water directly affects the following FEPs:
- Corrosion of the cladding tubes and metallic parts of the fuel assembly [3.2.7]
- Alteration and dissolution of the fuel matrix [3.2.8]
- Aqueous solubility and speciation [3.3.1]
- Precipitation and co-precipitation [3.3.2]
- Corrosion of the cast iron insert [4.2.6]
- Aqueous solubility and speciation (in the canister) [4.3.1]
- Precipitation and co-precipitation (in the canister) [4.3.2]

**References:**

### 3.2.7 Corrosion of cladding tubes and metallic fuel assembly parts

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th><strong>Class:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Alternative names:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Metal corrosion; Corrosion of the cladding; Cladding failure</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Section in 2007-09:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7, 2.6</td>
</tr>
</tbody>
</table>

**General description:**
The cladding and other metallic components of the fuel assembly will contain neutron activation products of the alloying elements and impurities. The activation products likely to be present in zirconium alloy and other metal parts of the assembly are C-14, Cl-36, Zr-93 and Nb-94. As these metals are corroded by water in a failed canister, the
activation products will be released at a rate controlled by the corrosion of these metallic structures (with the exception of C-14, as discussed below).

The metallic structures of the fuel assembly are made of highly corrosion-resistant metals such as stainless steel, zirconium and nickel based alloys. The cladding material is zirconium alloy, containing small amounts of alloying metals such as Cr or Nb depending on the fuel type. For the time being, it is pessimistically assumed that the PWR control rods from OL3 will also be encapsulated with the fuel elements. These control rods are made of an alloy containing 80 wt.% Ag, 15 wt.% In and 5 wt.% Cd, and have a zirconium alloy cladding. The amount of zirconium alloy (including that in the cladding) is about ten times greater than that of the other metals in the fuel assemblies.

High temperature corrosion of the fuel cladding in the reactor creates a thin, tightly bound zirconium dioxide (ZrO₂) passivating layer. Hydrogen dissolved in the cooling water or generated by radiolysis of the cooling water is partly absorbed into the cladding (the hydrogen pick-up fraction). This can lead to hydride formation and long-term embrittlement (delayed hydrogen cracking) of the fuel cladding.

Prior to encapsulation, the fuel assemblies will be stored underwater in cooling pools for up to 50 years. During reactor operations and in the cooling pools, there is the potential for corrosion of the cladding and metallic structures. Based on operational experience at the Olkiluoto and Loviisa nuclear power plants, there is a low probability (less than one in ten thousand) that the fuel cladding will be leaking and, therefore, that the fuel pellets will be in contact with cooling pool water (Rossi et al. 2009).

Failed cladding can allow cooling pool water to enter into a fuel pin. If not completely dried prior to encapsulation, this water will be decomposed by radiolysis forming acids that will corrode the exposed internal surfaces of the copper canister and the fuel assembly [3.2.5]. The amount of corrosion of the fuel assembly that can occur before the canister fails is, however, very small due to the small amount of cooling pool water that may be present inside each canister.

Alpha decay of actinides in the spent nuclear fuel will cause a build-up of helium gas in the matrix [3.2.10] but this pressure increase is not sufficient to cause any damage to the cladding. This process is independent of the state of the canister, and is controlled directly by radioactive decay within the spent nuclear fuel.

After the canister has failed, water will enter the internal spaces and may also begin to corrode the exposed metallic surfaces of the fuel assembly and the fuel cladding. Under the chemically reducing conditions expected at the time of canister failure, the rate of general corrosion of the cladding will be very low due to the inherent corrosion resistance of zirconium alloy and the passivating ZrO₂ layer on its surface. Estimates of the rates of general corrosion of zirconium alloy under repository conditions gave a conservative upper limit of 20 nm/a and a ‘reasonable’ value of 5 nm/a, although rates as low as < 1 nm/a are possible (Shoesmith & Zagidulin 2010). Using a corrosion rate of 5 nm/a and an average cladding thickness of 0.5 mm, the lifetime of the cladding is estimated to be around 50,000 years, assuming it may corrode both from the inside and outside simultaneously. This is equivalent to a fractional corrosion rate of 10⁻⁵/a.

An alternative approach to estimating the zirconium alloy corrosion rate takes into account the solubility of ZrO₂ in the immediate vicinity of the fuel, and the removal of dissolved zirconium species, which then leads to zirconium alloy corrosion. The solubility of ZrO₂ in water is very low, in the order of 10⁻⁹ mol/L (Brown et al. 2005,
Bruno et al. 2007). This solubility is so low that it results in a negligible release of activation products from the zirconium alloy, consistent with the fractional release approach.

After canister failure, corrosion of the cast iron insert of the canister by water will generate hydrogen [4.2.6], which may be absorbed by the cladding and lead to zirconium alloy embrittlement.

During leaching tests of cladding samples, C-14 has been observed to be released relatively rapidly from the oxide part of the zirconium alloy cladding. The fraction of C-14 in the cladding inventory can be up to 20 % (Johnson & McGinnes 2002, Yamaguchi et al. 1999). The chemical form of C-14 in the cladding is not clear, although there is a possibility that it may exist as elemental carbon (graphite) or possibly the compound ZrC (zirconium carbide). These forms are generally stable but can be released as organic carbon compounds in a metal/water system (Yamaguchi et al. 1999).

Corrosion rates of the other stainless steel and nickel-based alloy components of the fuel assembly are likely to be higher than for zirconium alloy, but only a few studies have been carried out under anoxic conditions. These studies indicate average rates of around 0.15 μm/a, with a range of 0.01–1 μm/a, where the highest rates correspond to saline groundwaters (SKB 2010, Section 3.2.7). Based on these rates, the minimum lifetime of the metallic parts of a fuel element (assuming a minimum thickness of 0.1 mm) would range from a hundred to ten thousand years. There are no natural analogues of relevance to these man-made alloys, but there are industrial analogues of stainless steel that provide bounding limits on the corrosion rate of this material under a variety of physico-chemical conditions.

The main constituent in the alloy used in the control rods is silver. Silver is a noble metal and, if the alloy is exposed to reducing water, no silver corrosion is expected unless the water contains dissolved sulphides. In that case, the corrosion rate will be controlled by the rate of supply of sulphide (McNeil & Little 1992).

At Olkiluoto, the current groundwater conditions at repository depth are saline, having a total dissolved solids (TDS) content of around 10–20 g/L containing mainly sodium, calcium and chloride. These saline waters may initiate stress corrosion cracking of the zirconium alloy components, although the conditions necessary for stress corrosion cracking are uncertain.

Mechanical cladding failure and metal corrosion do not depend on the specific conditions in KBS-3H (Gribi et al. 2007, Sections 2.6, 2.7).

Overall, corrosion of the cladding tubes and metallic parts of the fuel assembly is influenced by the following features of the repository system.

- Radionuclide inventory: controls the rate of radiolysis and helium gas generation, thus affecting the pressure and stress.
- Temperature: because corrosion rates tend to increase with temperature.
- Mechanical stress: acting on the cladding (e.g. from internal helium pressure) can exacerbate stress corrosion cracking.
- Material composition: particularly the presence of impurities in the metallic components can accelerate the corrosion rate.
- Water composition: particularly strongly saline groundwaters can increase corrosion rates for some metals and induce stress corrosion cracking.
**Uncertainties in the understanding of the FEP:**

The corrosion processes for cladding and other metallic components are well understood, although there are some uncertainties regarding the rates of corrosion and the time to failure of the cladding under repository conditions. The uncertainties in the measured corrosion rates depend, among other things, on the method used to measure corrosion rates, especially for very low rates (Posiva 2013e). Due to these uncertainties, pessimistic values for the radionuclide fractional release rates from the cladding and other metal parts are used in the radionuclide release and transport calculations.

The release rates of activation products are conservatively based on the corrosion rates of the metallic parts of the fuel assembly under repository conditions. There are sufficient data of good quality to support much lower corrosion rates for zirconium alloy, which is the most abundant metal in the fuel assembly by weight (Kursten et al. 2004, White et al. 1966, Smart et al. 2004).

**Couplings to other FEPs:**

Corrosion of the cladding tubes and metallic parts of the fuel assembly is directly affected by the following FEPs:

- Heat transfer [3.2.3]
- Radiolysis of residual water (in an intact canister) [3.2.5]
- Radiolysis of canister water [3.2.6]
- Corrosion of the copper overpack [4.2.5]
- Corrosion of the cast iron insert [4.2.6]

Corrosion of the cladding tubes and metallic parts of the fuel assembly directly affects the following FEPs:

- Alteration and dissolution of the fuel matrix [3.2.8]
- Release of the labile fraction of the inventory [3.2.9]
- Criticality (if it were to occur) [3.2.11]
- Aqueous solubility and speciation [3.3.1]
- Precipitation and co-precipitation [3.3.2]
- Sorption [3.3.3]
- Aqueous solubility and speciation (in the canister) [4.3.1]
- Precipitation and co-precipitation (in the canister) [4.3.2]

**References:**


### 3.2.8 Alteration and dissolution of the fuel matrix

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:**

Fuel dissolution; Fuel matrix corrosion

**Section in 2007-09:**

2.7

#### General description:

On contact with water, the fuel matrix will alter, with formation of secondary phases, and eventually dissolve. This results in the slow congruent release of uranium and other radionuclides contained in the fuel matrix. This process is controlled by the chemical environment in the fuel/clad gap, and by the fuel composition and structure. This process does not depend on the specific conditions in KBS-3H (Gribi et al. 2007, Section 2.7).

**Effect of alpha activity on alteration and dissolution**

Under repository conditions at the expected time of water penetration in the canister, the conditions will be strongly reducing, because of the presence of massive amounts of metallic iron in the insert (and its corrosion products later on). It can be assumed, therefore, that the water coming into contact with the fuel will be free of oxygen and that the conditions inside the canister will be reducing.

At the time of groundwater penetration into the canister, the radiation field will be predominantly alpha [3.2.1]. Evidence from experiments suggests that alpha radiation exhibits only a weak oxidising effect that may lead to slow oxidative dissolution if no reducing agents are present, but that this may be countered effectively by the presence of dissolved H₂ gas and Fe(II) species that would be present in the repository near field. There is experimental evidence for a threshold in alpha activity below which radiation seems to become unable to sustain oxidative dissolution. The dissolution is then controlled by the solubility of UO₂ and not by radiolytic dissolution (Figure 3-5). This threshold is in the range 18–33 MBq/g of UO₂ in carbonate solution (Poinssot et al. 2005). This activity range equates to a decay time of between 10,000 to 30,000 years for BWR fuel with a burn-up of 40 MWd/kgU and PWR fuel with a burn-up of 60 MWd/kgU (Anttila 2005). However, the results of dissolution rate measurements by VTT (Ollila et al. 2004, Ollila & Oversby 2005, Ollila 2008) with ²³³U-doped UO₂ samples in 0.01 to 0.1 M NaCl solutions under anoxic conditions did not show any effect of alpha radiolysis with doping levels of 5 and 10 % ²³³U (corresponding to 32–63 MBq/g UO₂). This suggests that the radiolysis threshold depends on the environmental conditions, such as the reducing buffer capacity of the solution. Particularly low dissolution rates are observed in the presence of hydrogen. In the absence of radiolysis, under reducing conditions, U(IV) solubility controlled fuel matrix dissolution would dominate. The detailed mechanism of the fuel alteration and dissolution process is not well known because of the highly heterogeneous nature of the fuel.
Figure 3-5. Effect of alpha activity on solubility and decay rate controlled release of U from alpha-doped UO$_2$. Below the threshold, the fuel dissolution process is solubility-controlled, above the threshold it is controlled by alpha radiolysis. The darker shaded areas illustrate the spread in measured rates of the influence of alpha activity on fuel corrosion. Adapted from Poinssot et al. (2005, Figure 2).

Several modelling approaches have been proposed but none of them can fully explain the experimental results (MICADO 2010). In particular, the occurrence of oxidative dissolution of the UO$_2$ matrix is controversial. The solubility of U(VI) compounds being considerably higher than the less oxidised U(IV) species, if oxidative alteration were to occur, then the radionuclide release rate could become controlled directly by the rate of alteration rather than the rate of uranium dissolution. Dissolution rate measurements using unirradiated UO$_2$ under reducing conditions suggest that the release rate of uranium depends on the UO$_2$ surface area to water volume (SA/V) ratio, which may be related to the preferential dissolution of high-energy sites from the surface (Ollila 2008). The mechanism seemed to involve dissolution and subsequent precipitation of uranium because its concentration in solution remained constant.

The dissolution rate of spent nuclear fuel under the conditions caused by alpha radiolysis has been studied using UO$_2$ doped with U-$^{233}$ to simulate alpha activity levels expected at times of 3000 and 10,000 years after disposal (Ollila et al. 2004, Ollila & Oversby 2005, Ollila 2008). The data show that the presence of corroding iron in solution under anaerobic conditions is very effective at controlling the redox conditions and limiting the solubility of UO$_2$ and that H$_2$ is more effective than aqueous Fe(II) in lowering the uranium concentration in solution. The reduction of U(VI) carbonate and hydroxide complexes by aqueous Fe(II) has been studied experimentally.
by Myllykylä & Ollila (2008, 2011). The results suggest that Fe(II) reduced U(VI) in solution in spite of the U(VI) stabilising effect of the carbonate ions in solution. No enhanced corrosion rates or solubility effects that could be attributed to alpha radiolysis were observed in these tests. This result was corroborated by a literature review of radiolysis effects on UO₂ release (Ollila 2011). A solubility study (measurement of dissolution rates) of alpha-doped UO₂ using a high ionic strength solution (0.1 M NaCl) simulating groundwater conditions at repository depths at Olkiluoto is ongoing within the framework of the European REDUPP project (Evins & Vähänen 2012). Ollila (2008) also investigated the effect of 1 ppm sulphide ions under anoxic conditions (N₂, O₂ < 1 ppm) on the dissolution rates of 5 % and 10 % alpha-doped UO₂ samples. Ollila’s (2008) results indicate that sulphide ions are also able to counteract any oxidising effects due to alpha radiolysis since no effects of alpha-radiolysis could be observed in these tests either. These results have been confirmed by Yang et al. (2012), who studied experimentally the reaction between H₂O₂ and H₂S/HS⁻ as well as the effect of H₂S/HS⁻ on γ-radiation induced dissolution of a UO₂ pellet. Yang et al. (2012) show that the reaction of H₂O₂ and H₂S/HS⁻ is rapid and that H₂S/HS⁻ can effectively protect UO₂ from oxidative dissolution. The effect depends on sulphide concentration in combination with dose rate.

Radionuclides in the fuel matrix, cladding and in other metal parts are assumed to be released congruently as these components corrode. The congruency assumption is substantiated by experimental data (e.g. Röllin et al. 2001), which include supporting arguments related to crystal chemistry of spent nuclear fuel and microstructural analysis of fuel. Congruent release may be modified by the precipitation of some of the radionuclides embedded in the matrix material (e.g. isotopes of barium and radium) [3.3.1]. The available experimental data obtained under reducing conditions have been reviewed by Ollila (2011). This fractional release rate under reducing conditions is 10⁻⁷ per year.

In oxidising conditions, the measured fuel dissolution rate is higher because uranium is promptly oxidised to U(VI), which is considerably more soluble than U(IV). The fractional release rate assumed in oxidising conditions is 10⁻⁶ per year (Hanson et al. 2004). In principle, oxidising conditions may be achieved in the repository in the case of penetration of oxygenated glacial meltwaters during the melting period of a glacier located in the vicinity of the repository. The duration of the period of oxygenated meltwater penetration would, however, be very short and the redox conditions would be buffered by the bentonite and the cast iron insert during diffusion through the engineered barriers. Furthermore, there is no palaeohydrogeological evidence to suggest that there has been any influence of glacial waters from any past glaciations, and especially no oxygen containing glacial meltwaters, on the deep groundwater conditions at Olkiluoto [10.2.7]. Fuel pellets may be in contact with aerated water in the spent nuclear fuel cooling pool, in case of a leaking fuel rod. Part of this water may be trapped in the fuel pin at the time of encapsulation. In this case, the fuel would dissolve at a tenfold higher dissolution rate but the volume of water available for dissolution is limited (at most 50 cm³ of water per pin based on the void volume in a pin) and will be mostly in vapour form because of the high temperature of the fuel.

There is a considerable body of information on UO₂ dissolution processes and rates available from natural analogues, from a wide range of locations and geochemical environments, including the crystalline rocks at Palmottu in Finland (Ahonen et al.
These studies have indicated that the rate of dissolution is extremely slow in chemically reducing environments and in line with the laboratory data (Miller et al. 2000).

**Hydrogen effect**

The majority of experimental studies conducted in the presence of hydrogen show that dissolved hydrogen suppresses or significantly reduces UO$_2$ dissolution (e.g. Broczkowski et al. 2007, Carbol et al. 2005, 2009, Cera et al. 2006, Fors et al. 2009). The impact of hydrogen observed in different studies has been summarised by Broczkowski et al. (2010). A number of mechanisms have been either demonstrated or proposed to explain the H$_2$ effect, all of which involve the activation of hydrogen to produce the strongly reducing H’ radical, which scavenges radiolytic oxidants and suppresses fuel oxidation and dissolution. Evidence of a surface-catalysed reaction, taking place in the H$_2$-UO$_2$-H$_2$O system where molecular hydrogen is able to reduce oxidants originating from α-radiolysis has also been reported (Carbol et al. 2009). Jonsson et al. (2007) demonstrated by modelling that H$_2$ produced from radiolysis of groundwater alone will be sufficient to inhibit the dissolution completely for spent nuclear fuel older than 100 years.

**Effect of epsilon particles**

Epsilon particles are micrometre- to nanometre-sized metallic particles (containing Mo-Ru-Pd-Tc-Rh) that are formed in the spent nuclear fuel matrix during reactor operation. These particles embedded in the UO$_2$ matrix are shown to lower the hydrogen pressure needed to inhibit fuel dissolution to very low values, as low as 0.01–0.1 MPa. It is thought that epsilon particles play a catalyst role in the activation of molecular hydrogen (Broczkowski et al. 2010, Trummer et al. 2009). Since the corrosion of the insert could produce hydrogen pressures up to 5 MPa [4.2.6], it is expected that fuel dissolution will be completely suppressed at all times under the long-term conditions expected in repositories (Jonsson et al. 2007, Eriksen & Jonsson 2007, Eriksen et al. 2008). Yang et al. (2012) studied the reduction of U(VI) in the presence and absence of H$_2$ and Pd particles in anoxic aqueous solution. They showed that H$_2$S/HS$^-$ is a less powerful catalyst for molecular H$_2$ than Pd. Poisoning of the Pd catalyst by sulphide ions was not observed. Concerning the dissolution of the spent fuel matrix, epsilon particles have also been shown to dissolve much more slowly than the rest of the UO$_2$ matrix (Martinez-Esparza et al. 2002); therefore, the assumption of congruent dissolution of the fuel matrix can be considered pessimistic.

**Fuel matrix dissolution as a function of burn-up**

It was initially believed that burn-up may increase the spent nuclear fuel dissolution rate because it increases the content of fission products and higher actinides, and the surface area of the fuel, especially at the fuel rim [3.2.4]. More recent studies on a range of fuels with different burn-up histories under oxidising conditions indicate, however, that releases do not increase proportionally with burn-up (e.g. Clarens et al. 2008, Fors et al. 2009, Zwicky et al. 2011). The highest cumulative fractional releases are observed for fuels with an intermediate burn-up (40–50 MWd/kgU), a slight decrease being observed for fuels with the highest burn-up (over 60 MWd/kg). The increased amount of doping of the UO$_2$ matrix with non-uranium fission product and actinide atoms has been suggested to cause an increased resistance to oxidative dissolution of the UO$_2$ matrix.
The fuel dissolution rate has been measured also in the rim around a high burn-up pellet, which is the region with a higher concentration of actinide and fission products [3.2.4]. Experimental fuel leaching results showed that the releases of almost all radionuclides were slightly lower from the outer part, which contained the rim and had higher local burn-up compared with those from the centre of the pellet (Clarens et al. 2008). Similar trends in flow-through dissolution tests for high burn-up fuel in oxidising conditions have been reported (Hanson et al. 2004).

Overall, dissolution of the spent nuclear fuel matrix is influenced by the following features of the repository system.

- Temperature: affects the rate of alteration and dissolution reactions.
- Fuel geometry: both the radiation field and the surface area of the fuel in contact with water affect the dissolution rate.
- Material composition: the composition of the spent nuclear fuel is a primary control over the rate of dissolution and alteration.
- Water composition: the redox condition, in particular, is the most important control on spent nuclear fuel dissolution, with the rate of dissolution being very low under the expected near-field conditions.
- Gas composition: the presence of H₂ from anaerobic corrosion of iron may suppress dissolution.

**Uncertainties in the understanding of the FEP:**

The specific mechanism of fuel dissolution is still somewhat uncertain although a large number of experimental data has been produced to clarify the effect of hydrogen and that of burn-up. The effect of high burn-up on the initial releases of radionuclides in anoxic conditions has been investigated in the framework of the EU project ‘First nuclides’ (http://www.firstnuclides.eu).

The effect of high ionic strength of the Olkiluoto natural groundwater and surface chemistry on UO₂ dissolution has been investigated within the framework of the European project REDUPP (Evins & Vähänen 2012).

Experimental uncertainties are high when measuring UO₂ dissolution rates because this material is extremely sensitive to surface oxidation (as may occur in the case of damaged fuel rods), especially in the presence of a few layers of water undergoing radiolysis (Jégou et al. 2005, Muzeau et al. 2009). Thus, the large spread of dissolution rates published in the literature reflects more the dissolution rate of a (partially) oxidised UO₂ layer on the surface than the long-term dissolution rates of UO₂ in anaerobic conditions.

**Couplings to other FEPs:**

Alteration and dissolution of the spent nuclear fuel matrix is directly affected by the following FEPs:

- Heat transfer [3.2.3]
- Structural alteration of the fuel pellets [3.2.4]
- Radiolysis of the canister water [3.2.6]
- Corrosion of the cladding tubes and metallic parts of the fuel assembly [3.2.7]
- Diffusion in fuel pellets [3.3.4]
- Corrosion of the copper overpack [4.2.5]
- Corrosion of the cast iron insert [4.2.6]
Alteration and dissolution of the spent nuclear fuel matrix directly affects the following FEPs:

- Criticality (if it were to occur) [3.2.11]
- Aqueous solubility and speciation [3.3.1]
- Precipitation and co-precipitation [3.3.2]
- Sorption [3.3.3]
- Diffusion in fuel pellets [3.3.4]
- Aqueous solubility and speciation (in the canister) [4.3.1]
- Precipitation and co-precipitation (in the canister) [4.3.2]
- Sorption (in the canister) [4.3.3]
- Diffusion (in the canister) [4.3.4]
- Advection (in the canister) [4.3.5]
- Colloid transport (in the canister) [4.3.6]
- Gas transport (in the canister) [4.3.7]

References:


3.2.9 Release of the labile fraction of the inventory

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:**
- Dissolution of gap inventory; Instant release fraction

**Section in 2007-09:**
- 2.7

**General description:**

During irradiation of the fuel in a reactor, a certain fraction of the radionuclide inventory migrates into cracks in the fuel pellets and to grain boundaries, or accumulates in the available gaps between the fuel and the cladding. The migration process is by thermal diffusion during reactor operation [3.3.4]. When the copper canister and cladding fail and water contacts the spent nuclear fuel, this enriched (labile) fraction becomes available for release. These radionuclides usually have high solubilities and so may be rapidly released from the fuel on a time scale in the order of days. They are also generally non-sorbing, so can result in an early peak release from the near field. The canister water composition is not a controlling parameter because the gap release is highly soluble in all likely canister waters. This process does not depend on the specific conditions in **KBS-3H** (Gribi et al. 2007, Section 2.7).

This early release fraction of the inventory is modelled in the radionuclide release and transport calculations as a fraction of the inventory released instantaneously at the time of canister failure (known as the ‘instant release fraction’ or IRF). In reality, the release is not likely to be instantaneous and may continue for an extended period of time, but it is still rapid compared with the release rates of radionuclides embedded in the fuel matrix. The behaviour of fission gases in the IRF is best known, whereas the behaviour of other potentially segregated radionuclides is more uncertain. The IRF is independent of the bulk dissolution rate of the spent nuclear fuel [3.2.8] but depends on the irradiation history of the fuel.

The fraction of the radionuclides that is incompatible with the UO₂ matrix and accumulates in the gaps and void spaces within the fuel rods is generally considered to be correlated to the fission gas release measured in post-irradiation examination of fuel rods (Johnson & Tait 1997, Werme et al. 2004, Ferry et al. 2004). The fission gas release increases with increasing burn-up. Typically, values are < 1 % at burn-ups below 40 MWd/kgU, below 5 % for burn-up in the range 40–50 MWd/kgU (Nordström 2009, Oldberg 2009) and for very high burn-up (> 60 MWd/kgU) the fission gas release may exceed 10 %.

The currently average burn-up in Finnish reactors is 37 to 47 MWd/kgU depending on the reactor type (Table 3-1). The release of fission gas is also strongly correlated to the linear heat generation rate (i.e. the amount of heat generated per unit length of fuel rod) of the fuel. Modelling fission gas release as a function of irradiation history continues to develop (Van Uffelen 2006, Blair 2008) to improve fuel performance and for operational safety purposes.

The maximum burn-up of fuel in Finnish reactors has been limited to 45 MWd/kgU but, over the next few decades, the planned burn-up of fuel will increase to an estimated average assembly burn-up of 55 MWd/kgU or possibly higher, which would go beyond the limit considered in the data previously evaluated (Anttila 2005). Modelling of the
Fission gas release from the knowledge of the fuel power history has, however, improved (Van Uffelen 2006, Blair 2008, Nordström 2009, Oldberg 2009). Recently, calculations of the fission gas release of Swedish BWR and PWR reactors for various burn-up and linear power ratings have been carried out (Oldberg 2009, Nordström 2009). It has been experimentally shown that small fractions of the content of the fission gases Cs and I can leave the fuel matrix during reactor operation.

Fission product leaching studies on spent nuclear fuels with a range of burn-up and irradiation histories, and their correlations with fission gas release, can provide reliable estimates for the IRF of several important long-lived radionuclides (e.g. I-129 and Cs-135) for moderate burn-up UO₂ fuel, up to 45 MWd/kgU (Johnson et al. 2012, Serrano-Purroy et al. 2012). In this range of burn-up, the values chosen for the radionuclide transport calculations correspond to pessimistic, upper limits (Posiva 2013e). The radionuclides of most significance in the IRF in determining dose for early canister failure are C-14, Cl-36, Se-79, Tc-99, Pd-107, Sn-126, I-129 and Cs-135.

Overall, release of the labile fraction of the inventory is influenced by the following features of the repository system.

- Radionuclide inventory: controls the nature and concentrations of radionuclides present that may be released and their distribution in the fuel pellets.
- Temperature: can affect the rate of diffusion of the labile fraction.
- Mechanical stress: can cause cracking of the fuel pellets and increase the rate of release of the labile fraction.

**Uncertainties in the understanding of the FEP:**

There are uncertainties regarding the extent and, in some cases, the very existence of segregation of certain radionuclides. The process uncertainty is related to the lack of information on the diffusion mechanisms and rates of transfer of certain nuclides to the void spaces inside or near the fuel pellet. The current knowledge is empirical, based on the correlation with measurements of fission gas release. Moreover, the IRF values depend on fission gas release measurements for high burn-up fuel, for which there are few experimental data.

Any mechanistic and conceptual uncertainties are handled pessimistically, and immediate release after water contact is assumed.

**Couplings to other FEPs:**

Release of the labile fraction of the inventory is directly affected by the following FEPs:

- Radioactive decay (and in-growth) [3.2.1]
- Heat transfer [3.2.3]
- Structural alteration of the fuel pellets [3.2.4]
- Corrosion of the cladding tubes and metal parts of the fuel assembly [3.2.7]
- Production of helium gas [3.2.10]
- Aqueous solubility and speciation [3.3.1]
- Diffusion in fuel pellets [3.3.4]
- Corrosion of the copper overpack [4.2.5]
- Corrosion of the cast iron insert [4.2.6]
- Diffusion (in the canister) [4.3.4]
Release of the labile fraction of the inventory directly affects the following FEPs:

- Diffusion (in the canister) [4.3.4]
- Advection (in the canister) [4.3.5]

**References:**


### 3.2.10 Production of helium gas

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th><strong>Class:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:** Helium production

**Section in 2007-09:** 2.7

**General description:**

Alpha decay of actinides in the spent nuclear fuel results in the formation of helium (He) atoms in closed pores in the fuel matrix. Alpha particles (helium nuclei) form gaseous helium after they have slowed down in the fuel matrix. The helium gas is stable and unreactive with other elements and, therefore, the total amount of helium gas in the fuel elements will increase over time as alpha decay continues. The production of helium proceeds for as long as there is uranium or other actinides left in the spent nuclear fuel.

If helium gas was to accumulate in the annular gap between the fuel pellets and the cladding in an intact cladding tube, this would result in a build-up in pressure and could lead to mechanical failure of the tube. In an intact cladding tube (with a void volume of 50 cm³), the increase in gas pressure is calculated to be in the range of 3.4 to 4.4 MPa after 100,000 years (SKB 2010, p. 70). If all of this accumulated helium was released to the void inside the canister after the mechanical rupture of the cladding tube, the pressure increase would be about 0.5 to 0.65 MPa, which is considerably lower than the external pressure on the canister and, therefore, will have negligible consequences for deformation of the canister [4.2.3].

This process does not depend on the specific conditions in KBS-3H (Gribi et al. 2007, Section 2.7). The rate of helium production depends on the burn-up history of the fuel. It has been calculated that the amounts produced after 1000 and 50,000 years would be $7 \times 10^{18}$ and $2.6 \times 10^{19}$ atoms per gram of UO₂, respectively, for fuel with burn-up of 52 MWd/kgU (Ferry et al. 2010). For a burn-up of 60 MWd/kgU, the amount of He produced is higher by about 15 % at 1000 years but the difference decreases thereafter. Most of the helium generated will, however, remain trapped within the fuel matrix. It has been shown that the internal helium pressure build-up in the spent nuclear fuel over time will not lead to micro-cracking or affect the physical integrity of the UO₂ matrix [3.2.4]. Studies of helium accumulation in 320 million year old natural UO₂ (pitchblende) from Pen-ar-Ran in France, showed that it retained less than 5 % of the total amount of radiogenic helium formed (Roudil et al. 2008). This corresponds roughly to the expected solubility of helium in UO₂. The sample had not been subjected to any events that could have caused helium loss and, therefore, it was concluded that the rate of helium diffusion in the pitchblende was nine orders of magnitude higher than that expected in well-crystallised spent nuclear fuel. The reason for this is not presently clear.

Overall, the production of helium gas is influenced by the following features of the repository system.

- Radionuclide inventory: the burn-up of the fuel and the initial fission product inventory is a primary control on the rate of helium production.
- Temperature: controls the diffusion of helium in the fuel pellets.
- Mechanical stress: can cause cracking of the fuel pellets and increase the release rate of helium from the fuel.
**Uncertainties in the understanding of the FEP:**

The production of helium gas due to radioactive decay is well understood from the radioactive decay point of view. The effect of helium pressure build-up on UO₂ crack propagation in the rim of the fuel pellet is somewhat uncertain [3.2.4] but considered to be at an extremely low rate.

**Couplings to other FEPs:**

The production of helium gas is directly affected by the following FEPs:
- Radioactive decay (and in-growth) [3.2.1]
- Diffusion in fuel pellets [3.3.4]

The production of helium gas directly affects the following FEPs:
- Structural alteration of the fuel pellets [3.2.4]
- Release of the labile fraction of the inventory [3.2.9]

**References:**


**Related bibliography not cited in the text:**


### 3.2.11 Criticality

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th><strong>Class:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Event</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:**
Induced fission (criticality); Induced fission; Self-sustaining chain reaction; Uncontrolled chain reaction

**Section in 2007-09:**
2.3.1

**General description:**

Criticality is discussed here in analogy with TURVA-2012 FEP report (Posiva 2012d), although this event would normally be screened out as having vanishingly low probability based on the canister and the repository design, and the strategy for loading spent fuel assemblies into the canisters, which are intended to ensure the low likelihood of its occurrence in the long term.

A measure of the reactivity of a system containing fissile mass is the effective neutron multiplication factor ($k_{eff}$), which is the ratio of the number of neutrons produced in the system to the number of neutrons absorbed in or lost from the system. When $k_{eff} = 1$, the system is critical. The system is prompt critical when $k_{eff} = 1 + \beta$, where $\beta$ is the fraction of delayed neutrons.

A criticality accident is the occurrence of an uncontrolled nuclear chain reaction in a system containing fissile material. A prompt supercritical event could potentially cause energy release in a timescale of a few milliseconds, sufficient for fuel damage and release of radionuclides. All types of critical events would also change the radionuclide inventory of the system. In the repository, a criticality excursion could cause a mechanical failure of the engineered barriers and, potentially, a transfer of radionuclides from the canister to the geosphere [4.3.5, 5.3.5].

According to YVL B.4 (Guide YVL B.4), the effective multiplication factor $k_{eff}$ shall not exceed the value 0.95 under normal conditions or in anticipated operational occurrences and the value 0.98 in other design basis scenarios. These administrative margins have been designed so that any unknown uncertainties potentially missed in the criticality safety assessment cannot jeopardise subcriticality. Technological uncertainties, reactor operating history, changes in the storage conditions and uncertainties in the calculations shall be taken into account. In the long-term analysis it has to be assumed that leak-tightness of the disposal canister is lost and the container has sustained deformations (Guide YVL D.5). Subcriticality is one of the fundamental premises of the canister design (Raiko 2013).

The short-term criticality safety has been demonstrated in Haavisto (2014), which covers all operations in the encapsulation plant and the disposal facility when the disposal canisters are assumed to be intact. According to the analyses, criticality during encapsulation and disposal operations can be reliably ruled out.

The criticality hazard of the spent fuel lasts for a long time, due to the long-lived fissile nuclides (U-233, Pu-239 and particularly U-235). For a high burnup fuel, the reactivity maximum occurs at the time of disposal compared to all subsequent times. For a low burnup fuel, a peak around 20000 years may give the highest reactivity. In practice the limiting cooling time depends on the possible geometrical forms the fuel can take. Long-term changes in the fuel and container geometry, the diffusion of nuclides and
the dissolution of the fuel matrix may affect the reactivity remarkably. Theoretically, the potential for criticality persists until U-235 has decayed to the extent that the minimum critical mass exceeds the mass of uranium available for a given configuration. That is, for hundreds of millions of years.

The potential for long-term criticality in disposal conditions has been studied by several authors: Behrenz & Hannerz (1978), Van Konynenburg (1995), Oversby (1996a, 1996b, 1998), Nicot (2008), NDA (2010) and has been more recently reassessed by SKB (SKB 2010, Section 2.1.3) and Hedin et al. (2013).

Short and long-term criticality safety of a KBS-3V canister has been assessed for BWR, PWR and VVER-440 fuels (Haavisto 2014). Resembling analyses have been carried out for the Swedish disposal concept (Agrenius 2010) mainly for intact BWR and PWR fuel. The analyses (Haavisto 2014) are limited to in-vessel configurations and the long-term scenarios have been treated with bounding geometrical configurations and assumptions. The analyses provide information as to the boundary conditions (initial enrichment, burnup, geometrical configuration, fuel dissolution) within which subcriticality is ensured.

Out-of-canister criticality events caused by the transport (e.g. by diffusion [4.3.4]) and reaccumulation (e.g. by precipitation [4.3.2]) of radionuclides in the buffer, backfill or geosphere have also been assessed (SKB 2010, Section 2.1.3). It was concluded that criticality due to uranium outside the canister would require dissolution and transport of uranium under oxidising conditions and subsequent deposition of uranium under reducing conditions. There is no credible mechanism to achieve both oxidising and reducing conditions in the near field of the repository even in the long term. For these reasons, all out-of-canister criticality events are considered to have a vanishingly small probability.

In summary, in the short term, subcriticality is ensured by the control of the enrichment and the burnup (spent fuel inventory) and the fixed geometry of the fuel assemblies and the canister. The most recent analyses by Nicolet, NDA and SKB agree on the extremely low probability of a criticality event and on its low consequences. Nonetheless, in response of requests by the regulatory authorities in Finland and Sweden, long-term criticality scenarios will be formulated and analysed in 2017‒2018 for both KBS-3H and KBS-3V.

Overall, the reactivity of the disposal canister is controlled by the following features of the repository system.

- Radionuclide inventory: the enrichment and burnup of the fuel assemblies control the concentrations of fissile nuclides and neutron absorbers.
- Fuel geometry: controls the reactivity in the short term (moderator-to-fuel ratio)
- Canister composition and geometry: control the reactivity in the short term (moderator-to-fuel ratio, scattering, moderation).
- Canister composition: reactivity control in the long term. The corrosion-resistant copper overpack is designed to keep the canister leak-tight sufficiently long to ensure that most of the fissile Pu-239 decays to U-235, thus making criticality due to plutonium highly improbable.
− Water presence: Criticality can be ruled out if water is not present inside the canister. If water is present, neutrons will be slowed down and the system reactivity will be increased.
− Water composition: Impurities in the water can decrease the multiplication factor considerably compared with pure water.

**Uncertainties in the understanding of the FEP:**
The uncertainties in the calculated spent fuel composition will be taken into account in the criticality safety analysis.
Uncertainty in the assigned burnup value will be taken into account.

**Couplings to other FEPs:**
Criticality (if it were to occur) would be directly affected by the following FEPs:
− Radioactive decay and in-growth [3.2.1]
− Corrosion of the cladding tubes and metallic parts of the fuel assembly [3.2.7]
− Alteration and dissolution of the fuel matrix [3.2.8]
− Radiation attenuation (by canister metal) [4.2.1]
− Advection (in the canister) [4.3.5]
− Precipitation and co-precipitation (in the buffer) [5.3.2]
− Sorption (in the buffer) [5.3.3]
− Diffusion (in the buffer) [5.3.4]
Criticality (if it were to occur) would directly affect the following FEPs:
− Radioactive decay and in-growth [3.2.1]
− Heat generation [3.2.2]
− Advection (in the canister) [4.3.5]
− Advection (in the buffer) [5.3.5]

**References:**


Related bibliography not cited in the text:


US DOE 2008. Screening analysis of criticality features, events and processes for license application. DOC.20080208.0001. QA ANL-DS0-NU-000001 REV 00 February.
3.3 Migration FEPs

Radionuclides may migrate within, and out of, the spent nuclear fuel pellets by diffusion and become associated with the secondary alteration products formed by the degradation of the spent nuclear fuel matrix and the metallic components of the fuel assembly.

Other migration processes that occur in different repository components, such as advection, colloid transport and gas transport, do not occur within the spent nuclear fuel and so are not considered here. The migration processes that affect radionuclides released from the spent nuclear fuel to the water in the canister void space are described in Section 4.3.

### 3.3.1 Aqueous solubility and speciation

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
</tr>
</tbody>
</table>

**Alternative names:** Speciation of radionuclides; Colloid formation

**Dissolution and speciation; Solubility and speciation**

<table>
<thead>
<tr>
<th>Section in 2007-09:</th>
<th>2.7</th>
</tr>
</thead>
</table>

**General description:**

Radionuclides will be released by slow dissolution of the spent nuclear fuel matrix [3.2.8] and from the labile fraction of the inventory contained in the cladding gap and grain boundaries [3.2.9]. Solubility refers to the total aqueous concentration of an element in all dissolved chemical forms, which are in equilibrium with each other and with the solid mineral phases in the system. Radionuclides may form different solid phases, with different solubilities, depending on the geochemical conditions. For example, the UO₂ spent nuclear fuel matrix is poorly soluble under the geochemical conditions expected in the repository near field. If equilibrium is reached, a maximum concentration of all soluble species can be estimated from the solubility products of the species that can co-exist, including the solubility determining solid phase. The chemical form (speciation) that a radionuclide will take once in the aqueous phase will depend on the presence of other dissolved inorganic and organic compounds in the water with which it can bond.

The most important parameters that affect solubility and speciation are water composition, redox potential and pH. High salinity groundwater affects the solubility equilibria through the ionic strength. The presence of strong complexing ligands, such as carbonate and chloride ions, also affects the speciation and solubility. This process does not depend on the specific conditions in **KBS-3H** (Gribi et al. 2007, Section 2.7).

The redox conditions are relevant for elements with several oxidation states (e.g. U, Pu, Se), in terms of redox potential and reducing capacity of the system. In the case of uranium, for example, reducing conditions in the canister due to the presence of hydrogen gas and corroding iron are the most important factors limiting solubility. The temperature affects the kinetics of dissolution/precipitation processes as well as solubilities and the complexes formed. In addition, the reactivity of redox active surfaces (e.g. those of the iron insert) may strongly affect the kinetics of precipitation [3.3.2].

The inflow and outflow of water in the canister void space, and within the cladding tubes, will be controlled by the slow rate of groundwater movement and diffusion through the buffer. Consequently, the water inside the canister will readily become saturated with...
respect to low-solubility elements (e.g. uranium). Under these conditions, the migration of low-solubility elements from the spent nuclear fuel matrix to the aqueous phase is solubility limited. Further dissolution of the spent nuclear fuel will be controlled by the rate at which the dissolved species can diffuse out of the canister [4.3.4] and the dissolution process will be congruent, meaning that radionuclides will be released in the same proportions they occur in the spent nuclear fuel.

The corrosion of the cast iron insert will have important implications for controlling the solubility and speciation, and, therefore, the transport of radionuclides dissolved in the water within the canister void spaces. The generation of hydrogen due to anaerobic iron corrosion [4.2.6] will impose a reducing environment. This will decrease the solubility limit for most of the redox-sensitive radionuclides, such as actinides, thus decreasing the potential mass fluxes out of the system. Solubility limits play an important role in constraining the transport of many radionuclides within the canister, in contrast to the geosphere where radionuclide concentrations are likely to remain below solubility limits.

Similarly, the cladding and metallic components of the fuel assembly are also poorly soluble and, therefore, the release of the activation products they contain will also be slow and be solubility limited.

Radionuclide solubilities and speciation depend on the chemical environment in the canister cavity and several assessments have been made of the radionuclide solubility limits expected within the repository near field (Duro et al. 2006, Grivé et al. 2007, Wersin et al. 2014). Solubility limits relevant to the different canister water compositions expected at Olkiluoto have been defined, and in the solubility calculations, a solubility-limiting phase is assumed for each radioelement (Wersin et al. 2014). The most probable solid phases expected to form under the specified chemical conditions are identified. The results of chemical thermodynamic modelling can be compared with the measured concentrations in natural and laboratory studies.

Radionuclide solubility and transport may also be affected by microbes which can affect the geochemical conditions in the near field [5.2.8]. Sulphate-reducing bacteria can, for example, affect those elements whose solubility is considered to be limited by sulphate or sulphide phases, such as Sr, Ra, Se and Sn.

Overall, aqueous solubility and speciation is influenced by the following features of the repository system.

- Radionuclide inventory: controls the radionuclides that may be released from the spent nuclear fuel by congruent dissolution.
- Temperature: a control on the solubility of the spent nuclear fuel.
- Pressure: the hydrostatic pressure will influence solubility and speciation, but is a second-order control in the repository environment.
- Material composition: the composition of the spent nuclear fuel is a primary control over its solubility.
- Water composition: in particular, pH and redox potential (Eh) directly control the solubility and speciation of radionuclides through defining the type and concentration of dissolved species in canister water.
Uncertainties in the understanding of the FEP:

The general process of spent nuclear fuel dissolution and the solubility limits that will apply are well understood. There are uncertainties in the composition of the water penetrating into the canister, reflecting the uncertainty in the spatial and temporal variation in geochemical conditions in the repository (in particular pH, Eh and CO₂ concentration) during system evolution. This leads to uncertainties in the estimation of the solubility of the radionuclides and their speciation. This is accounted for to a large extent by defining reference and bounding groundwaters and porewaters as a function of the climatic evolution. For many elements, the geochemical uncertainty is larger than the thermodynamic uncertainty.

The thermodynamic uncertainty is estimated from the uncertainty in the main species that are present in solution, and the solubility constants associated with those species. The thermodynamic uncertainty also depends on the quality of the data in the database. For example, it includes various types of uncertainties, such as the extrapolation procedure of the original experimental data to zero ionic strength and the effects of the omission of relevant complexes in data processed for inclusion in the database.

Other uncertainties relate to metal carbonate complexation data, and solubility/speciation data for hyperalkaline conditions (pH > 10). For actinides, where carbonate complexation is of particular relevance, the uncertainty can be estimated to a large extent from the uncertainty in logK reported in the thermochemical database.

Furthermore, specific mechanisms and rates of dissolution in the high ionic strength groundwaters at Olkiluoto are uncertain. Most data are available for more dilute, oxidising groundwater systems. The current approach is to use thermodynamic data that are applicable both to low and high ionic strength and to take into account the uncertainties in the ionic strength extrapolation and in the overall uncertainty in the solubility value. The uncertainty treatment is based on conservative assumptions, thus leading to derived upper solubility limits that are generally higher than measured ones and therefore it is considered as robust.

Couplings to other FEPs:

Aqueous solubility and speciation is directly affected by the following FEPs:
- Radioactive decay (and in-growth) [3.2.1]
- Heat generation [3.2.2]
- Heat transfer [3.2.3]
- Radiolysis of the canister water [3.2.6]
- Corrosion of the cladding tubes and metal parts of the fuel assembly [3.2.7]
- Alteration and dissolution of the fuel matrix [3.2.8]
- Precipitation and co-precipitation [3.3.2]
- Sorption [3.3.3]
- Corrosion of the cast iron insert [4.2.6]

Aqueous solubility and speciation directly affects the following FEPs:
- Release of the labile fraction of the inventory [3.2.9]
- Precipitation and co-precipitation [3.3.2]
- Sorption [3.3.3]
- Diffusion in fuel pellets [3.3.4]
3.3.2 Precipitation and co-precipitation

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
<th>Alternative names:</th>
<th>Section in 2007-09:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**General description:**

The solubility limits of radionuclides in the canister and the buffer of a KBS-3V repository at Olkiluoto have been updated (Wersin et al. 2014). The same values are applicable to a KBS-3H repository as the canister and buffer materials are the same as in 3V and this process is not dependent on the type of design. Radionuclides generally will precipitate if their solubility limits are exceeded. Precipitation could occur, for example, if there is a change in the geochemical conditions, such as a drop in temperature or inflow of water from the rock with a different composition. Co-precipitation of a radionuclide with other major or more abundant, generally stable, isotopes of the same element. In addition, precipitation could be with a relatively “minor” element present at a low concentration, if it had a low solubility limit. This process is strongly influenced by the water conditions within the canister and, in turn, by the evolving bentonite porewater.

The possibility of solid solution formation under repository conditions has been investigated. It is thought that, at the relatively low temperatures expected in a repository at which ion diffusion in the solid phase is negligible, the transition from adsorbed layer or surface precipitate to solid solution is expected to occur only in solids with high recrystallisation rates (Bruno et al. 2007). Radionuclides released from the spent nuclear fuel may also become associated with secondary phases caused by oxidative alteration of the UO₂ matrix, if it occurs, but this is not seen experimentally [3.2.8].

Experimental tests on the dissolution of spent nuclear fuel pellets in water provide indications of the co-precipitation of Np and Pu with U (Cui et al. 2008, Fors et al. 2008). In performance assessments, usually no credit is taken for the expected co-precipitation.
of elements with similar chemical properties, since the solubilities of the component elements in ideal solid solutions are lower than those of the corresponding pure components. Furthermore, co-precipitation could also give rise to a stable deposit in which radionuclides could be produced by decay of the parent nuclides and be released at a later time.

There is overwhelming evidence of the co-precipitation of Ra, Ca and Ba in the presence of sulphate (Berner & Curti 2002). Sulphate is an abundant species in groundwater at Olkiluoto. The co-precipitation of Ra-226 with Ba is of particular interest as a potential mechanism to retard the migration of this mobile nuclide [4.3.2]. This process has been studied in the context of the KBS-3V type repository (Grandia et al. 2008, Bosbach et al. 2010) to derive radium solubility limits. If Ra and Ba are released simultaneously from spent nuclear fuel, it is suggested that Ra will be readily incorporated into the precipitating BaSO₄ to form Ra-Ba-sulphate solid solution, which would immobilise the otherwise mobile Ra. The inventory of stable barium in the waste is largely in excess compared to that of Ra-226, which forms by decay of thorium and uranium isotopes. The amount of stable Ba increases with its ingrowth as a decay product (from caesium). The calculated Ra/Ba at maximum Ra inventory (100 000 years) for different fuel types from Olkiluoto and Loviisa reactors are 2.2 *10⁻⁴ to 3.2*10⁻⁴ (Wersin et al. 2014).

Experimental results show that, even if Ra and Ba do not precipitate at the same time, in the long term there is a significant uptake of Ra into the bulk of barite crystals already formed (Bosbach et al. 2010). Barium is also present as a trace element in bentonite (approximately 325 ppm in commercial MX-80, i.e. the reference bentonite buffer material) (Curti & Wersin 2002, Table 5.3) and in groundwater (1–2 ppm at Olkiluoto, Pitkänen et al. 2004). The chemical form of Ba in the bentonite is, however, uncertain and it is not obvious whether it will co-precipitate with radionuclides to form insoluble barite. Precipitation and co-precipitation will retard radionuclide transport if they occur on solid surfaces. Precipitation is considered to be irreversible unless a change in geochemical conditions causes the solid phases to redissolve.

As the iron insert corrodes, and solid secondary alteration products are formed, there is the potential for radionuclides to be directly incorporated into these phases (mineralisation). Similarly, as radionuclides reach their solubility limits they may be incorporated in solid phases precipitated or co-precipitated from solution. Therefore, this will contribute to the retardation of migration of radionuclides out of a breached canister.

Radionuclides can form intrinsic colloids (e.g. an assemblage of very small fuel-derived particles) or pseudo-colloids (radionuclides adsorbed on the surface of colloidal particles) inside the canister. Suspended colloids can enhance the transport of certain radionuclides (e.g. Pu) within the canister [4.3.6]. It is unlikely, however, that colloids could be readily transported out of the canister to the buffer and beyond, because the buffer is designed to filter colloids [5.3.6]. In general, the stability and thus the mobility of colloidal systems are controlled by the grain size (1 nm to 450 nm) and the absolute surface potential (≥ ± 20 mV) of the dispersed particles and by the density of the particle. The stability of colloids depends on canister water salinity. In saline water, colloids will form a sediment due to aggregation and flocculation because the salinity reduces the electrostatic repulsion between the clay particle surfaces.
Overall, precipitation and co-precipitation are influenced by the following features of the repository system.

- Radionuclide inventory: controls the radionuclides that are available for inclusion in precipitates.
- Temperature: has a first-order control on the solubility of radionuclides.
- Pressure: can influence solubility limits and, thus, precipitation, but is a second order control in the repository environment.
- Material composition: the composition of the residual materials and natural compounds that may migrate into the canister may affect the precipitates that are formed.
- Water composition: is a first-order control on the solubility limits and the presence of other dissolved elements controls the potential for co-precipitation to occur.

**Uncertainties in the understanding of the FEP:**

Although the precipitation of mineral phases including radionuclides can be derived in a straightforward way from thermodynamic data, kinetic constraints may inhibit the formation of any given solid phase. There is a lack of kinetic data under relevant conditions for many radionuclides (Wersin et al. 2014).

Co-precipitation and solid solution formation have been studied only for specific systems, such as for pure carbonate and sulphate systems. The uncertainty in the evolution of near-field conditions is large and, therefore, this process is usually not considered in radionuclide transport modelling, which is a conservative approach. There are also few reliable thermodynamic data for solid solutions (Bruno et al. 2007).

**Couplings to other FEPs:**

Precipitation and co-precipitation are directly affected by the following FEPs:

- Radioactive decay (and in-growth) [3.2.1]
- Heat transfer [3.2.3]
- Radiolysis of the canister water [3.2.6]
- Corrosion of the cladding tubes and metallic parts of the fuel assembly [3.2.7]
- Alteration and dissolution of the fuel matrix [3.2.8]
- Aqueous solubility and speciation [3.3.1]
- Sorption [3.3.3]
- Corrosion of the cast iron insert [4.2.6]

Precipitation and co-precipitation directly affect the following FEPs:

- Aqueous solubility and speciation [3.3.1]
- Sorption [3.3.3]
- Diffusion in fuel pellets [3.3.4]
- Aqueous solubility and speciation (in the canister) [4.3.1]
- Precipitation and co-precipitation (in the canister) [4.3.2]
References:


### 3.3.3 Sorption

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th><strong>Class:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Alternative names:</strong></th>
<th><strong>Section in 2007-09:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Ion exchange; Physical adsorption</td>
<td>2.8</td>
</tr>
</tbody>
</table>

**General description:**

Sorption is a general term describing the attachment of dissolved species to mineral surfaces. It includes ion exchange, physical adsorption and surface complexation. Sorption can also be considered as the precursor to precipitation.

The updated geochemical database for a KBS-3V type repository at the Olkiluoto site (Wersin et al. 2014) includes sorption data for actinides (Th, Pa, U, Np, Pu, Am, Cm), elements of the groups IA to VIIA (C, Cs, Sr, Ra, Se, Sn, I, Cl), transition elements (Zr, Ni, Nb, Co, Mo, Tc, Pd, Ag) and lanthanides (Eu, Sm). The database is also applicable to the KBS-3H type repository as it does not depend on repository design.

Sorption is element specific and depends strongly on the surface characteristics of the solid phase. Under the ambient geochemical conditions, the likely sites for sorption associated with spent nuclear fuel will be the alteration products from UO₂ degradation [3.2.8] and the corrosion products of the steel components of the fuel assembly [3.2.7]. Due to the non-reactive nature of zirconium and nickel based alloys, sorption onto the cladding tubes and other components of the fuel assembly is not likely to be significant.

The greatest sorption potential within the canister will, however, be provided by the very large surface area of the cast iron insert and its corrosion products [4.3.3].

Overall, sorption is influenced by the following features of the repository system.

- Radionuclide inventory: controls the radionuclides that are available for sorption.
- Temperature: is a control over the kinetics of radionuclide sorption.
- Material composition (of the solid sorbing phase): the composition of the fuel and the metallic components of the fuel assembly will affect their sorption capacity.
- Water composition: particularly redox and the concentration of dissolved species can affect the solubility and sorption potential.

**Uncertainties in the understanding of the FEP:**

Although the conceptual understanding of sorption is well established, radionuclide sorption onto spent nuclear fuel and the metallic parts of the fuel assembly is not precisely quantified, but it does not add uncertainties to the understanding of the process itself.

**Couplings to other FEPs:**

Sorption is directly affected by the following FEPs:

- Radioactive decay (and in-growth) [3.2.1]
- Corrosion of the cladding tubes and metal parts of the fuel assembly [3.2.7]
- Alteration and dissolution of the fuel matrix [3.2.8]
- Aqueous solubility and speciation [3.3.1]
- Precipitation and co-precipitation [3.3.2]
- Corrosion of the cast iron insert [4.2.6]
Sorption directly affects the following FEPs:
- Aqueous solubility and speciation [3.3.1]
- Precipitation and co-precipitation [3.3.2]
- Diffusion in fuel pellets [3.3.4]

References:

### 3.3.4 Diffusion in fuel pellets

<table>
<thead>
<tr>
<th>Type:</th>
<th>Process</th>
</tr>
</thead>
<tbody>
<tr>
<td>Class:</td>
<td>Migration</td>
</tr>
</tbody>
</table>

**Alternative names:**
- Athermal diffusion

**Section in 2007-09:**
- 2.8

**General description:**
Athermal diffusion is radiation-induced diffusion of the most mobile radionuclides (e.g. Cs-137 and Cs-135, I-129, Cl-36, C-14) present in the UO$_2$ lattice to void spaces such as cracks in the fuel pellets, gaps between the fuel and the cladding or grain boundaries. Under repository conditions, fission and activation products generated in the fuel will slowly migrate within the spent nuclear fuel pellet (UO$_2$ matrix) by athermal diffusion. This process does not involve heat or a change in temperature. It does either depend on the specific conditions in KBS-3H (Gribi et al. 2007, Section 2.7).

Radiogenic heat will cause the peak temperature of the fuel to be reached within a few years after disposal, and it will then take around 5000 years for the spent nuclear fuel and the canister to cool to around 20 °C, assuming that the ambient temperature is about 10 °C [3.2.2]. Although these temperatures do not allow solid state thermal diffusion after disposal, they do allow athermal diffusion of the mobile radionuclides in the fuel pellet to the gaps and grain boundaries from which they can be rapidly released [3.2.9].

Alpha radiation is the only type of radiation capable of inducing athermal diffusion because it has the potential to change the physical and chemical behaviour of the fuel over the long term by forming defects in the UO$_2$ lattice and by helium generation [3.2.10]. The rate of athermal diffusion is dependent on the rate of alpha decay which reduces over time but continues for hundreds of thousands of years due to the long half-life of some of the alpha emitters [3.2.1].

Athermal diffusion is such a slow process that it cannot be experimentally studied in disposal conditions. A number of theoretical models have been applied to estimate the significance of this process with respect to the migration of fission products in fuel pellets (Lovera et al. 2003, Olander 2004, Ferry et al. 2005, 2008, Van Brutzel & Crocombette 2007, Martin et al. 2009).

Most theoretical studies estimate diffusion coefficients due to alpha self-irradiation to be low and in the range $10^{-25}$ to $10^{-29}$ m$^2$/s after 100 years of alpha decay. A diffusion
The diffusion coefficient of $10^{-25}$ m$^2$/s has been proposed for the first few decades, decreasing over time proportionally with the alpha activity of the spent nuclear fuel (Lovera et al. 2003). However, this value is probably an overestimation, because the authors did not take into account alternative mechanisms for the loss of Pb from the Oklo uraninite, on which their diffusion coefficient is based (SKB 2010, Section 2.4.2).

Analyses of the thermal spike produced in the UO$_2$ lattice due to alpha decay, typically producing a particle of kinetic energy 5 MeV and a recoil atom of ~ 100 keV, showed that it could cause athermal diffusion (Olander 2004). The diffusion coefficient calculated for Xe as a result of the thermal spike integrated over all alpha decays was $10^{-30}$ m$^2$/s.

It has been concluded that the athermal diffusion mechanism does not influence radionuclide release if the diffusion constant is less than $10^{-26}$ m$^2$/s (Werme et al. 2004). This corresponds to an atomic average movement of 0.5 microns in 10$^6$ years. For spent nuclear fuel with an assumed burn-up of up to 60 MWd/kg and a minimum cooling time of 20 years, this means that athermal diffusion is not expected to increase the instant release fraction of the inventory (Olander 2004).

This conclusion is supported by other studies. Investigation of the behaviour of iodine in UO$_2$ irradiated with heavy ions to simulate the effect of alpha radiation showed no measurable displacement (< 50 nm) within the matrix (Ferry et al. 2005, 2008). It was concluded from the modelling and experimental results, that the release of fission products to grain-boundaries would not be of consequence even in the long term. This conclusion is valid both for the centre of the fuel pellet and for the rim although there are higher uncertainties in the latter case.

Modelling of ballistic collisions and the additional point defects created during cascades showed that, in all cases, the derived athermal diffusion coefficients were < $10^{-26}$ m$^2$/s (Van Brutzel & Crocombette 2007). Additional molecular dynamics modelling of the contribution of radiation-induced diffusion to the diffusion of lattice atoms in UO$_2$ over a large temperature range of 300–1400 K showed that the effect of radiation-induced diffusion was negligible compared with thermally activated diffusion under long-term storage conditions (Martin et al. 2009).

The natural analogue observations from Oklo support a low value for the diffusion coefficient for alpha self-irradiation enhanced diffusion. It has been concluded that the diffusion coefficient of Pb at low temperatures in the Oklo uraninites was vanishingly small (Evins et al. 2005).

Combined, these studies all indicate that athermal diffusion is insignificant for the accumulation of the labile fraction in the gaps and grain boundaries after waste emplacement.

Overall, diffusion of radionuclides within the fuel rods (including gaps and grain boundaries) is influenced by the following features of the repository system.

- Radionuclide inventory: controls the radionuclides that are available for diffusion.
- Temperature: is relevant in the reactor but not in the repository, where temperatures will be much lower.
- Mechanical stress: can cause cracking of the fuel pellets (during reactor operation) and increase the rate of bulk diffusion from the pellets after emplacement.
Uncertainties in the understanding of the FEP:
Athermal diffusion cannot readily be measured experimentally, so the diffusion coefficient in the fuel pellet is, therefore, known only to the nearest order of magnitude. It is concluded, however, that the diffusion coefficient is so low that the process will make a negligible contribution to the instant release fraction.

Couplings to other FEPs:
Diffusion of radionuclides in the fuel pellet is directly affected by the following FEPs:
- Radioactive decay (and in-growth) [3.2.1]
- Heat transfer [3.2.3]
- Structural alteration of the fuel pellets [3.2.4]
- Alteration and dissolution of the fuel matrix [3.2.8]
- Aqueous solubility and speciation [3.3.1]
- Precipitation and co-precipitation [3.3.2]
- Sorption [3.3.3]
Diffusion of radionuclides in the fuel pellet directly affects the following FEPs:
- Alteration and dissolution of the fuel matrix [3.2.8]
- Release of the labile fraction of the inventory [3.2.9]
- Production of helium gas [3.2.10]

References:


4 CANISTER

4.1 Description

The canister, which is the same for both KBS-3V and KBS-3H designs, is designed for the encapsulation of entire fuel assemblies, and includes a number of sub-components, as shown in Figure 4-1:

- the copper overpack, which provides corrosion resistance;
- the cast iron insert, which provides mechanical strength and contains a number of channels for the fuel assemblies; and
- the internal void spaces between the fuel assemblies and the cast iron insert.

Initially, all of the void spaces will be filled with argon but, if the canister fails, the voids will become water filled. This canister water will be derived from groundwater that has first equilibrated with the bentonite buffer and later with the corrosion products of the cast iron insert.

Copper is used for the overpack material because of its well-known properties, its good thermal and mechanical characteristics, and for its resistance to corrosion in general and especially in the water-saturated and chemically reducing environment at repository depth in the Olkiluoto bedrock. Cast iron is used for the insert to provide mechanical strength and radiation shielding, and to maintain the fuel assemblies in a sub-critical configuration. The iron also provides a redox buffer to ensure chemically reducing conditions under which many radionuclides are poorly soluble. To enable fabrication of the canister, there will initially be a narrow annular gap between the cast iron insert and the copper overpack (Raiko et al. 2012).

There are currently three versions of the canister, one for each spent nuclear fuel type from the Olkiluoto and Loviisa reactors (Figure 4-1). The design and dimensioning analyses of the copper-iron canisters for spent nuclear fuel are presented in Raiko (2013) and the principal dimensions are summarised in Table 4-1.
The canister materials and the casting process are being developed to achieve specific design objectives and tolerances. The copper is oxygen-free, high conductivity copper (Cu-OF) with the addition of 30 to 100 ppm of phosphorus (Raiko 2013). This micro-alloying improves the creep strain properties of Cu-OF, thus lowering the risk of cracking in hot deformation processes during manufacturing and during postulated mechanical loads in the repository. The insert is made of nodular graphite cast iron. The lid of the insert is made of structural steel.

The spent nuclear fuel will be sealed in the canisters as whole fuel assemblies, one per channel in the cast iron insert. The assemblies will be vacuum dried to remove residual cooling pool water, and the void spaces in the canister will be purged with argon to expel air. This is to minimise the potential for the generation of corrosive radiolytic oxidants and nitric acid (see 3.2.4 and 3.2.5) inside the canister. Nonetheless, it is conservatively assumed that a maximum of 600 grams of residual water may be present inside a sealed canister within fuel rods that leaked in the cooling pools.

After loading of the fuel assemblies, the canister will be closed and the lid welded into place. The outer surfaces of the weld will be machined and the entire weld inspected with non-destructive means to ensure it is water and gas tight. After loading, the canister will be stored prior to emplacement in the repository. The canister temperature (measured on the external surfaces) increases within a few days by 50–100 °C, depending on the internal radiogenic heat generation and the ventilation conditions in the canister storage area.
Table 4-1. Main dimensions and masses of canisters for different types of spent nuclear fuel. From Raiko (2013).

<table>
<thead>
<tr>
<th></th>
<th>Loviisa 1–2 (VVER-440)</th>
<th>Olkiluoto 1–2 (BWR)</th>
<th>Olkiluoto 3 (PWR)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outer diameter (m)</td>
<td>1.05</td>
<td>1.05</td>
<td>1.05</td>
</tr>
<tr>
<td>Height with flat bottom end* (m)</td>
<td>3.552</td>
<td>4.752</td>
<td>5.2225</td>
</tr>
<tr>
<td>Thickness of copper cylinder, nominal, (mm)</td>
<td>49</td>
<td>49</td>
<td>49</td>
</tr>
<tr>
<td>Thickness of copper lid and bottom, nominal, (mm)</td>
<td>50</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>Thickness of iron insert bottom nominal** (mm)</td>
<td>70</td>
<td>60</td>
<td>85</td>
</tr>
<tr>
<td>Number of fuel assemblies</td>
<td>12</td>
<td>12</td>
<td>4</td>
</tr>
<tr>
<td>Amount of spent nuclear fuel (tU)</td>
<td>1.4</td>
<td>2.2</td>
<td>2.1</td>
</tr>
<tr>
<td>Void space with fuel assemblies (m³)</td>
<td>0.61</td>
<td>0.95</td>
<td>0.67</td>
</tr>
<tr>
<td>Mass of fuel assemblies (ton)</td>
<td>2.6</td>
<td>3.6</td>
<td>3.2</td>
</tr>
<tr>
<td>Mass of iron (ton)</td>
<td>8.6</td>
<td>10.6</td>
<td>15.8</td>
</tr>
<tr>
<td>Mass of steel (ton)</td>
<td>2.0</td>
<td>3.0</td>
<td>2.1</td>
</tr>
<tr>
<td>Mass of copper* (ton)</td>
<td>5.6</td>
<td>7.3</td>
<td>8.0</td>
</tr>
<tr>
<td>Total canister mass gross* (ton)</td>
<td>18.8</td>
<td>24.5</td>
<td>29.1***</td>
</tr>
<tr>
<td>Total area of canister outside surface* (m²)</td>
<td>13.67</td>
<td>17.63</td>
<td>19.18</td>
</tr>
<tr>
<td>Total volume of canister* (m³)</td>
<td>3.03</td>
<td>4.07</td>
<td>4.46</td>
</tr>
</tbody>
</table>

* If the welded base alternative is used for the copper overpack, then the total length increases +75 mm, the total surface area +0.45 m², the total canister volume +0.024 m³ and the copper mass and the total canister mass +0.21 ton.

** The total bottom thickness is the sum of cast iron thickness and the steel cassette bottom plate thickness.

Posiva and SKB are carrying out a joint programme to develop methods to manufacture, seal and inspect copper-iron canisters for spent nuclear fuel. Since TURVA-2012, Posiva has changed their reference welding method (see Posiva 2014b) from electron beam welding to friction stir welding (FSW), which is the same method as used by SKB, and this new method is assumed in this report.

4.1.1 Long-term safety and performance

The safety function of the canister is to ensure a prolonged period of containment of the spent nuclear fuel. This safety function rests first and foremost on both the mechanical strength of the canister’s cast iron insert and the corrosion resistance of the copper overpack surrounding it. It is intended that the canister shall retain its favourable properties over hundreds of thousands of years (Design Basis – KBS-3H, Posiva 2016c).

The ability of the canister to provide its containment safety function over the long term depends on its initial state, and on the corrosion process and mechanical loads applied during its evolution. The majority of canisters will be intact at the time of emplacement.
A few canisters may, however, have an initial defect (penetrating or non-penetrating) that, if present, is most likely to be located in the lid weld. Although the welds will be inspected, it is possible that a small number of these defective canisters may be emplaced in the repository, thus affecting the canister’s initial state.

The main driver for corrosion of the copper overpack, in the short term, will be residual oxygen introduced during operation of the repository and, in the longer term, the sulphide ions present in the groundwater, buffer and backfill. The main mechanical loads applied to the canister will be caused by uneven swelling of the buffer, isostatic loads from the presence of a future ice sheet, and the possibility of a shear load due to a rock displacement.

4.1.2 Overview of the potentially significant FEPs

There are a number of processes that are considered to be potentially significant for the long-term safety performance of the canister that relate to system evolution and to the migration of radionuclides and other substances.

Processes related to system evolution are:
4.2.1 Radiation attenuation
4.2.2 Heat transfer
4.2.3 Deformation
4.2.4 Thermal expansion of the canister
4.2.5 Corrosion of the copper overpack
4.2.6 Corrosion of the cast iron insert
4.2.7 Stress corrosion cracking

Processes related to the migration of radionuclides and other substances are:
4.3.1 Aqueous solubility and speciation
4.3.2 Precipitation and co-precipitation
4.3.3 Sorption
4.3.4 Diffusion
4.3.5 Advection
4.3.6 Colloid transport
4.3.7 Gas transport

These processes are the same as those in TURVA-2012 (Posiva 2012d). According to Gribi et al. (2007, Section 3.2) the list of canister processes considered for KBS-3V is appropriate also for KBS-3H.
These processes are each potentially affected by a number of features of the repository system that can influence the occurrence, rate, activity and potential couplings between the processes. These features relate either to aspects of the design of the repository or to parameters (characteristics) of the copper canister that might be time dependent during the repository lifetime. The most significant features are:

- Radionuclide inventory
- Temperature
- Pressure
- Canister geometry
- Mechanical stresses
- Material composition
- Water composition
- Gas composition.

The possible influences of these features on the processes considered to be significant for the long-term safety of the canister are described in each FEP description, and are summarised in Table 4-2.

Many of the processes occurring within the canister are interdependent and directly coupled to each other. For example, corrosion of the cast iron insert [4.2.6] will affect the sorption capacity [4.3.3] (via material and water composition). The direct couplings are listed in each FEP description, and are summarised in the matrix shown in Table 4-3.

Similarly, due to the complex interactions between the various parts of the disposal system, the evolution of the canister can influence (or be influenced by) processes occurring in other parts of the repository through the interactions between various FEPs. For example, heat transfer in the canister [4.2.2] will drive heat transfer in the bentonite buffer [5.2.1]. The interactions between the canister and other components of the disposal system are summarised in Table 4-4.
References


Table 4-2. Possible influences of features of the disposal system on the processes considered to be significant for the long-term performance of the canister (marked with Y). These influences and couplings are discussed in more detail in each FEP description.

<table>
<thead>
<tr>
<th>Processes</th>
<th>Features</th>
<th>Radionuclide inventory</th>
<th>Temperature</th>
<th>Pressure</th>
<th>Canister geometry</th>
<th>Mechanical stresses</th>
<th>Material composition</th>
<th>Water composition</th>
<th>Gas composition</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Processes related to system evolution:</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.2.1 Radiation attenuation</td>
<td>Y</td>
<td></td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td>Y</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.2.2 Heat transfer</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td>Y</td>
<td></td>
<td></td>
<td>Y</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.2.3 Deformation</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.2.4 Thermal expansion of the canister</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.2.5 Corrosion of the copper overpack</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td></td>
</tr>
<tr>
<td>4.2.6 Corrosion of the cast iron insert</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td>Y</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td></td>
</tr>
<tr>
<td>4.2.7 Stress corrosion cracking</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Processes related to the migration of radionuclides and other substances:</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.3.1 Aqueous solubility and speciation</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td>Y</td>
<td>Y</td>
<td></td>
</tr>
<tr>
<td>4.3.2 Precipitation and co-precipitation</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td>Y</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.3.3 Sorption</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td>Y</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.3.4 Diffusion</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td>Y</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.3.5 Advection</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.3.6 Colloid transport</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.3.7 Gas transport</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td></td>
</tr>
</tbody>
</table>
Table 4-3. Possible couplings between FEPs within the canister considered significant for the long-term performance of the disposal system. The numbers on the leading diagonal refer to the FEPs listed in Section 4.1.2. As an example of how to read this table, the blue coloured square means that “Corrosion of the cast iron insert” [4.2.6] directly affects “Sorption” [4.3.3].

<table>
<thead>
<tr>
<th></th>
<th>4.2.1</th>
<th>X</th>
<th>X</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.2.2</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>4.2.3</td>
<td>X</td>
<td></td>
<td></td>
</tr>
<tr>
<td>X</td>
<td>4.2.4</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>X</td>
<td>4.2.5</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>X</td>
<td>4.2.6</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>X</td>
<td>X</td>
<td>4.2.7</td>
<td></td>
</tr>
<tr>
<td>4.3.1</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>4.3.2</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>X</td>
<td>4.3.3</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>X</td>
<td>4.3.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.3.5</td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>4.3.6</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>X</td>
<td>X</td>
<td>4.3.7</td>
<td></td>
</tr>
</tbody>
</table>
**Table 4-4.** Interaction matrix for the canister. FEPs in italics are addressed in other chapters. A short name for some of the FEPs is used in the table: IRF (Release of the labile fraction of the inventory), Precipitation (Precipitation and co-precipitation).

<table>
<thead>
<tr>
<th>Spent fuel</th>
<th>Heat transfer</th>
<th>Radiation attenuation</th>
<th>Alteration and dissolution of the fuel matrix; Diffusion; Precipitation; IRF</th>
<th>Radiation attenuation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer; IRF; Advection; Colloid transport; Diffusion</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer; Thermal expansion of the canister</td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer</td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Deformation</td>
<td>Heat transfer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Deformation</td>
<td>Overpack</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Advection Diffusion Sorption</td>
<td>Buffer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Inadvertent human intrusion</td>
<td>External</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Insert</th>
<th>Heat transfer</th>
<th>Radiation attenuation</th>
<th>Alteration and dissolution of the fuel matrix; Diffusion; Precipitation; IRF</th>
<th>Radiation attenuation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer; IRF; Advection; Colloid transport; Diffusion</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer; Thermal expansion of the canister</td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer</td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Deformation</td>
<td>Heat transfer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Deformation</td>
<td>Overpack</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Advection Diffusion Sorption</td>
<td>Buffer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Inadvertent human intrusion</td>
<td>External</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Void spaces</th>
<th>Heat transfer</th>
<th>Radiation attenuation</th>
<th>Alteration and dissolution of the fuel matrix; Diffusion; Precipitation; IRF</th>
<th>Radiation attenuation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer; IRF; Advection; Colloid transport; Diffusion</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer; Thermal expansion of the canister</td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer</td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Deformation</td>
<td>Heat transfer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Deformation</td>
<td>Overpack</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Advection Diffusion Sorption</td>
<td>Buffer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Inadvertent human intrusion</td>
<td>External</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Water</th>
<th>Heat transfer</th>
<th>Radiation attenuation</th>
<th>Alteration and dissolution of the fuel matrix; Diffusion; Precipitation; IRF</th>
<th>Radiation attenuation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer; IRF; Advection; Colloid transport; Diffusion</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer; Thermal expansion of the canister</td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer</td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Deformation</td>
<td>Heat transfer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Deformation</td>
<td>Overpack</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Advection Diffusion Sorption</td>
<td>Buffer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Inadvertent human intrusion</td>
<td>External</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Thermal expansion of the canister</th>
<th>Heat transfer</th>
<th>Radiation attenuation</th>
<th>Alteration and dissolution of the fuel matrix; Diffusion; Precipitation; IRF</th>
<th>Radiation attenuation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer; IRF; Advection; Colloid transport; Diffusion</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer; Thermal expansion of the canister</td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer</td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Deformation</td>
<td>Heat transfer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Deformation</td>
<td>Overpack</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Advection Diffusion Sorption</td>
<td>Buffer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Inadvertent human intrusion</td>
<td>External</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Deformation</th>
<th>Heat transfer</th>
<th>Radiation attenuation</th>
<th>Alteration and dissolution of the fuel matrix; Diffusion; Precipitation; IRF</th>
<th>Radiation attenuation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer; IRF; Advection; Colloid transport; Diffusion</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer; Thermal expansion of the canister</td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer</td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Deformation</td>
<td>Heat transfer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Deformation</td>
<td>Overpack</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Advection Diffusion Sorption</td>
<td>Buffer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Inadvertent human intrusion</td>
<td>External</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Overpack</th>
<th>Heat transfer</th>
<th>Radiation attenuation</th>
<th>Alteration and dissolution of the fuel matrix; Diffusion; Precipitation; IRF</th>
<th>Radiation attenuation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer; IRF; Advection; Colloid transport; Diffusion</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer; Thermal expansion of the canister</td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer</td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Deformation</td>
<td>Heat transfer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Deformation</td>
<td>Overpack</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Advection Diffusion Sorption</td>
<td>Buffer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Inadvertent human intrusion</td>
<td>External</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Buffer</th>
<th>Heat transfer</th>
<th>Radiation attenuation</th>
<th>Alteration and dissolution of the fuel matrix; Diffusion; Precipitation; IRF</th>
<th>Radiation attenuation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer; IRF; Advection; Colloid transport; Diffusion</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer; Thermal expansion of the canister</td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer</td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Deformation</td>
<td>Heat transfer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Deformation</td>
<td>Overpack</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Advection Diffusion Sorption</td>
<td>Buffer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Inadvertent human intrusion</td>
<td>External</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Surface environment</th>
<th>Heat transfer</th>
<th>Radiation attenuation</th>
<th>Alteration and dissolution of the fuel matrix; Diffusion; Precipitation; IRF</th>
<th>Radiation attenuation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer; IRF; Advection; Colloid transport; Diffusion</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer; Thermal expansion of the canister</td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Heat transfer</td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Deformation</td>
<td>Heat transfer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Deformation</td>
<td>Overpack</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Advection Diffusion Sorption</td>
<td>Buffer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Inadvertent human intrusion</td>
<td>External</td>
</tr>
</tbody>
</table>
4.2 System evolution FEPs

The key function of the canister is to contain the spent nuclear fuel and, hence, limit the release of radionuclides into the host rock and the surface environment by natural transport processes. This is achieved through the resistance of the copper canister to corrosion and the structural strength of the cast iron insert. Various radiation, thermal, chemical and mechanical processes (and their couplings) will affect the evolution of the cast iron insert and the copper overpack of the canister. The most important potential consequence is failure of the canister that would ultimately allow groundwater to penetrate the void space and come into contact with the fuel. The following descriptions summarise each of these processes and the effects of the different features on them. The couplings between processes are identified, but the analyses and consequences of these couplings will be dealt with in Posiva (2016b).

Whenever the FEP description is affected by the specific characteristics of the KBS-3H design, the term “KBS-3H” (in bold) is included in the text.

References

Posiva 2016b. Safety evaluation for a KBS-3H spent nuclear fuel repository at Olkiluoto – Performance Assessment. Eurajoki, Finland: Posiva Oy. POSIVA 2016-02 (in prep.).

4.2.1 Radiation attenuation

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
<tr>
<td><strong>Alternative names:</strong></td>
<td><strong>Section in 2007-09:</strong></td>
</tr>
<tr>
<td>Radiation attenuation/heat generation</td>
<td>3.3.1</td>
</tr>
</tbody>
</table>

**General description:**

Radiation will be emitted due to radioactive decay within the spent nuclear fuel and some of this radiation will penetrate out to the iron and copper metal of the canister. The radiation field will reduce over time in a direct relationship to decay, although ingrowth of daughter radionuclides will also affect the radiation field over time [3.2.1]. The alpha and beta radiation is poorly penetrating and will largely be attenuated by the fuel matrix itself. The primary radiation-related process in the canister is, therefore, attenuation of gamma and neutron radiation within the massive cast iron insert and, to a lesser extent, the copper overpack of the canister.

The rate of radiation attenuation is, in part, controlled by the design of the canister, with the gamma dose rate being halved for every 20 to 25 mm thickness of the iron insert. Radiation attenuation by the canister has been calculated to reduce the maximum post-encapsulation radiation dose rates from 100 Sv/h at the spent nuclear fuel surface to 200 mSv/h at the outer surface of the copper canister for gamma radiation, and from 30 mSv/h to 10 mSv/h for neutron radiation (Anttila 2005).

This substantial radiation attenuation will have a number of effects, the most significant being the generation of thermal energy (heat) directly in the metal. The greatest
influence on the near-field temperature will, however, be the decay heat generated directly by radioactive decay in the spent nuclear fuel pellets [3.2.2].

A secondary effect of gamma and neutron radiation attenuation is minor material changes to the canister metals (e.g. altered yield stress and creep rates, enhanced solute segregation, dimensional changes and increased brittleness). Of these, embrittlement of iron could be the most problematic because it can affect the mechanical strength of the cast iron insert and make it more prone to failure under loading.

The radiation sensitivity of iron and steel materials is determined by their chemical composition. Phosphorous, copper and nickel contents increase the susceptibility of steel to radiation embrittlement. Empirical relationships between fast neutron fluence and the chemical composition of steels, and the degree of radiation embrittlement, have been developed from a large body of experimental data on reactor pressure vessel steels. These studies indicate that detectable embrittlement effects do not occur until the fast neutron fluence exceeds a threshold of around $10^{19}$ neutrons/cm² (ASME 1983).

In comparison, the calculated neutron fluence that will impinge upon the canister metal over 100,000 years is several orders of magnitude less than this threshold, at $4 \times 10^{15}$ neutrons/cm² (Ranta-aho 2008). The peak radiation field and, therefore, attenuation will be reached shortly after disposal and is directly related to gamma and neutron radiation. The gamma radiation is due largely to the radioactive decay of Cs-137 which has a half-life of approximately 30 years. The period of gamma radiation attenuation is, therefore, limited to less than the first thousand years.

Studies on the effect of radiation on the canister during long-term disposal have shown that the magnitude of any physical property changes, e.g. yield stress, creep rates, enhanced solute segregation, dimensional changes, or brittleness, resulting from radiation exposure will be negligible (e.g. Guinan 2001). In some recent studies, however, it has been claimed that even if dose rates are low, they can have adverse effects on material properties in some cases (Brissonneau et al. 2004, Sandberg & Korzhavyi 2009). It has been argued that long time scales and, for instance, low temperature may increase the effects of neutron and gamma radiation in disposal canisters. Copper has been shown to increase the susceptibility of steel to radiation embrittlement (Brissonneau et al. 2004). The highest degree of embrittlement was observed in steel containers with copper contents in the range of 0.05 to 0.25 %. To minimise the risk of radiation embrittlement in the disposal canister, the copper content of the iron used to manufacture the insert is specified to be less than 0.05 %.

Taking account of the dose rate from the fuel and the composition of the canister metal, it is considered very unlikely that the mechanical integrity of a canister will be significantly affected by radiation attenuation and embrittlement processes, and no detectable material damage or ageing effects are expected (Raiko 2013).

Overall, radiation attenuation by the canister metal is influenced by the following features of the repository system.

- Radionuclide inventory: defines the time (decay) dependent radiation intensity and, therefore, the dose rate experienced by the metal.
- Canister geometry: particularly the canister thickness, which controls the total amount of radiation attenuation that occurs.
- Material composition: alters the susceptibility of metals to embrittlement.
Uncertainties in the understanding of the FEP:
The time-dependent radiation field and dose to the canister metals is readily calculated, as is the amount of attenuation in the canister metals. There are no significant uncertainties.

Couplings to other FEPs:
Radiation attenuation by the canister metals is directly affected by the following FEP:
- Radioactive decay (and in-growth) [3.2.1]
Radiation attenuation by the canister metal directly affects the following FEPs:
- Heat transfer [4.2.2]
- Thermal expansion of the canister [4.2.4]
- Radiolysis of porewater (in the buffer) [5.2.5]

References:

<table>
<thead>
<tr>
<th>Type:</th>
<th>Heat transfer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Class:</td>
<td>System evolution</td>
</tr>
<tr>
<td>Alternative names:</td>
<td>Heat transport</td>
</tr>
<tr>
<td>Section in 2007-09:</td>
<td>3.4</td>
</tr>
</tbody>
</table>

General description:
Heat will be generated primarily by radioactive decay in the fuel [3.2.2] and, to a lesser extent, by radiation attenuation in the canister metals [4.2.1]. This heat will be transferred through the copper canister to the bentonite buffer by conduction directly through the metals and by radiation across the void spaces within
the canister. Convection may also be an important means of heat transfer after the canister has been breached and groundwater has flooded the void spaces.

The rate of heat transfer through the copper canister is controlled by:

- the thermal conductivity of the iron and copper metals;
- heat transfer processes in the canister void spaces and the bentonite buffer that control the time-dependent temperature gradient across the canister metals; and
- heat transfer processes between the buffer and the rock through the supercontainer shell and through air or water or extruded buffer in the gap around the perforated shell.

Thermal processes in the cast iron insert and copper canister do not depend on the specific conditions in KBS-3H (identical fuel and canister as in KBS-3V). Differences arise only due to the specific repository geometry, materials (e.g. titanium) and conditions outside the canister.

Both iron and copper have very high thermal conductivities and, thus, there are only very small temperature differentials in them. The gap between insert and overpack, however, causes a steep change in the temperature that depends on the thermal emissivity of the respective surfaces on both sides of the gap. In addition, the gas content of the gap has an effect on the thermal conductivity over the gap. Argon or air is much better than vacuum in the gap (Ikonen 2006, p. 22, 29) because they enhance the thermal conductivity. Argon will probably be used as gas-shield around canisters when the FSW method is applied. When using FSW, the possibility of having a vacuum between the insert and the overpack is avoided.

Heat transfer through the copper canister will occur in all time frames, but the rate will be greatest immediately after emplacement when the maximum radiogenic heat output occurs [3.2.2], and there is the greatest thermal gradient across the canister and the near field.

The strategy for emplacing waste and the thermal dimensioning of the repository are both designed to ensure that the temperature on the outside surface of the canister never exceeds 100 °C in the repository. In the thermal analysis for a KBS-3H repository (Ikonen & Raiko 2015), the allowable calculated maximum canister temperature was set to 95 °C allowing a safety margin of 5 °C for uncertainties in thermal analysis parameters (e.g. local scattering in rock conductivity). The highest allowable temperature of 95.0 °C is encountered after about 15 years, assuming a (BWR) canister spacing of 9.0 m and drift spacing of 25 m. The results for canisters in the horizontal direction were very similar to the results for canisters in the vertical direction. The analyses showed that the temperature of the canister-buffer-interface is slightly lower than in KBS-3V configuration of canisters. The small differences are based on the differences in buffer configuration between KBS-3H and KBS-3V variants. There are three details that improve the cooling process in KBS-3H, namely:

1. the air gap between canister and buffer is smaller in KBS-3H,
2. the canister always lies horizontally on the buffer, with a tight contact with buffer under the canister, and
3. the outer gap between the supercontainer and drift wall (rock) is open and allows radiation heat transfer in addition to conduction in air (the pellet filling in KBS-3V prevents the radiation heat transfer mode).
Two disadvantages in the heat transfer chain in the KBS-3H configuration are that:
1. there is an axial gap between top-lid-end of the canister and the bentonite buffer, and,
2. the horizontal orientation of the canisters increases slightly the temperature of the canisters, because, the canister ends are closer to each other causing more effective local interaction between adjacent canisters in the KBS-3H configuration.

However, the disadvantageous effect of these two is compensated by the three advantageous differences listed above. All factors considered, the KBS-3H configuration results in maximum temperatures that are 2.9 to 3.7 °C lower, depending on the canister type, as compared with KBS-3V using equal canister centre-to-centre distances (Ikonen & Raiko 2015).

Overall, heat transfer through the canister is influenced by the following features of the repository system.
- Radionuclide inventory: defines the radiogenic heat output and the heat generated by attenuation.
- Temperature: the temperature gradient controls the rate of heat transfer.
- Canister geometry: controls the heat flow across the canister, especially the material thicknesses and void spaces.
- Material composition: controls the rate of heat transfer by conduction across the canister metals.
- Gas composition (and thermal conductivity): controls the rate of heat transfer by conduction over the gaps or voids.
- Material composition: thermal emissivity: controls the transport of radiation from the spent nuclear fuel to the insert metal and over the gas-filled gaps inside the canister.

Uncertainties in the understanding of the FEP:
The thermal conductivities of the cast iron insert and copper overpack materials are well known. However, the emissivity of copper surfaces and the width of the copper-iron gap and its evolution are less well known. Overall, the uncertainties associated with heat transfer within the canister are small.

Couplings to other FEPs:
Heat transfer through the canister is directly affected by the following FEPs:
- Heat transfer (in the spent nuclear fuel) [3.2.3]
- Radiation attenuation [4.2.1]
- Heat transfer (in the buffer) [5.2.1]

Heat transfer through the canister directly affects the following FEPs:
- Deformation [4.2.3]
- Thermal expansion of the canister [4.2.4]
- Corrosion of the copper overpack [4.2.5]
- Corrosion of the cast iron insert [4.2.6]
- Stress corrosion cracking [4.2.7]
- Aqueous solubility and speciation [4.3.1]
- Precipitation and co-precipitation [4.3.2]
- Sorption [4.3.3]
- Diffusion [4.3.4]
- Advection [4.3.5]
- Colloid transport [4.3.6]
- Gas transport [4.3.7]
- Heat transfer (in the buffer) [5.2.1]

References:

4.2.3 Deformation

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

Alternative names:
Deformation of cast iron insert; Deformation of copper canister from external pressure; Deformation from internal corrosion products; Deformation of the canister

Section in 2007-09:
3.6.1

General description:
Large loads and pressures will be imposed on the canister due to both internal and external sources. The nature of these loads and their potential for causing deformation is, to some extent, dependent on whether the canister is intact or has been breached.

The overpack is made of hot-deformed copper that is a soft, very ductile and highly corrosion-resistant material. Consequently, the overpack will deform when subjected to increased loads. The ability of the canister as a whole to resist deformation is, therefore, largely provided by the strength and stiffness of the massive cast iron insert.

The deformation of canister cast iron insert and copper canister by external loads depends on the relative orientation of the canister in the stress field. For this reason, some differences are expected between the behaviour in KBS-3V and KBS-3H (Gribi et al. 2007, Section 3.6).

Internal loads whilst the canister is intact
Whilst the canister remains intact, any internal pressures that are imposed on it may be due to either the development of a gas pressure or from thermal loading. Gases can be produced inside an intact canister by a number of processes. Any free water present (e.g. trapped within fuel rods) can produce hydrogen gas by either direct corrosion of the iron insert or by radiolysis [3.2.5]. The amount of residual water in the canister is so small, however, that it cannot lead to any significant increase in the internal pressure and will not result in deformation of the canister. Helium gas will also be produced inside the
canister as a direct consequence of radioactive decay within the spent nuclear fuel [3.2.10] but, again, this will not result in any significant gas pressure or deformation of the canister. Heat transfer and the resulting thermal gradients across the canister [4.2.2] may cause larger internal loads due to thermal deformation and expansion [4.2.4]. After emplacement, the temperature on the outside of the copper overpack will rise rapidly to a maximum of around 100 °C and it will then cool to around 10 °C within a few thousand years. The thermal expansion coefficient of iron is sufficiently low that it will not cause excessive deformation during expansion and shrinkage.

When the overpack is forced to deform plastically onto the surface of the insert (see below), due to the hydrostatic and swelling pressure, the copper overpack will remain in a compressive stress state until the temperature decreases. This will affect the heat transfer properties of the canister. Cooling will then eliminate the compressive stress or convert it to a small tensile stress in the worst assumed combination of conditions (Raiko 2013, Section 8.4.3).

**Internal loads after the canister is breached**

Except for the possibility of an initial penetrating defect, canister failure is not expected to occur for many tens of thousands of years, and after near-field temperatures have cooled to ambient levels. At this time, the thermal output from the spent nuclear fuel will be very low and, consequently, thermal loading is not expected to result in any increased rates of deformation after canister failure.

After the canister has failed, however, groundwater will penetrate into the void spaces and begin to corrode the iron insert under anaerobic conditions causing hydrogen gas generation and the formation of solid corrosion products [4.2.6]. The gas pressure will be equalised across the canister due to the penetrations and, consequently, will not result in any net increase in the load.

The solid products of anaerobic iron corrosion are iron oxides and iron oxy-hydroxides, both of which are associated with a volume increase. Their formation may, therefore, cause an increase in pressure within the canister, especially if they form within the annular gap between the iron insert and the copper overpack. The larger volume occupied by the corrosion products may cause, with time, an increase of the internal mechanical pressure against the copper overpack, which may eventually lead to local deformation of the canister (SKB 2010, Section 3.4.5). In time, the corrosion rate slows down when a protective layer of corrosion products is formed.

**External loads**

Continuous, time-dependent external loads will be imposed on the canister due to the hydrostatic pressure and swelling of the bentonite buffer.

The hydrostatic pressure from groundwater is a symmetric and evenly distributed external load. Its magnitude depends on the height of the groundwater column and, under normal conditions in Finland, this approximates to the depth of the repository below ground. During glaciation, however, the hydrostatic pressure will be increased in proportion to the thickness of the ice sheet present at the site [see 10.2.2 in Posiva 2012d].

The bentonite swelling pressure is caused by expansion of the bentonite mineral grains as they absorb first water from artificial watering (see below) and then groundwater [5.2.2]. During water uptake and saturation, the rate of swelling may be uneven, which will impose differential pressures on a canister, but, as complete swelling is achieved,
the swelling pressure is expected to become symmetric and evenly distributed on the copper canister. Any differences in initial bentonite density may, however, cause some variation in the final swelling pressure and the potential differential loads were examined in canister mechanical design (Raiko 2013).

The combined loading due to the hydrostatic and bentonite swelling pressures will be imposed on the copper overpack, which will deform plastically or by creep, causing the annular gap between it and the cast iron insert to close. These external pressures will, therefore, be transmitted to the cast iron insert. Plastic collapse of the cast iron insert due to the gradual increase in hydrostatic and bentonite swelling pressures has been tested and modelled under postulated repository conditions, and the results show that the cast iron insert can withstand these external pressures (including glacial loading) by a large margin and retain its structural integrity. This is summarised in the Canister Design Report (Raiko 2013) and the Design Analysis Report for the Canister (Raiko et al. 2010, Section 8.3).

The creep of copper and especially the copper weld has been examined for canister reliability and lifetime (Aalto 1998, Holmström et al. 2013, Purhonen 2014; the last report handles specifically friction stir welding). The copper overpack undergoes creep due to external loading at elevated temperature until the copper overpack comes into contact with the cast iron insert that is essentially the load bearing member of the canister structure. The gap between the copper overpack and the insert is designed to avoid excessive copper creep during the external loading by the buffer. The maximum creep strain will affect the inner corners near the lid or the bottom. It will however reach only some per cent, at maximum (Holmström et al. 2013). In the cylindrical wall of the canister the creep strains remain low. Thus, the copper and even the copper weld are ductile enough to bear this kind of deformation. Savolainen et al. (2012) studied the plastic deformation of the base materials compared to that of FSW and EBW welds. They found that, while the base material deforms uniformly, the deformation in the weld material is localised. Differences in plastic deformation have been observed between the FSW and EBW processes (Savolainen et al. 2012). The FSW method is assumed in this safety case, as it is Posiva’s current reference welding method. Since FSW has better creep ductility than EBW, a change to FSW is favourable to long-term safety from the point of view of swelling loads (even and uneven) from the bentonite and the hydrostatic pressure from groundwater (the benefits of FSW are discussed in more detail in Posiva’s response to STUK’s request 12/H42252/2014).

The conclusions for the KBS-3V case are also likely to apply to KBS-3H, although there may be some differences due to the development of saturated conditions (Gribi et al. 2007, Section 3.6.1). The KBS-3H design now adopts the DAWE (Drainage, Artificial Watering and air Evacuation) system and the change of supercontainer shell material from steel to titanium with a lower gas production rate helps to accelerate buffer saturation, and the KBS-3H alternative is probably not more sensitive to uneven buffer swelling and related canister deformation than the KBS-3V alternative. Processes with a different significance to, or potential impact on, KBS-3H compared with KBS-3V that could give rise to increases in buffer density over time are discussed in Sections 3.6.1 and 4.6.1 of Gribi et al. (2007).

Creep movements due to the glacial loading are omitted in KBS-3V because the additional stresses are not sufficiently high (e.g. Rasilainen 2004). This conclusion is also valid for KBS-3H (Gribi et al. 2007, Section 3.6.1).
In addition to continuous hydrostatic and bentonite swelling pressures, the canister may be subjected to instantaneous external shear loads due to rock movements initiated by either isostatic (glacial) or tectonic processes [see 10.2.2 in Posiva 2012d]. If the shear plane intersects the KBS-3H deposition drift in the most unfavourable location (i.e. mid-height of a canister and perpendicular to its axis) it may cause high plastic strains in the rounding radii of the lid or bottom and in the singularities in the lid weld root, potentially leading to canister failure. It has been estimated that the canister would survive a rock shear displacement of 5 cm with a 1 m/s velocity but would fail if the displacement was 10 cm (Raiko et al. 2010, Hernelind 2010). Such rock movements are considered unlikely at Olkiluoto except, possibly, during deglaciation periods and the likelihood will be minimised by locating the canister positions away from pre-existing fractures in the rock (La Pointe & Hermanson 2002; McEwen et al. 2012). The risk of rock shear damaging the canisters is slightly different for KBS-3H and KBS-3V because of the different orientation of the canisters with respect to the main fractures sets at Olkiluoto [10.2.3]; see also Pekkarinen (2014). The rheological properties of the buffer play an important role in determining the consequences of a rock shear movement on the canister. Regarding the welding method, a change to FSW is favourable to long-term safety from the point of view of rock shear displacements, since FSW has better creep ductility than EBW.

For the fracture conditions at Olkiluoto it is unlikely to be possible to locate all KBS-3H deposition drifts free of fractures having the possibility of damaging shear displacements (Pekkarinen 2014). This is not a problem as long as these fractures do not intersect any canister positions.

Creep of the cast iron insert has been disregarded in the canister strength analyses based on the results of Martinsson et al. (2010). However, brittle fracture of the cast iron insert under rock shear conditions has been assessed. Brittle fracture is possible only for brittle materials, and the tendency for it to occur depends on material quality and the temperature. Testing of the cast iron material at 0 °C showed, however, that it displays ductile, not brittle, behaviour (Raiko et al. 2010). A series of high loading-rate tests were also conducted and the results showed that the static fracture resistance curves are representative even for dynamic loads, and higher loading rates do not lower the fracture resistance of the insert material at low temperatures (Raiko et al. 2010). Brittle fracture of the insert is, therefore, not considered to be an issue.

Overall, deformation of the canister is influenced by the following features of the repository system.

− Radionuclide inventory: controls the radiogenic heat output and the generation of helium gas pressure inside the intact canister.
− Temperature: many material properties are temperature dependent.
− Pressure: the internal and external pressures are the primary control on deformation, particularly the external hydrostatic and bentonite swelling pressures.
− Canister geometry: in particular, the dimensions and shape of the canister have a significant control on its overall strength, stiffness, stress concentrations and stability against buckling.
− Mechanical stress: is the dominant control on the deformation of the canister.
− Material composition: is a direct control on the mechanical properties of the cast iron insert and copper overpack (strength, ductility, thermal expansion).
Uncertainties in the understanding of the FEP:
The mechanical behaviour of cast iron and copper is well known from industrial analogues. The dimensions and fitting of the overpack and the insert are defined so that the gap is large enough for installation and for moderate thermal deformation yet small enough that there is no possibility for excessive plastic deformation or creep of the copper overpack.

The main uncertainties concern the long-term evolution of the geosphere and the possibility of a rock shear in the vicinity of a canister. In particular, the rock-shear magnitude and velocity are uncertain as well as the evolution of the rheological properties of the buffer bentonite and the canister metals at low temperature (if it is assumed that a rock shear movement could happen in conjunction with a glaciation). The application of Rock Suitability Classification (RSC) (McEwen et al. 2012; Posiva 2016c, App. C) will diminish this uncertainty.

Couplings to other FEPs:
Deformation of the copper canister is directly affected by the following FEPs:
- Heat transfer [4.2.2]
- Thermal expansion of the canister [4.2.4]
- Corrosion of the copper overpack [4.2.5]
- Water uptake and swelling (in the buffer) [5.2.2]
- Reactivation-displacement along existing fractures [10.2.3]
- Glaciation [see 10.2.2 in Posiva 2012d]

Deformation of the copper canister directly affects the following FEPs:
- Stress corrosion cracking [4.2.7]

References:


Sweden: Swedish Nuclear Fuel and Waste Management Co. (SKB). Report R-10-64. 31 p. ISSN 1402-3091.


### 4.2.4 Thermal expansion of the canister

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th><strong>Class:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Alternative names:</strong></th>
<th><strong>Section in 2007-09:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal expansion (both cast iron insert and copper canister); Deformation of the canister</td>
<td>3.6</td>
</tr>
</tbody>
</table>

**General description:**

The temperature of the canister metal and the thermal gradients across it are controlled by the rate of internal (radiogenic) heat generation [3.2.2], and the rates of heat transfer through the canister [4.2.2], the bentonite buffer [5.2.1] and the near-field rock [10.2.1]. This description is applicable to both a KBS-3V and a **KBS-3H** type repository. The canisters will reach their maximum temperature in the repository within 10 to 15 years after disposal. The maximum temperature on the outside surface of the canister will not exceed 100 °C by design, but the internal temperature at the surface of the fuel may be
close to 200 °C (Ikonen 2006). It has been shown that the temperature drop between the insert and the overpack at the beginning of the service life of the canister is 65 °C at the most (Raiko 2013).

The cast iron insert and the copper overpack will react to this initial heating and the resulting thermal gradient across the canister by thermal expansion. Copper has a higher thermal expansion coefficient than iron, and consequently the copper overpack will expand more than the iron insert (Figure 4-2 and Figure 4-3). In the absence of external pressure, this differential thermal expansion would cause the annular gap between the insert and the overpack to widen from its nominal size of 1.5 mm. Figures 4-3 and 4-4 show that the gaps in the axial and radial directions are wide enough to allow thermal deformation of the canister materials even when there is a temperature difference between the insert and copper overpack (up to 65 °C) and there is no contact between the copper overpack and the insert.

**Figure 4-2.** The thermal expansion of canister components in the axial direction. The red arrow shows the allowable temperature difference (~65 °C) before there is contact between the insert and the copper overpack. The green line shows the evolution of the gap in a constant temperature regime. From Raiko (2013, Figure 26).
Contact would lead to tensile stress in the overpack and that would increase the risk of stress corrosion. Later, under saturated repository conditions, however, the external hydrostatic and bentonite swelling pressures will cause plastic or creep deformation of the copper and the annular gap will close once swelling pressure builds up in the buffer. After this deformation, the general residual stress state in the copper overpack will be compressional. Furthermore, the closure of the gaps will lead to a significant decrease in the thermal gradient between the insert and overpack.

The thermal conductivity of the metal body of the canister is two orders of magnitude higher than the conductivity of the surrounding bentonite buffer and the near-field rock. Due to this difference, the thermal gradient will dissipate and a uniform temperature will exist across the canister metal once a state of thermal equilibrium has been reached in the near field.

Over a period of around 50,000 years, as the radiogenic heat generation reduces, the canister will cool to the initial ambient temperature of around 10 °C [4.2.2]. The canister metals will contract due to cooling and some tensile strain will be generated in the copper overpack because it contracts faster than the cast iron insert due to the difference in the thermal expansion coefficients of the two metals. The assessment of the thermal loading shows that there is no risk of failure of the canister metals due to thermal expansion (Raiko 2013, Sections 8.4.2 and 8.4.3).
Overall, thermal expansion of the canister is influenced by the following features of the repository system.

- Radionuclide inventory: defines the radiogenic heat output and the heat generated by attenuation, though indirectly via temperature.
- Temperature: particularly the rate of change of temperature and the thermal gradient across the canister, because this affects the amount of expansion and any differential expansion that may occur.
- Pressure: the external hydrostatic and bentonite swelling pressures will resist thermal expansion, and affect creep of the copper overpack.
- Canister geometry: particularly the dimensions and shape of the canister control the amount of expansion and differential expansion.
- Mechanical stress: the tensile and compressive stresses in the canister metals will affect the deformation response to internal and external pressures.
- Material composition: the composition of the copper and iron metals in the canister will affect their coefficients of thermal expansion.

Uncertainties in the understanding of the FEP:
The maximum temperature inside the canister and the thermal expansion of the canister metals are well known and can be readily calculated.

Couplings to other FEPs:
Thermal expansion of the copper canister is directly affected by the following FEPs:
- Radiation attenuation [4.2.1]
- Heat transfer [4.2.2]
Thermal expansion of the copper canister directly affects the following FEPs:
- Deformation [4.2.3]
- Stress corrosion cracking [4.2.7]

References:

4.2.5 Corrosion of the copper overpack

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

Alternative names: Corrosion of copper canister; Corrosion

Section in 2007-09: 3.7

General description:
The copper overpack is made of an alloy referred to as oxygen-free copper (Cu-OF) with added phosphorus. Corrosion of the copper overpack can take place by either general (uniform) corrosion mechanisms or by localised corrosion mechanisms. Both are potentially important for the performance of the canister, and for the migration of...
radionuclides out of the canister by diffusion [4.3.4], advection [4.3.5], colloid-mediated transport [4.3.6] or gas-mediated transport [4.3.7]. Stress corrosion cracking is addressed separately [4.2.7]. Corrosion of the copper overpack does not depend on the specific conditions in KBS-3H (Gribi et al. 2007, Section 3.6.1).

General corrosion

The copper overpack is made of high purity, oxygen-free, high conductivity copper (Cu-OF). In pure water, this metal is thermodynamically stable but, in natural groundwaters, it will corrode by reactions and at rates controlled largely by the composition of the water, particularly the redox conditions and the nature of dissolved species. Much is known about the mechanism of general corrosion of the copper overpack in repository conditions. The most important parameters controlling the rate of general corrosion are: the rates of mass transport of species to and from the canister surface, the availability of O₂, the influx of Cl⁻ ions from the groundwater, and the supply of sulphide ions to the canister.

Immediately after the canister has been emplaced, near-field conditions will be oxidising due to the presence of trapped air in the bentonite buffer. Some of this oxygen will be used by Cu in the general corrosion of the external surface of the copper overpack and the formation of oxide phases. The rate of general corrosion under these conditions will be limited by the availability of O₂ or of Cu(II) formed by the homogeneous oxidation of Cu(I) by O₂. Any carbonate, sulphate and hydroxide present may also be incorporated into the oxide phases. These phases will coat the copper surface, forming a passivating layer, which will inhibit further corrosion. However, the presence of any naturally occurring chloride in the groundwater will tend to maintain the canister in an ‘active’ corrosion state rather than in a ‘passive’ one. However, Saario et al. (2004) concluded that the corrosion of copper stopped in compacted bentonite when the O₂ was locally exhausted at the surface and anoxic conditions had been established. There is no evidence that copper corrodes in oxygen-free concentrated Cl⁻ solutions at neutral pH, consistent with thermodynamic predictions (SKB 2010, Section 3.5.4) and observations in geological occurrences of metallic copper (e.g. Marcos 2002).

After a period of time, the near field will become anaerobic due to the consumption of residual oxygen by the iron minerals present in the rock, buffer materials and KBS-3H filling components. Once anaerobic conditions have been established, the only available species that will be corrosive to copper is sulphide.

Copper corrosion by sulphides

From a thermodynamic point of view, there is a wide range of possible S species in aqueous solution at near-neutral pH: sulphide can be in the form of bisulphide HS⁻, polysulphides Sₓ⁻², polythionates SₓOᵧ²⁻ or elemental sulphur. Macdonald & Sharifi-Asl (2011) carried out extensive thermodynamic analyses of those S species that could corrode copper using corrosion-domain diagrams and volt-equivalent diagrams. They found that sulphide, polysulphides and certain polythionates may “activate” copper. The interfacial dissolution reaction in the process can be expressed by:

\[
\text{Cu} + \text{HS}^- \rightarrow \text{Cu}_2\text{S} + \text{H}_2\text{S} + e^- \\
\text{Cu} + \text{HS}^- \rightarrow \text{Cu}_2\text{S} + \text{H}_2\text{S} + e^- \\
\text{Cu(HS)}_{\text{adsorbed}} + 2\text{Cl}^- \rightarrow \text{CuCl}_2 + \text{HS}^- 
\]

At high sulphide concentration (> 15 mg/L) a protective film forms with second-order kinetics. The film grows at the film/solution interface. The film contains Cu⁺ ions that
diffuse in the HS\textsuperscript{-} solution. At lower sulphide concentrations (< 2 mg/L) a non-protective film forms following first-order kinetics. The rate-limiting step is the transport of HS\textsuperscript{-} in aqueous solution (Chen et al. 2011a, 2011b, Smith et al. 2011). Sulphide is present naturally in the groundwater at repository depth at Olkiluoto generally in concentrations of less than 1 mg/L; the highest reliably measured sulphide content is about 31 mg/L at a (vertical) depth of 531.5 m in borehole OL-KR46 (Posiva 2016c) and it is also present as a minor impurity (e.g. pyrite) in some commercially available bentonites. The basic reactions involved in the corrosion of copper in the presence of sulphide have been incorporated into a mixed-potential model to predict the evolution of the corrosion behaviour of the canister as the environment evolves from the initial aerobic phase to the long-term sulphide-dominated period (King et al. 2011).

General corrosion can also be induced by sulphate-reducing bacteria (SRB) which can, under favourable conditions, reduce sulphate in groundwater [10.2.8]. Microbial activity has been demonstrated to decrease exponentially with increasing buffer densities and approaches nil at densities above 2000 kg/m\textsuperscript{3} (Pedersen & Hallbäck 2013), which is the expected density of the buffer after complete swelling [5.2.8]. Corrosion of the canister by SRB could be possible due to microbial activity at the bentonite-rock interface or other interfaces in the KBS-3H deposition drift, and the subsequent diffusion of the produced sulphide to the canister. The concentration of sulphide will depend on the SRB growth conditions and the presence of Fe(II), which will control the solubility of sulphide. The impact of microbially produced sulphide on the canister lifetime is expected to be limited because of the slow migration of sulphide through the bulk of the bentonite buffer and the likelihood of precipitation as iron sulphide [5.2.8].

The MiniCan in situ test on copper corrosion at the Åspö Hard Rock Laboratory has been carried out to investigate a range of corrosion issues associated with the canister, including the possibility of expansion of the outer copper canister as a result of the anaerobic corrosion of the cast iron insert. The project started in 2006 and the results are available up to the end of 2011 (Smart & Rance 2008, Smart et al. 2011, 2012). Part of the copper samples have been embedded in a bentonite test parcel in oxic bentonite/saline groundwater conditions and corrosion rates have been measured (Rosborg & Pan 2008, Rosborg et al. 2011). Gravimetric data on these samples showed an average corrosion rate of 0.5 μm/a. Electrochemical impedance spectroscopy studies on a three-year old sample of pure copper showed a corrosion rate range of 0.4–0.7 μm/a (Rosborg et al. 2011). This is somewhat lower than the value of 1.0 μm/a obtained from the electric resistivity measurements (Rosborg & Pan 2008).

Copper corrosion may, in principle, also be affected by γ-radiolysis of the moist air/vapour and porewater close to the canister surface. The maximum surface dose rate for the copper canister is limited by design to 1 Gy/h. At this low dose rate, the effect of the products of radiolysis is expected to be small to negligible (Shoesmith & King 1999). Furthermore, the canister surface is expected to be dry during the period of highest dose rates, further limiting the production of radiolysis products. The available data (King et al. 2012 and references therein) show no evidence for enhanced corrosion rates except, possibly, at very high dose rates (> 100 Gy/h). Given that the γ-dose essentially ceases after 1000 years (due mostly to Cs-137 decay with a half-life of about 30 years) the experimental results suggest that the influence of radiation on general corrosion of the copper overpack will be negligible. More recent laboratory studies do, however, show that irradiated copper samples can be more corroded than corresponding reference samples (Björkbacka et al. 2012). In these studies, corrosion
was associated with an increased concentration of copper in water after irradiation, and surface examination revealed local corrosion features in the irradiated samples. Assessments of the general corrosion rate of the copper overpack have taken account of the various sources of sulphide and the possibility for microbi ally induced corrosion. Depending on the model used and on the assumptions, the calculated general corrosion depths range from a few to tens of micrometres over one million years (King et al. 2012, Table 8-1).

In any case, the general corrosion rate is expected to be very low because it is limited by the diffusive supply of sulphide ions through the bentonite barrier to the canister surface. A higher rate of corrosion would, however, be expected in the case of a defective buffer around a canister if advective conditions were to be established [5.2.3, 5.2.4]. Numerous natural analogue studies support the view that geochemical conditions in the repository may limit copper corrosion (Miller et al. 2000, Milodowski et al. 2002). Elemental copper has persisted for millions of years in several geological environments, including those found in Finland. Copper corrosion by oxidation and sulphidation occurs at very low rates even in natural copper ores (Marcos & Ahonen 1999).

Localised corrosion
Uneven water uptake and swelling of the bentonite buffer around the canister [5.2.2] could lead to localised electrochemical corrosion of the copper overpack at the areas where the wetted bentonite contacts the copper surface. Those areas are possible locations for the spatial separation of anodic and cathodic processes. Once the bentonite has completed swelling, however, there will be uniform contact between the bentonite and the copper overpack. The fact that some sites have been exposed to conditions that enable electrochemical corrosion longer than others may cause slightly uneven corrosion over the copper surface. Apart from that, the gradual closing of the gap between the bentonite buffer and the canister is not likely to result in any significant localised effects. Mechanistic copper pitting studies indicate that an oxidant, either O₂ or Cu(II), is a prerequisite for pit propagation during localised corrosion. As the repository near-field environment will evolve from initially oxidising to ultimately reducing conditions, this implies that pitting will only be possible (if at all) in the early stages of repository evolution and, consequently, general corrosion is expected to be the dominant corrosion mechanism that affects the copper overpack.

A major limiting factor for pitting would be the amount of O₂ contained in the buffer material. As water uptake continues, eventually the entire canister surface will be wetted and the differential O₂ concentration that acted initially as the driving force for localised corrosion will disappear. Corrosion experiments under simulated repository conditions suggest that canisters will not undergo classical pitting but rather a form of homogeneous surface roughening, in which there is no permanent separation of anodic and cathodic sites (King et al. 2012, Section 5.3). The localised corrosion depth of copper during the post-closure thermal phase is expected to be between a few tens and a few hundreds of micrometres (King et al. 2012, Table 8-1).

As the bentonite buffer progressively takes up water, the chloride concentration in the porewater composition will gradually increase. The presence of chloride tends to support general corrosion, not localised corrosion. It is also reasonable to assume that copper chlorides or hydroxy chlorides may form as an initial corrosion product in saline groundwaters during the water saturation phase in compacted pure bentonite. High salinity causes
localised corrosion only at low pH (pH < 4). In the early evolution of the near field, the pH is expected to be slightly alkaline due to the buffering effect of the bentonite.

The effect of alkaline leachates from degradation of cementitious materials in the near field [9.2.8] on localised corrosion of the copper overpack has been investigated (King et al. 2012, Section 5.3.2). If the pH increases prior to the establishment of reducing conditions, the canister surface will become passivated by the formation of a duplex Cu$_2$O/Cu(OH)$_2$ film when conditions exceed pH 9. The corrosion potential will be determined by the equilibrium potential for the Cu$_2$O/Cu(OH)$_2$ couple under oxidising conditions or by the Cu/Cu$_2$O redox couple under reducing conditions (in the absence of sulphide). Localised corrosion is only likely to occur for a short time during the evolution of the repository environment when the canister is still relatively cool (< 40 °C) and there is sufficient O$_2$ available to support localised corrosion and prior to the increase in porewater pH and salinity. The subsequent increase in canister surface temperature, porewater pH and salinity, and decrease in O$_2$ concentration will make pit initiation less likely, although the canister will remain passivated provided the porewater pH is maintained above pH 9. The higher the pH, the more strongly the canister is passivated and the less likely the surface is to undergo localised attack. It should be noted that the amount of alkaline leachates in the near field of a KBS-3H repository will be smaller than in KBS-3V, because no cement-based grout will be used in the deposition drifts (as no rock bolts are planned to be used in them). In addition, the plugs in the drift will be composed mainly of titanium, not concrete.

If the salinity increases prior to the increase in pH, the corrosion potential will be a true mixed potential, determined by the relative kinetics of Cu dissolution as CuCl$_2$ and of the reduction of O$_2$. A mixed-potential model for predicting the long-term corrosion behaviour of the copper in compacted sulphide-containing bentonite has been developed (King 2008, King et al. 2011). During the initial post-emplacement period, the heat from the canister can cause the surrounding bentonite to dry out and solid phases to precipitate from the porewater as a consequence of evaporation. At this time, the canister surface will be progressively covered by a duplex corrosion product layer comprising an inner layer of Cu$_2$O and an outer layer of basic Cu(II) salts (most likely either malachite (Cu$_2$CO$_3$(OH)$_2$) or atacamite (CuCl$_2$•3Cu(OH)$_2$)) depending upon the relative concentrations of CO$_3^{2-}$ and Cl$^-$ in the porewater (King et al. 2012, Section 5.1). Salt deposition has been investigated in the Long Term Test of Buffer Material (known as the LOT experiment) at Åspö, where copper heaters are buried in bentonite (Karnland et al. 2009). Two of these packages have been retrieved and analysed (Wersin 2013). These two heaters had surface temperatures of 90 °C and 130 °C. Examination of the copper surfaces showed coverage by a thin layer of calcium sulphate/calcium carbonate but no chloride enrichment even if the groundwater had high chloride content (over 8000 mg/L). It is not clear whether the precipitates were caused by evaporation or by the lower solubility of the calcium salts at elevated temperatures. The second LOT recovery after 6 years exposure at 130 °C showed the same surface coverage of anhydrite and calcite. The longer exposure did not, however, seem to cause more precipitation (Karnland et al. 2009). Salt accumulations on steel heaters and in the surrounding clay were also discovered in hydrothermal experimental field tests in Stripsa (Pusch et al. 1992). The long-term safety relevance of salt precipitation on the copper surface has been ranked low in the updated state-of-the-art copper corrosion report (King et al. 2012).
Additional postulated uniform corrosion mechanism

The possibility of copper corrosion in pure water has been suggested due to observations in laboratory studies of a transition from O$_2$-consuming to H$_2$-evolving corrosion of oxygen-free, high conductivity copper (Cu-OF) in deionised water (Szakálos et al. 2007). These researchers suggest that a previously unknown copper hydroxy compound is formed when copper corrodes in pure water in the absence of O$_2$. The authors propose the following mechanism:

$$\text{Cu} + y\text{H}_2\text{O} \rightarrow \text{H}_x\text{CuO}_y + (2y - x)\text{H}_{\text{ads}}$$

As a consequence, it is suggested that copper corrodes with the evolution of H$_2$, with an equilibrium H$_2$ partial pressure of approximately 0.001 atm at 70–80 °C. The authors propose an anaerobic corrosion rate up to 5 micrometres/year, which increases with time. For the time being it has not been possible to reproduce the results. King (2010) carried out a critical review of the literature and concluded that the scientific evidence for this mechanism is still weak and that, even if it were to happen, it would be a self-limiting process, because the repository can be considered an almost completely closed system in which hydrogen is able to build up and suppress corrosion (King 2010, Section 3.6). The corrosion rate would then be determined by the rate of diffusion of H$_2$ away from the container. MacDonald & Sharifi-Asl (2011) demonstrated that copper is only thermodynamically stable in pure anoxic water with very low concentrations of [Cu$^+$] and very low partial pressures of hydrogen gas (10$^{-14}$ atm). The H$_2$ partial pressure in the normal atmosphere is higher than this value and corrosion of steel components in the repository will result in a H$_2$ partial pressure in the repository much higher than that below which copper would be unstable in water. Becker & Hermansson (2011) carried out experimental studies of copper corrosion in pure anoxic water in order to reproduce Szakálos’ results. Hydrogen formation was observed in their conditions although the origin is yet unclear. The total amount of hydrogen detected after the test is lower than what would be possible with respect to the copper amounts found in the test solutions after the experiments. The same observation was made in previous experiments mentioned above. In addition, in this work, the test solutions were shown to contain unexpected amounts of metals, which might be related to the observation of hydrogen. Becker & Hermansson (2011) emphasise that even if copper will corrode in pure anoxic water, no conclusions about how copper canisters at repository depth will behave with regard to corrosion can be drawn. The rate of corrosion will be affected by the thermodynamic driving force associated with hydrogen gas formation but this has not yet been addressed (Becker & Hermansson 2011). Johansson & Brink (2012) performed a literature review on the mechanism and energy of surface reactions at the copper-water interface, which sheds additional light on surface reactions and the proposed mechanism of copper corrosion in anoxic water. They concluded that the H$_2$ detected by Hultquist et al. (2009; see also Hultquist et al. 2013) is likely to originate from surface oxidation and passivation reactions in which the H$_2$O molecule is cleaved and H$_2$ forms until the surface is passivated.

Using a similar setup as Hultquist et al. (2008), Becker & Hermansson (2011) demonstrated the production of hydrogen in oxygen-free water containing metallic copper, but the experiment was stopped before a steady-state pressure was reached. An analogous experiment has been done in Finland (Ollila 2013). Sealed flasks allowing hydrogen to escape through a Pd membrane and with copper foils in oxygen-free water stored in a glove box with N$_2$ or Ar atmosphere did not show any visible copper
corrosion while the equivalent sealed flasks stored in air showed clear signs of corrosion indicating oxygen penetration through the seal (Ollila 2013). The production of hydrogen was confirmed but the amounts of hydrogen were not measured.

Recently a series of H₂ pressure measurements in oxygen-free water containing copper (canister material grade) samples have also started in several sets of test tubes under a variety of conditions (Bengtsson et al. 2013). Preliminary results show hydrogen production but no clear steady-state pressure for the hydrogen-generating process, though higher pressures are reached than those measured by Hultquist et al. Furthermore, hydrogen production rates seem to be sensitive to the experimental conditions such as sample grinding techniques, sampling methods, test tube characteristics etc.

Electrochemical studies of copper in water provide an insight into the kinetics of the H₂ production process (Bojinov et al. 2010, Betova et al. 2013). These studies show initially electrochemically more active properties of the copper surface layer, which, however, stabilised after 2000 to 2500 hours. Preliminary results from the measurements with an amperometric hydrogen microsensor indicate concentrations of H₂ corresponding to higher pressures at room temperature compared with the Hultquist et al. (2011) steady state pressure at higher temperature (Bengtsson et al. 2013). Quantum mechanical calculations by Korzhavyi et al. (2012) and experimental observations by Soroka et al. (2013) have potentially identified an unstable compound, resembling CuOH, but further experimental and theoretical work is ongoing.

Theoretical studies of reactions at the copper surface suggest that the observed H₂ is the result of the dissociative adsorption of H₂O on the copper surface and does not involve oxidation of the bulk material (Johansson & Brinck 2012). These studies show that it is possible to produce hydrogen from the cleavage of water molecules in the first one or two monolayers of water on a copper surface, but the amount of hydrogen produced is too small to explain the experimental observations.

Additional mechanistic considerations about the copper corrosion in anaerobic water are provided by King et al. (2012, Section 5.2.2), and King & Lilja (2011). SKB (2010) evaluated the implications for the canister: if the proposed mechanism exists, the corrosion rate will be limited by the rate of H₂ transport away from the canister. Based on this, the corrosion rate would be of the order of 1 nm/a. Therefore, the consequence for the canister lifetime is minimal even over one million years.

Various authors have also attempted to determine whether copper corrodes in sulphide containing anaerobic water (Betova et al. 2003, 2004, Bojinov et al. 2004). Arilalhti et al. (2011, 2012) studied the exposure of pre-cracked copper to high concentrations of sulphides in anoxic conditions. Their results and implications for stress corrosion cracking are discussed in Section 4.2.7. Recent studies have examined copper corrosion electrochemically and proposed a kinetic model to interpret the impedance measurements of copper in a deoxygenated neutral aqueous solution (Bojinov et al. 2010). They showed that no sustainable active corrosion was occurring in the experimental conditions in spite of the observation of Cu(II) in solution.

Experiments are underway to study the process. Based on experiments carried out so far by SKB (e.g. Bengtsson et al. 2013), it would seem that copper is not significantly corroded in oxygen-free conditions, and the minor hydrogen amounts observed in the experiments originate from the copper material itself and no hydrogen has been...
generated by corrosion. Future experiments commissioned by Posiva aim to confirm and demonstrate reproducibility of SKB’s results (Posiva 2015). The change to FSW is relevant to galvanic and grain boundary corrosion as well as to stress corrosion cracking. Other types of corrosion affect equally EBW and FSW welds, as they do not depend on those intrinsic material properties (e.g., residual stress) that differentiate FSW from EBW. Uniform corrosion, mainly due to sulphide, depends on environmental conditions and on the initial copper thickness, not on the welding method per se. The controversial issue related to formation of hydrogen gas from anaerobic water samples containing copper strips (Hultquist et al. 2008) is still under investigation but, regardless of the process involved, it would affect both FSW and EBW in the same way (Posiva’s response to STUK’s request 12/H42252/2014).

**Galvanic corrosion**

Galvanic corrosion occurs when two dissimilar metals are in direct electrical contact (i.e. there is free passage of electrons through the metals) in an electrolyte (e.g. seawater, LaQue 1975). The galvanic series shows that titanium in the passive state (i.e. having a film of TiO$_2$) is more positive in the galvanic series in seawater than copper. So, in any metal couple the copper would be expected to corrode preferentially to titanium, but they would have to be in direct electrical contact (i.e. physically touching with no insulating layer between them) as well as be in the same electrolyte (i.e. saturated clay). The extent of any damage would depend on the relative surface areas of the cathode (i.e. titanium) and the anode (i.e. copper). The extent of the corrosion would also depend on the relative corrosion potentials of the two metals, which will be governed by the oxygen concentration. As the oxygen concentration decreases any effect will decrease. Copper-titanium couples have been investigated by Du et al. (2014) and Kunieda et al. (1980), who examined the effects of such factors as relative areas of the copper and titanium electrodes, oxygen concentration and temperature for galvanic corrosion in seawater.

In the current design, the copper and titanium components will not come into direct electrical contact (i.e. in which electron currents could pass between the two metals) and since this is a prerequisite for galvanic corrosion, the risk of galvanically enhanced corrosion of the copper is vanishingly small under normal operating conditions. However, there are some highly unlikely scenarios under which metal-to-metal contact could arise, as follows:

- if bentonite was to be completely eroded away, a possibility considered in Posiva (2013f) and the supercontainer shell, or pieces of it, could come into contact with the copper canister
- the copper canister sinks within the bentonite under the influence of gravity and comes into contact with the titanium shell.

If these cases the possibility of galvanic corrosion needs to be considered. The actual effect would be localised around the pieces of titanium in contact with the copper and its magnitude would depend on the relative areas of the metals. It is assumed that by the time any galvanic coupling occurred the conditions would be fully anoxic. In order for galvanic corrosion to occur there would need to be electronic conductivity through the corrosion product layers on both metals, namely titanium and copper. The corrosion products present on the copper surface (e.g. copper sulphide) and on titanium (comprising mainly TiO$_2$) are semi-conductors, so it is possible that there will be
sufficient conductivity to enable galvanic corrosion to take place. In this situation, the
titanium would act as the cathode and the copper would be the anode, which could
corrode at an accelerated rate. The anodic activity would be concentrated on the contact
point or line contact between the copper and the titanium shell. The galvanic corrosion
current would be determined by the passive current density on the surface of the
titanium, which would be very low under anoxic conditions. However, the available
surface area would be very large, so there is a theoretical possibility of galvanically-
enhanced corrosion at the point of contact between the two metals. The extent of any
enhancement of corrosion rate would depend on the geometric layout of the touching
pieces of metal and the current ‘throwing power’ in the medium of interest. As the
titanium would be the cathode in the couple the rate of hydrogen uptake in the metal
would be increased compared to the uncoupled material.

_stray current corrosion_
Stray current corrosion is in practice a common problem in systems like e.g. those with
power cables in the rail transportation, or with cathodic protection (CP) systems, where
it might affect underground pipelines in their vicinity (Revie & Uhlig 2008). It occurs
when currents present in the surrounding environment (e.g. soil or seawater) enter a
metallic structure and then leave at a different location on the structure. In some cases,
enhanced corrosion can occur at the entry and exit points, and the damage is more
severe for direct rather than alternating currents (ibid.). It is most likely to affect the
corrosion of long structures such as pipelines, rather than relatively short objects such
as an individual isolated canister. There are no known reported examples of this type
of corrosion affecting titanium structures. The issue was modelled by Taxén et al.
(2014) for stray currents from a high voltage direct current (HVDC) power
transmission system for the KBS-3V design alternative and it was concluded that this
is not a significant problem for the corrosion of the copper canisters. In the KBS-3H
alternative the currents along the deposition drifts and voltage differences between
system components are somewhat different, though in any of those studies the
heterogeneity of the bedrock accounted for and the electrical field assumed will not
keep as uniform as assumed in the assessment.
Overall, corrosion of the copper overpack is influenced by the following features of the
repository system.

- Temperature: controls the rate of corrosion reactions and, in the case of a canister
  with initial defect, general corrosion may begin at high near-field temperatures and
  be accelerated.
- Mechanical stress: the combination of stress and a chemically aggressive
groundwater may promote corrosion.
- Material composition: the corrosion processes (especially the rate) and the nature
  of the corrosion products are dependent on the composition of the copper metal,
  particularly any impurities and oxygen content.
- Water composition: specifically, for general copper corrosion the most important
  parameters in the long term (after the short period with oxygen present) are the
  concentrations of dissolved chloride and sulphide in the groundwater, and the
  supply of these species to the canister surface.
**Uncertainties in the understanding of the FEP:**

There are no uncertainties concerning the general understanding of copper corrosion under aerobic and anaerobic conditions. Uncertainties in the general corrosion rate are relatively small and the rate can be expected to be less than 1 mm in 100,000 years. The main uncertainties relate to the evolution of the near-field geochemical conditions, i.e. the time-dependent variable amounts of sulphide that can reach the copper surface of the canisters. The sulphate reduction process and its kinetics are being experimentally investigated in ONKALO (Posiva 2009, Sections 3.1.2.4 and 6.5.7). The effects of stray currents are expected to be in the same period even significantly smaller.

**Couplings to other FEPs:**

Corrosion of the copper overpack is directly affected by the following FEPs:

- Heat transfer [4.2.2]
- Stress corrosion cracking [4.2.7]
- Water uptake and swelling (in the buffer) [5.2.2]
- Radiolysis of porewater (in the buffer) [5.2.5]
- Alteration of accessory minerals (in the buffer) [5.2.7]
- Microbial activity (in the buffer) [5.2.8]
- Diffusion (in the buffer) [5.3.4]

Corrosion of the copper overpack directly affects the following FEPs:

- Radiolysis of the canister water [3.2.6]
- Corrosion of the cladding tubes and metallic parts of the fuel assembly [3.2.7]
- Alteration and dissolution of the fuel matrix [3.2.8]
- Release of the labile fraction of the inventory [3.2.9]
- Deformation [4.2.3]
- Corrosion of the cast iron insert [4.2.6]
- Diffusion [4.3.4]
- Advection [4.3.5]
- Colloid transport [4.3.6]
- Gas transport [4.3.7]

**References:**


Johansson, A.J. & Brink, T. 2012. Mechanisms and energetics of surface reactions at the copper-water interface. A critical literature review with implications for the debate


Posiva 2016c. Results of monitoring at Olkiluoto in 2013 – Hydrogeochemistry (to be published).


4.2.6 Corrosion of the cast iron insert

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:**
Corrosion of cast iron insert; Galvanic corrosion

**Section in 2007-09:**
3.7

**General description:**
Corrosion of the cast iron insert can take place by either general (uniform) corrosion mechanisms or by localised corrosion mechanisms. Both are potentially important for the performance of the canister, and for the migration of radionuclides out of the canister by diffusion [4.3.4], advection [4.3.5], colloid-mediated transport [4.3.6] or gas-mediated transport [4.3.7]. Corrosion of the cast iron insert does not depend on repository geometry and thus this description applies to both a KBS-3V and a KBS-3H-type repository (Gribi et al. 2007, Section 3.6.1).

**General corrosion**

General corrosion of the insert can only occur in the presence of water. Prior to failure of the canister, there may be some water present inside the canister from the time of encapsulation due to residual water contained in the fuel rods [3.2.5]. The volume of
this water will, however, be small and any corrosion it causes on the internal surfaces of the cast iron insert will be very limited and, thus, this process is not considered to be significant.

After the canister has failed, however, larger volumes of groundwater will penetrate into the void spaces and begin to cause general corrosion of the cast iron insert. In the case of an initial canister defect, aerobic corrosion of the insert could occur if bentonite is not properly emplaced but it will be restricted by the slow rate of water inflow into the canister and by the limited dissolved oxygen content. Aerobic corrosion can, therefore, take place for only a short period of time before the chemistry of the penetrating water becomes anoxic as the dissolved oxygen in the groundwater is consumed by oxidation of the iron insert.

In the likely evolution of the repository, the copper overpack is expected to remain intact for several hundreds of thousands of years after emplacement. The initially trapped oxygen will be consumed during the saturation phase by reducing species in the groundwater (e.g. methane) and reactions with minerals in the barriers and with the copper overpack. Thus, the groundwater will be chemically reducing well before the canister fails. Near-field conditions are expected to remain chemically reducing indefinitely.

Under anaerobic conditions, corrosion of iron will generate hydrogen gas, small concentrations of dissolved Fe(II) and magnetite (Fe₃O₄) as the most likely corrosion end products. The formation of alternative solid secondary phases is possible, especially in the presence of higher contents of dissolved (reduced) sulphur species (CuFeS₂ or Fe₃S), carbonate species (FeCO₃ or Fe₂(OH)₂CO₃) or, in the case of more oxidising conditions, goethite (FeOOH) and haematite (Fe₂O₃). In the absence of pH buffering provided by carbonates, chloride-dominated solutions favour extremely slow corrosion accompanied by the formation of a thin magnetite film (Lee et al. 2006). Results from literature surveys showed magnetite to be the most common corrosion product on archaeological and industrial iron objects under reducing conditions (Smart & Adams 2006).

The solid secondary alteration products may form a passivating layer on the exposed surfaces of the iron insert, slowing further reaction, and reducing the likelihood of localised corrosion. The probable ranking order of the passivating ability of the different possible corrosion products is Cu₅S < CuFeS₂ < Fe₃S < CuFeO₂ < Fe₃O₄.

The solid secondary alteration products occupy a larger volume than the equivalent quantity of iron and, over time, will fill the available void spaces inside the canister. If the annular gap between the cast iron insert and the copper overpack has not closed due to thermal expansion and plastic deformation of the copper [4.2.4], then the iron corrosion products will also begin to fill this space. It has been estimated that the annulus would become completely filled with corrosion products between 10,000 and 20,000 years after failure of the copper overpack (SKB 2010). Once groundwater can access the internal void spaces of the canister, growth of secondary alteration products will fill these spaces also. In the long term, growth of the corrosion products will limit further access of groundwater to the cast iron insert and, potentially, generate mechanical deformation of the canister [4.2.3]. However, this has not been observed in natural analogues preserved under reducing conditions or in the ‘stress cell’ apparatus, which did not detect any expansion from anaerobic corrosion of cast iron after more than 900 days of exposure (Smart & Adams 2006).

The solid secondary alteration products will provide abundant and very active sorption sites for radionuclides released from the spent nuclear fuel. Some radionuclides may
be directly incorporated into the corrosion products through mineralisation and precipitation reactions. The sorption of radionuclides onto the surface of these solid phases will retard their migration, although this retardation cannot be quantified [4.3.3].

The rate of general corrosion of the insert has been estimated from laboratory and natural analogue studies to be below 1 μm/a after a few thousand years due to the passivation of the metal surfaces (e.g. Smart et al. 2001, Hermanson 2004, Smart & Adams 2006). Once the passivating film has developed, the subsequent corrosion rate of the insert will depend on the availability of water (which will be constrained by the diffusive properties of the bentonite buffer in the main scenario) and the transport properties of ions through the passivating layer. Continued general corrosion of the insert will consume the residual water inside the canister. When all of the void spaces are filled with alteration products, very little water can enter and corrosion will drop to a very low rate. Anaerobic corrosion of the iron insert will then continue, controlled by diffusion rates, until all iron is consumed. Hydrogen pressures inside the canister during the corrosion of the insert have been estimated by Bond et al. (1997) and can reach values of up to 5 MPa, assuming an insert corrosion rate of 0.1 μm/a and a breach in the canister wall of 5·10^{-6} m².

**Localised corrosion**

Localised corrosion (‘pitting’) of the cast iron insert is not expected to occur under repository conditions because the passivating oxide layer formed by generalised corrosion will protect the metal from localised attack. If it did occur, however, it would be after the copper overpack had failed and groundwater had penetrated the void spaces within the canister and, thus, its consequences would be minimal because the containment function of the canister would have already been lost.

Galvanic corrosion may occur after plastic deformation of the copper overpack, because the bentonite swelling pressure closes the annular gap between it and the cast iron insert (Smart et al. 2005). At the points of contact between the two metals, localised corrosion of the iron could occur in the presence of groundwater to act as an electrolyte. Galvanic corrosion is affected by the same factors as other corrosion processes (e.g. pH, temperature and salinity) but, in addition, the localised points of contact may lead to more pronounced galvanic attack. Experimental work indicates, however, that galvanic corrosion does not result in increased corrosion rates under the reducing conditions that would be expected in the repository near field (Smart et al. 2004). Studies on archaeological items also demonstrate that, in reducing conditions, galvanic coupling between iron and copper alloy does not cause accelerated corrosion rates of the iron (Smart & Adams 2006). Therefore, galvanic corrosion is considered not to be a significant process for the cast iron insert.

King et al. (2012) have reviewed the existing literature about galvanic and grain boundary corrosion comparing EBW and FSW. Overall, there were no indications of preferential corrosion of the weld. Galvanic currents between the weld and base material for FSW were low and no significant potential difference could be detected between the materials. The FSW tool is cathodic to the weld material, so that any particles from the tool that become incorporated into the weld material would be cathodically protected and would not corrode to create locally aggressive conditions (as can occur when Fe particles from carbon steel tools become embedded in fabricated structures) (King et al. 2012, p. 125). It should be noted that the used conditions to study grain boundary attacks and galvanic corrosion are far from real conditions present in the repository. Also, the FSW
tool has nowadays been redesigned and it is surface coated to limit the amount of impurities that could affect the corrosion behaviour of the FS weld.

Concerning the influence of grain size, Fennell et al. (2001) showed that the growth of grains during welding can concentrate impurities at the grain boundary due to a decrease in the relative volumes of the grain body and the grain boundaries. In this respect FSW is a better option than EBW as the grain size of the weld material is smaller.

The effect of radiation on the corrosion of the cast iron insert has been investigated by Smart & Rance (2005). They observed that gamma radiation increases the anaerobic corrosion rate of carbon steel in artificial groundwater with a composition relevant to that at Olkiluoto. At a dose rate of 11 Gy/h the increase only lasts for approximately 7000 hours, but at 300 Gy/h the enhancement is longer lasting and may be continuous. The enhancement in the corrosion rate is greater in simulated groundwater than in bentonite-equilibrated groundwater, which had a higher ionic strength and a higher initial pH.

Overall, corrosion of the cast iron insert is influenced by the following features of the repository system.

- **Temperature**: controls the rate of corrosion reactions and, in the case of a canister with initial defect, general corrosion may begin at high near-field temperatures and be accelerated.
- **Canister geometry**: the dimensions and shape of the canister have an effect on the exposed surface area for general corrosion and the void space into which solid corrosion products can expand. It also affects the contacts for galvanic corrosion to occur.
- **Mechanical stress**: the combination of stress and a chemically aggressive groundwater/porewater may promote stress corrosion cracking.
- **Material composition**: the corrosion processes (especially the rate) and the nature of the corrosion products depend on the composition of the iron.
- **Water composition**: is the primary control on the corrosion mechanism and its rate, and the nature of any solid and gaseous corrosion products that may be formed.

### Uncertainties in the understanding of the FEP:

There are no uncertainties concerning the general understanding of iron corrosion under aerobic and anaerobic conditions. Uncertainties in the general corrosion rate of the cast iron insert are relatively small and the rate can be expected to be less than 1 μm/a. There is, however, conceptual and numerical uncertainty about how coupled processes will operate under repository conditions to control the long-term evolution of the canister, in terms of the availability of groundwater through the bentonite buffer, the growth of secondary alteration products in the available void spaces and the mechanical impact on the failed canister.

The greatest uncertainties relate to the evolution of the near-field geochemical conditions. If oxygen-rich groundwater were to reach to repository depths and the buffer was disrupted, then considerably faster corrosion rates could occur. There is, however, evidence of a very long-term persistence of reducing conditions in the deep bedrock in Finland (Posiva 2009, Section 3.1.2.4). The capacity of the hydrobiogeochemical system present on the geosphere fractures to buffer infiltration of acidic and oxygenated water from the surface has been investigated and demonstrated to have substantial buffering capacity (e.g. Pitkänen et al. 2008).
Couplings to other FEPs:

Corrosion of the cast iron insert is directly affected by the following FEPs:
- Radiolysis of residual water (in an intact canister) [3.2.5]
- Radiolysis of the canister water [3.2.6]
- Heat transfer [4.2.2]
- Corrosion of the copper overpack [4.2.5]
- Stress corrosion cracking [4.2.7]

Corrosion of the cast iron insert directly affects the following FEPs:
- Radiolysis of the canister water [3.2.6]
- Corrosion of the cladding tubes and metallic parts of the fuel assembly [3.2.7]
- Alteration and dissolution of the fuel matrix [3.2.8]
- Release of the labile fraction of the inventory [3.2.9]
- Aqueous solubility and speciation (in the spent nuclear fuel) [3.3.1]
- Precipitation and co-precipitation (in the spent nuclear fuel) [3.3.2]
- Sorption (in the spent nuclear fuel) [3.3.3]
- Aqueous solubility and speciation [4.3.1]
- Precipitation and co-precipitation [4.3.2]
- Sorption [4.3.3]
- Diffusion [4.3.4]
- Advection [4.3.5]
- Colloid transport [4.3.6]
- Gas transport [4.3.7]
- Alteration of accessory minerals (in the buffer) [5.2.7]

References:


4.2.7 Stress corrosion cracking

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:**
- Stress corrosion cracking of cast iron insert
- Stress corrosion cracking, copper canister
- Corrosion

**Section in 2007-09:**
3.7

**General description:**
Stress corrosion cracking (SCC) may occur on metals that are subject to tensile stress in the presence of corrosive agents such as ammonia, nitric acid or acetate. If either of these conditions is missing, SCC cannot occur. Stress corrosion cracking does not depend on repository geometry and this description applies to both, KBS-3V and **KBS-3H** (Gribi et al. 2007, Section 3.7). With respect to the welding method, the FSW method (Posiva’s current reference method) is more favourable from the point of view of stress corrosion cracking compared with EBW, due to the lower initial residual stresses in the FS weld.
During the anaerobic phase, the initial residual stresses in the weld are deemed not to affect the performance of the canister because not all the conditions for SCC are fulfilled simultaneously during the canister evolution even in presence of such residual stresses (King & Newman 2010, p. 39). Furthermore, the likelihood of crack propagation is also smaller with smaller grain sizes, which is also favourable to FSW and its finer microstructure. Finally, as FSW induces lower initial stresses, the uncertainties concerning the potential for SCC are smaller with FSW than with EBW. Furthermore, as Gubner & Andersson (2007) showed, FSW would provide slightly better corrosion resistance than the EBW in very aggressive environments, though these were not representative of real repository conditions. The benefit of FSW is likely caused by the weld microstructure, which is closer to the base material in the case of FSW than EBW.

*Stress corrosion cracking of the cast iron insert*

During radiogenic heating, immediately after closure, the outer surface of the cast iron insert will be subject to a small tensile thermal stress due to the thermal gradient [4.2.4]. Subsequently, after complete swelling of the bentonite has occurred [5.2.2], the cast iron insert will be subject to a lower thermal gradient, due to increased thermal conductivity, and very low thermal stresses and the compressive stresses from external hydrostatic and swelling pressure become dominant. These compressive stresses are beneficial for the mechanical properties of the insert and they prevent the initiation of SCC on the insert surface. They tend to close surface cracks and increase the material strength, thereby improving the response to bending loads.

Residual tensile stresses in the insert can also result from the manufacturing process. The insert is heterogeneous, comprising the main cast iron body with steel tubes forming the spaces that hold the spent nuclear fuel assemblies. During fabrication of the insert, it has been observed that, after a long cooling phase, the steel tubes are affected by strong residual tensile stresses and the near-surface area of the insert is known to be in a high compressive stress state. During casting, the iron melt temperature is approximately 1350 °C, which causes the steel tubes to expand by more than 1 %. During subsequent cooling, the graphite spheres within the nodular iron grow causing swelling and generating tensile stresses in steel profiles and the internal parts deeper in the insert and compressive stresses on the near-surface part of the insert (Raiko et al. 2010, Section 13.6.2). The residual stresses have no practical influence on limit load or other higher loads that cause yielding because the residual stresses caused by manufacturing dissipate during yielding.

Some corrosive agents may accumulate within the insert, such as radiolytically generated nitric acid, but their volumes are likely to be small [3.2.5]. It has been estimated that the corrosion of the cast iron insert due to the nitric acid will be of the order of 10 µm, assuming all of the nitric acid corrodes only the insert (SKB 2010, Section 2.5.2). This combined with the limited magnitude of tensile stresses means that SCC is not thought to be a significant contributor to corrosion of the cast iron insert for as long as the copper overpack remains intact and no additional corrosive agents associated with the groundwater can come into contact with the insert.

*Stress corrosion cracking of the copper overpack*

Stress corrosion cracking of the copper overpack can occur if tensile stresses are present in the copper overpack. Tensile stresses in the copper overpack will be present due to different causes.
Shortly after deposition, the copper overpack may be subject to localised tensile stresses but the dominant stress will be compressive due to the external hydrostatic and bentonite swelling pressures that will force the copper overpack to be deformed onto the cast iron insert [4.2.3].

Residual tensile stresses may also form at the weld between the body of the canister and the lid during welding. Residual tensile stresses have been studied for the reference (FSW) and alternative welding methods (EBW). Residual stresses have been measured on EBW welds (Gripenberg 2009) and FS welds (Raiko et al. 2010, Section 13.6.1). Residual stresses in FSW have been found to be lower than in EBW, thus FSW is less prone to stress corrosion cracking.

Cold working (e.g. blows or dents on the copper surface) during canister handling can change the residual mechanical stresses on the canister surface. A stress concentration could then lead to crack initiation under some circumstances (e.g. a pre-existing flaw) but not all cracks that are initiated will propagate (King & Newman 2010). There is no evidence that discontinuities in the copper overpack will adversely affect the SCC behaviour of copper canisters (King et al. 2011, Section 6.1.2.3). SKB is carrying out research into the potential effects of handling and transportation on the long-term mechanical properties of the canister’s copper surface (Raiko et al. 2010).

Although tensile stresses will be present in the copper overpack, SCC would occur only if the geochemical conditions allow it. Shortly after deposition, the near-field environment is likely to be oxidising and other contaminants derived from repository excavation (e.g. nitrite and ammonia) may be present (although their amounts may be smaller in KBS-3H than in KBS-3V, since the drifts are bored, not blasted). Under oxidising conditions, such as in the presence of dissolved oxygen or Cu(II), the conditions under which SCC has been observed depend on the equilibrium potential and pH needed for Cu₂O/CuO formation. SCC also depends on redox potential (Eh) values. The likelihood of SCC of the copper overpack decreases, however, as the near field progressively becomes more reducing. This is confirmed by studies of SCC in the presence of acetate under reducing conditions and high pressure that show that neither Cu-OFP (oxygen free, phosphorous doped copper) nor the weld are susceptible to SCC under conditions that are more aggressive than expected in the repository near field (Kinnunen 2006). Although copper has been shown to be susceptible to SCC, particularly in the presence of phosphorous, which is sometimes present in commercial copper metal, Kinnunen (2006) showed that no phosphorus segregation at the grain boundaries or other interfaces occurred in Cu-OFP.

Some preliminary experimental evidence suggests that SCC of copper can be induced under reducing conditions by sulphide ions in highly saline seawater (Taniguchi & Kawasaki 2008), but the results cannot be reproduced. Indeed, many have tried, unsuccessfully, to replicate the observations of Taniguchi & Kawasaki (Arilahti et al. 2011, Bhaskaran et al. 2013). It is significant that Taniguchi & Kawasaki (2008) report an apparent threshold sulphide concentration for SCC. Under conditions where the transport of HS⁻ to the canister surface is rate limiting, the surface sulphide concentration will approach zero. Indeed, King & Newman (2010) have argued that, under such conditions, any mechanism that requires HS⁻ to enter the crack will be inoperative as the driving force for sulphide transport into the narrow crack will be infinitesimally small.

In the absence of corroborative evidence in support of Taniguchi & Kawasaki’s observations, and in the absence of a demonstrated mechanism involving vacancy...
injection, SCC of copper is deemed not possible under anaerobic conditions (King & Newman 2010).

Therefore, on the basis of the best available information, there is no evidence to suggest that SCC of the copper overpack, and specifically of the weld can be sustained during the long-term anaerobic phase under the geochemical conditions expected within the bentonite buffer.

Different models for SCC are available; the crack growth model used by Posiva and SKB predicts vanishingly small crack propagation rates of ≤ 0.1 µm in 100,000 years (King et al. 2011, Section 6.3). Furthermore, little hydrogen sulphide will reach the crack tip because the rate of corrosion of the canister surface by sulphide is limited due to the rate of diffusion through the compacted bentonite buffer. The absence of sulphidation at the crack tip precludes crack growth. Film-induced cleavage can also be ruled out because the properties of the non-adherent sulphide films formed on copper will not support the generation of a cleavage crack in the underlying copper.

Microbial production of ammonia, acetate and nitrite ions has also been taken into account in these models. As the available oxidants are consumed (e.g. acetate is consumed and CO₂ is the end-product of this reaction) and swelling of the bentonite buffer restricts the transport of SCC agents from the groundwater to the canister surface, the probability of SCC will diminish accordingly.

Experimental work has been performed in environments known to support SCC in repository conditions, including those in which significant amounts of ammonia, acetate and nitrite are present (Ikeda & Litke 2007, 2008, Litke & Ikeda 2008, 2011). The condition in which these experiments have been performed do not support the occurrence of the process in repository conditions as it is extremely unlikely to found the same significant amounts of ammonia, acetate and nitrite as used in the experiments.

Overall, stress corrosion cracking of the canister is influenced by the following features of the repository system.

- Temperature: SCC is more likely when the temperature drops because the metal is less likely to deform plastically and more likely to deform by cracking.
- Pressure: affects the mechanical stresses acting on the canister.
- Canister geometry: the dimensions and shape of the canister have an effect on the distribution of the mechanical stresses.
- Mechanical stresses: this is the main control on SCC, particularly the development of tensile stresses.
- Material composition: SCC is dependent on material composition.
- Water composition: SCC can only occur in the present of certain chemical species such as ammonia, nitric acid or acetate, which may be present as residual materials from repository construction or may be formed in microbial processes, e.g. acetate. In addition, the likelihood for SCC decreases strongly going from oxidising to reducing conditions. High porewater pH leads to a passivation of the copper surface and therefore reduces the potential for SCC.

**Uncertainties in the understanding of the FEP:**

There is extensive experience with, and knowledge of, the SCC of copper alloys, and considerable effort has gone into studying the SCC mechanism of copper canisters (King et al. 2011, Chapter 6). The mechanism of SCC is not, however, completely
understood. The conditions under which SCC takes place seem to be related to the equilibrium potential and pH for Cu₂O/CuO equilibrium.

Residual stresses in the cast iron insert resulting from the manufacturing process are currently being studied by SKB and Posiva. Preliminary results show that there are remarkably high compressive residual stresses in the insert, especially on the cylinder surface area and lower tensile stresses in the deeper parts of the material. Residual stresses in the weld of the copper canister resulting from the welding process are also currently being studied.

The possibility of SCC occurring under anoxic and reducing conditions, in the presence and absence of sulphides, is another area of ongoing investigation (Arilahti et al. 2011).

**Couplings to other FEPs:**

Stress corrosion cracking of the copper canister is directly affected by the following FEPs:
- Radiolysis of residual water (in an intact canister) [3.2.5]
- Heat transfer [4.2.2]
- Deformation [4.2.3]
- Thermal expansion of the canister [4.2.4]
- Water uptake and swelling (in the buffer) [5.2.2]
- Diffusion (in the buffer) [5.3.4]

Stress corrosion cracking of the canister directly affects the following FEPs:
- Corrosion of the copper overpack [4.2.5]
- Corrosion of the cast iron insert [4.2.6]

**References:**


4.3 Migration FEPs

Once the canister and then the cladding tubes are breached, radionuclides and other substances can be released from the fuel to the groundwater by various dissolution and alteration reactions. Following release, a number of physical and chemical processes will control the migration of radionuclides in the canister void spaces and through perforations in the canister wall to the buffer. The following descriptions summarise each of these processes and the effects of the different features on them. The coupling of the FEPs is also indicated, but the possible consequences of their interactions will be discussed in Posiva (2016b).

References

Posiva 2016b. Safety evaluation for a KBS-3H spent nuclear fuel repository at Olkiluoto – Performance Assessment. Eurajoki, Finland: Posiva Oy. POSIVA 2016-02 (in prep.).
### 4.3.1 Aqueous solubility and speciation

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th><strong>Class:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
</tr>
</tbody>
</table>

**Alternative names:**
Dissolution and speciation; Solubility and speciation

**Section in 2007-09:**
3.8

**General description:**
The processes that control radionuclide solubility and speciation within the canister are the same as those for spent nuclear fuel, and are discussed under FEP 3.3.1.

**Uncertainties in the understanding of the FEP:**
The uncertainties associated with radionuclide solubility and speciation within the canister are the same as those for spent nuclear fuel, and are discussed under FEP 3.3.1.

**Couplings to other FEPs:**
Aqueous solubility and speciation in the canister is directly affected by the following FEPs:
- Radiolysis of the canister water [3.2.6]
- Corrosion of the cladding tubes and metal parts of the fuel assembly [3.2.7]
- Alteration and dissolution of the fuel matrix [3.2.8]
- Precipitation and co-precipitation [3.3.2]
- Heat transfer [4.2.2]
- Corrosion of the cast iron insert [4.2.6]

Aqueous solubility and speciation directly affects the following FEPs:
- Precipitation and co-precipitation [4.3.2]
- Sorption [4.3.3]
- Diffusion [4.3.4]
- Advection [4.3.5]
- Colloid transport [4.3.6]

**Related bibliography not cited in the text:**


4.3.2 Precipitation and co-precipitation

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
</tr>
</tbody>
</table>

Alternative names: Radionuclide transport

Section in 2007-09: 3.7, 3.8

General description:
The processes that control precipitation and co-precipitation within the canister are the same as those for spent nuclear fuel, and are discussed under 3.3.2. The chemical processes in the canister do not depend on the specific conditions in KBS-3H (Gribi et al. 2007, Section 3.6.1).

Uncertainties in the understanding of the FEP:
The uncertainties associated with precipitation and co-precipitation within the canister are the same as those for spent nuclear fuel, and are discussed under FEP 3.3.2.

Couplings to other FEPs:
Precipitation and co-precipitation in the canister are directly affected by the following FEPs:
- Radiolysis of the canister water [3.2.6]
- Corrosion of the cladding tubes and metal parts of the fuel assembly [3.2.7]
- Alteration and dissolution of the fuel matrix [3.2.8]
- Precipitation and co-precipitation [3.3.2]
- Heat transfer [4.2.2]
- Corrosion of the cast iron insert [4.2.6]
- Aqueous solubility and speciation [4.3.1]
- Sorption [4.3.3]

Precipitation and co-precipitation in the canister directly affect the following FEPs:
- Sorption [4.3.3]
- Diffusion [4.3.4]
- Advection [4.3.5]
- Colloid transport [4.3.6]

References:

Related bibliography not cited in the text:
4.3.3 Sorption

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
</tr>
</tbody>
</table>

**Alternative names:**
- Ion exchange; Physical adsorption

**Section in 2007-09:**
- 3.8

**General description:**

The corrosion products of the cast iron insert will provide abundant and very active sorption sites for radionuclides. Sorption is element specific and depends on both, radionuclide speciation, and the solid phase composition and surface characteristics.

Under the ambient geochemical conditions, the primary iron corrosion product, magnetite, will be a strong scavenger of radionuclides from solution. The combination of the generation of chemically reducing conditions, under which many radionuclides are poorly soluble, mineralisation and precipitation reactions and sorption onto iron corrosion products will reduce the rate of radionuclide migration out of a canister.

Over time, the first-formed corrosion products, such as magnetite, may slowly react with the groundwaters to form a number of more stable solids such as goethite (FeOOH) and haematite (Fe₂O₃), if oxidising species are formed due to radiolysis of water or oxidising waters penetrate the canister. This in turn affects the sorption properties of these alteration products.

Potentially, the solid alteration products formed by the corrosion of the copper overpack may also retard radionuclides, but this is considered to be less significant than for the iron corrosion products because of their smaller volume due to the much lower reactivity of copper.

A number of natural analogue studies have examined the sorption of radionuclides on iron corrosion products, particularly in geological environments where naturally occurring uranium is in contact with iron minerals such as at Poços de Caldas and Morro do Ferro. These studies support laboratory evidence for the high sorption capacity for these iron corrosion products (Miller et al. 2000).
Overall, sorption is affected by a number of features:

- Radionuclide inventory: controls the radionuclides that are available for sorption.
- Temperature: significant control over the rate of iron corrosion and, thus, the total sorption capacity of the secondary corrosion products that are formed.
- Canister geometry: controls the available surface area on which sorbing corrosion products may form, and the void spaces into which they can grow.
- Material composition: the addition of other metals in the iron alloy can affect the nature of the solid corrosion products that form by reaction with the groundwater.
- Water composition: the porewater adjacent to the canister, particularly its redox potential and the concentration of dissolved species etc. can affect the nature of the solid corrosion products and their subsequent alteration.

**Uncertainties in the understanding of the FEP:**
Although the conceptual understanding of sorption is well established, the quantification of a bulk retardation rate for radionuclides due to the coupled processes of redox control, precipitation and sorption is not well defined.

Sorption is a reversible reaction, and the long-term retardation mechanism is conceptually well understood, although specifying the mechanisms responsible for retardation under repository conditions is less well established.

Radionuclides initially sorbed to iron corrosion products may be subsequently released (e.g. if the redox or temperature changes) or if the solid dissolves or undergoes other mineralogical transformations. This may be more likely to occur in the case of early canister failure when chemical conditions in the near field may be prone to more rapid change. The long-term sorption processes under these conditions are not well defined.

**Couplings to other FEPs:**
Sorption is directly affected by the following FEPs:

- Alteration and dissolution of the fuel matrix [3.2.8]
- Heat transfer [4.2.2]
- Corrosion of the copper overpack [4.2.5]
- Corrosion of the cast iron insert [4.2.6]
- Aqueous solubility and speciation [4.3.1]
- Precipitation and co-precipitation [4.3.2]
- Alteration of accessory minerals (in the buffer) [5.2.7]

Sorption directly affects the following FEPs:

- Precipitation and co-precipitation [4.3.2]
- Diffusion [4.3.4]
- Advection [4.3.5]
- Colloid transport [4.3.6]

**References:**
### 4.3.4 Diffusion

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Class:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Migration</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Alternative names:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Radionuclide transport (advection and diffusion)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Section in 2007-09:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>3.8</td>
</tr>
</tbody>
</table>

**General description:**

Diffusion is likely to be the dominant migration process operating within a failed canister and responsible for the transport of radionuclides to the buffer. This process is relevant for all time frames after groundwater penetrates the canister and the fuel cladding.

In a failed canister, groundwater will slowly flow into the canister void space [4.3.5]. Once the canister has become filled with water, and any hydraulic head gradients have dissipated, diffusion will be the primary mechanism for transporting any radionuclides released from the spent nuclear fuel through the canister void spaces.

Diffusion is driven by a potential gradient (typically a concentration gradient) and, consequently, there will be a slow net migration of radionuclides released from the spent nuclear fuel by dissolution through the canister void spaces and the perforations in the canister walls, to the buffer. The rate of radionuclide transport will, therefore, be controlled by the rate of radionuclide diffusion through the buffer [5.3.4] which effectively limits the concentration gradient in the near field.

It is possible, however, that all or a proportion of the canister void space will fill with hydrogen gas generated by anaerobic corrosion of the cast iron insert depending on the location of the perforations in the canister wall [4.3.7]. The formation of a gas phase (bubble) will expel groundwater from the canister and, therefore, cause diffusion through the groundwater to cease, although diffusion in gas is still possible for gaseous species (Wikramaratna et al. 1993).

Overall, diffusion is influenced by the following features of the repository system.

- Radionuclide inventory: controls the radionuclides that are available for diffusion.
- Temperature: the diffusion rate is partially controlled by temperature.
- Canister geometry: the location of any perforations in the canister wall will control the diffusion path and whether diffusion occurs largely in the gaseous or aqueous phase within the canister.
- Water composition: radionuclide concentration gradients in the water directly control the diffusion rate in the aqueous phase.
- Gas composition: radionuclide concentration gradients directly control the diffusion rate in the gaseous phase.

**Uncertainties in the understanding of the FEP:**

Generally, diffusion is a well understood process. The rate of water turnover and the transport of solutes within a failed canister void space are controlled by the hydraulic conductivity of the bentonite buffer, which will be very low, providing a diffusive barrier.
The greatest uncertainties related to diffusion from the canister into the buffer are the location, size and transport resistance (and its evolution) of any breach in the copper overpack due to, for example, corrosion or manufacturing defects or rock shear displacements.

**Couplings to other FEPs:**
Diffusion is directly affected by the following FEPs:
- Alteration and dissolution of the fuel matrix [3.2.8]
- Release of labile fraction of the inventory [3.2.9]
- Heat transfer [4.2.2]
- Corrosion of the copper overpack [4.2.5]
- Corrosion of the cast iron insert [4.2.6]
- Aqueous solubility and speciation [4.3.1]
- Precipitation and co-precipitation [4.3.2]
- Sorption [4.3.3]
- Diffusion (in the buffer) [5.3.4]

Diffusion directly affects the following FEPs:
- Release of labile fraction of the inventory [3.2.9]

**References:**

### 4.3.5 Advection

<table>
<thead>
<tr>
<th>Type: Process</th>
<th>Class: Migration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radionuclide transport (advection and diffusion)</td>
<td>Section in 2007-09: 3.8</td>
</tr>
</tbody>
</table>

**General description:**
Advection is the movement of water under a pressure gradient, and more exactly a transport mechanism of a substance or conserved property by a fluid due to the fluid’s bulk motion. When a canister fails, there will be a strong hydrostatic pressure gradient between the inside and the outside of the canister, which will force groundwater into the canister void space. Once the canister is filled with water, however, the hydrostatic pressure will equalise and further water movement inside the canister will be dominated by diffusion [4.3.4]. In the case of early canister failure, when there is still some radiogenic heat generation [3.2.2], thermal convection of water inside the canister may also occur.

It is possible, however, that all or a proportion of the canister void space will fill with hydrogen gas generated by anaerobic corrosion of the cast iron insert depending on the location of the perforations in the canister wall [4.3.7]. The formation of a gas phase...
(bubble) will expel groundwater from the canister and may, therefore, cause groundwater advection out of the canister.

Advection inside the canister, if it occurs, will cause a redistribution and homogenisation of the concentrations of dissolved radionuclides within the canister water, and transport radionuclides from the spent nuclear fuel to perforations in the canister wall. Advection will also cause the redistribution of any colloids within the canister.

Movement of groundwater and any dissolved radionuclides into and out of the canister will be controlled by the hydraulic conductivity of the bentonite buffer, which will provide a diffusive barrier [5.3.4]. This means that the rate of water turnover in the canister will be very slow and, consequently, the dissolution of the spent nuclear fuel [3.2.8] and the concentration of radionuclides in the water will be solubility limited. Advection will only be a significant process for radionuclide transport through perforations in the canister wall in cases where the buffer swelling pressure is much reduced due to its erosion [5.2.3, 5.2.4] and advection can occur through the buffer. As these conditions are very unlikely, advection in the canister is a much less significant transport process than diffusion.

Advection will also become less significant as the canister void spaces progressively fill with secondary alteration products formed by the anaerobic corrosion of the cast iron insert or by bentonite penetrating into a breached canister [4.2.6]. Eventually, these corrosion products or bentonite will fill the entire void space, groundwater will be expelled and migration pathways will become more tortuous and longer. In consequence, advection (and convection) processes will cease and radionuclide transport out of the canister will occur only by slow diffusion.

Overall, advection is influenced by the following features of the repository system.

- Radionuclide inventory: controls the radionuclides that are available for advective transport.
- Temperature: a temperature gradient will drive convection of groundwater.
- Pressure: the pressure at the canister outer wall and any gas pressure that develops in the canister will be the primary drivers for advection.
- Canister geometry: the location of any perforations in the canister wall will control the flow path and whether groundwater advection occurs or is stopped by a build-up of gas.

**Uncertainties in the understanding of the FEP:**

There are no conceptual uncertainties regarding the advection process, and its driving forces. The likelihood of advection being maintained inside the canister for a long period of time, or becoming a significant process causing transport through the canister wall to the buffer, is very low.
**Couplings to other FEPs:**

Advection is directly affected by the following FEPs:

- Criticality (if it were to occur) [3.2.11]
- Heat transfer [4.2.2]
- Corrosion of the copper overpack [4.2.5]
- Corrosion of the cast iron insert [4.2.6]
- Aqueous solubility and speciation [4.3.1]
- Precipitation and co-precipitation [4.3.2]
- Sorption [4.3.3]
- Gas transport [4.3.7]
- Advection (in the buffer) [5.3.5]

Advection directly affects the following FEPs:

- Release of labile fraction of the inventory [3.2.9]
- Criticality (if it were to occur) [3.2.11]
- Colloid transport [4.3.6]
- Gas transport [4.3.7]
- Advection (in the buffer) [5.3.5]

**Related bibliography not cited in the text:**


### 4.3.6 Colloid transport

<table>
<thead>
<tr>
<th>Type:</th>
<th>Process</th>
</tr>
</thead>
<tbody>
<tr>
<td>Class:</td>
<td>Migration</td>
</tr>
</tbody>
</table>

**Alternative names:**

Radionuclide transport; Colloid facilitated transport

**Section in 2007-09:**

3.8

**General description:**

In general, any particle that has a linear dimension between $10^{-9}$ and $10^{-6}$ m is considered to be a colloid (Hiemenz & Rajagopalan 1997). Larger solids are often termed ‘suspended particles’ and anything smaller is considered to be in solution.

The presence of colloids in the canister cavity may have a significant influence on radionuclide transport, but only after the canister has failed. Consequently, colloid formation and colloidal transport are particularly relevant to the defective canister scenarios. For the entire time the canister remains intact, no colloid-mediated...
radionuclide transport from the canister can occur, although colloids may form inside the canister before failure depending on the presence of water or vapour.

Most colloids will be formed after canister failure when groundwater begins to corrode the cast iron insert [4.2.6] and, eventually, the spent nuclear fuel [3.2.8]. Radionuclides can form either intrinsic colloids (eigen-colloids) or pseudo-colloids [3.3.2]. Furthermore, radionuclides may be incorporated in co-precipitates from solution so entering directly into colloidal form. These colloidal particles can provide radionuclides with low solubility (e.g. actinides) an alternative transport mechanism.

In general, the stability and thus the mobility of colloids are controlled by the grain size, the absolute surface charge (± 20 mV) of the dispersed particles and by the density of the particles. The stability of colloids depends significantly on groundwater salinity. In saline water, colloids tend to form a sediment due to aggregation and flocculation (e.g. Kranck 1973, IAEA 2003, Sutherland et al. 2014).

Although colloidal particles may move within the canister void space by advection or diffusion, they cannot migrate through the bentonite buffer due to the very high swelling pressure. The buffer acts as a filter for colloids, due to the small pore size that exists provided its dry density is above a threshold value (1650 kg/m$^3$) and is not reduced by erosion [5.2.3, 5.2.4].

Tetravalent actinides may form colloidal oxide particles. In particular, Pu(IV) is known to have a high tendency to form colloids (Choppin et al. 2002) and the formation of Pu colloids has been considered in data modelling in the SKB programme (Wold 2010). The measured concentrations of U, Pu and Np in tests simulating conditions inside a damaged canister are very low, and trends over time indicate the formation of an actinide co-precipitate rather than separate oxide phases (Carbol et al. 2009). The measured Pu concentrations do not suggest over-saturation with respect to the estimated solubility of Pu(OH)$_4$(am) indicating that colloids are not actively increasing the apparent Pu solubility in this case.

Overall, colloid transport is influenced by the following features of the repository system.

- Radionuclide inventory: controls the radionuclides that may be available for association with colloids.
- Temperature: the stability of colloids may be temperature dependent, although this is only a second-order control.
- Pressure: the pressure at the canister outer wall and any gas pressure that develops in the canister will be the primary drivers for colloid migration in flowing (advective) groundwater.
- Material composition: particularly of the canister metal, because corrosion of iron generates the majority of the colloidal particles in the canister.
- Water composition: the composition of the water in and close to the canister is a first-order control on the formation and stability of colloids.

**Uncertainties in the understanding of the FEP:**

The population of colloids inside the canister is uncertain but is not directly significant for safety provided the buffer remains intact and continues to act as a barrier to colloid transport. See also [10.3.6].
**Couplings to other FEPs:**

Colloid transport is directly affected by the following FEPs:
- Alteration and dissolution of the fuel matrix [3.2.8]
- Heat transfer [4.2.2]
- Corrosion of the copper overpack [4.2.5]
- Corrosion of the cast iron insert [4.2.6]
- Aqueous solubility and speciation [4.3.1]
- Precipitation and co-precipitation [4.3.2]
- Sorption [4.3.3]
- Advection [4.3.5]
- Gas transport [4.3.7]

Colloid transport directly affects the following FEPs:
- Colloid transport (in the buffer) [5.3.6]

**References:**


---

### 4.3.7 Gas transport

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
</tr>
</tbody>
</table>

**Alternative names:**
- Radionuclide transport;
- Two-phase flow;
- Water and gas transport

**Section in 2007-09:**
- 3.8

**General description:**

It is possible that a two-phase (water-gas) system will develop within the canister cavity in the post-closure evolution of the repository. The gas can be present as:
- hydrogen generated by anaerobic corrosion of iron,
- vapour caused by boiling of water if the boiling point is exceeded,
- argon used to purge the canister at the time of encapsulation,
- residual air, though insignificant compared to argon, or
- radiolysis products of water or water vapour.
Of these mechanisms, anaerobic corrosion of the cast iron insert generating hydrogen is likely to be the greatest contributor to the gas content within the canister cavity, and this can only occur after the canister has failed.

Gas generation by boiling of water is only possible when the internal temperature exceeds the boiling point and, therefore, is relevant only for cooling pool water trapped in leaking fuel rods and for groundwater in the early canister failure scenarios. The amount of gas that may be generated by radiolysis of canister water is considered to be very small [3.2.6].

A free gas phase (bubble) will form inside the canister if the partial pressure of the gas exceeds the hydrostatic pressure. Whether this occurs depends on the balance between the rate of gas generation and the rate of its transport out of the canister to the buffer. Unless the gas pressure exceeds the confining pressure of the bentonite buffer, gas release from the canister will be diffusion limited. If the gas pressure exceeds the confining pressure, then a gas bubble may push through the buffer [5.3.7].

Any free gas formed in the canister will rise to the uppermost part of the canister and will accumulate as a bubble if it is contained. As more gas is produced, the gas pressure and bubble volume will increase, and water will be expelled from the canister through any perforations. The maximum possible size of the bubble will be controlled by the internal geometry of the canister and the location of the perforations in the canister metal.

The case of hydrogen generation through anaerobic iron corrosion in a canister with different corrosion rates, perforation sizes and available internal surface areas for corrosion have been modelled (Bond et al. 1997).

The presence of a free gas phase in the canister may have a significant impact on the release of radionuclides. Any radionuclides that can partition into a free gas phase may be transported within and out of the canister as a gas (e.g. C-14). In addition, any water expelled from the canister due to a build-up of gas will carry dissolved radionuclides with it and, potentially, radionuclides in colloidal form [4.3.6]. In consequence, gas generation may enhance the total release of radionuclides from the canister.

If, however, a large gas bubble forms in the canister cavity, then further dissolution of the fuel [3.2.8] and corrosion of the internal surfaces of the iron insert [4.2.6] could be restricted because the presence of the gas may reduce the rate of water ingress into the canister.

If no free gas phase forms in the canister, then the cavity will become water filled after the canister fails and mainly diffusion [4.3.4] and to a lesser extent, advection [4.3.5] will become the dominant transport processes.

Overall, gas transport is influenced by the following features of the repository system.

- Radionuclide inventory: controls the radionuclides that may be available to form a free gas phase, and the radiation intensity controls the rate of radiolytic gas generation, although this is a less important gas generation process than anaerobic corrosion of iron.
- Temperature: the internal temperature and thermal gradients influence the rates of diffusion, advection and convection of gas, and also the solubility and pressure of the evolved gases.
- Pressure: is the primary control on whether gas will be dissolved into the groundwater or whether a free gas phase (bubble) will form.
- Canister geometry: the location of any perforations in the canister wall will control whether a gas phase (bubble) forms in the canister or not and the size and geometry of the region occupied by that gas phase.
- Material composition: particularly that of the iron insert will control the generation of gas under the anaerobic conditions that are expected inside the canister.
- Water composition: particularly redox will control the corrosion of iron and, therefore, the potential for gas generation inside the canister.
- Gas composition: the composition of the gases that are generated in the canister will control their solubility and, therefore, the potential for a free gas phase to form.

**Uncertainties in the understanding of the FEP:**

The greatest uncertainties for gas transport in the canister concern the timing and rate of water (or water vapour) penetration into the canister and the build-up of a free gas phase due to hydrogen production caused by corrosion of the cast iron insert. If the buffer prevents the hydrogen gas from escaping the canister, the gas overpressure is likely to decrease the rate of further water ingress into the canister.

**Couplings to other FEPs:**

Gas transport is directly affected by the following FEPs:
- Alteration and dissolution of the fuel matrix [3.2.8]
- Heat transfer [4.2.2]
- Corrosion of the copper overpack [4.2.5]
- Corrosion of the cast iron insert [4.2.6]
- Advection [4.3.5]
- Advection (in the buffer) [5.3.5]
- Gas transport (in the buffer) [5.3.7]

Gas transport directly affects the following FEPs:
- Advection [4.3.5]
- Colloid transport [4.3.6]

**References:**

5 BUFFER

5.1 Description

In the KBS-3H type repository, compacted bentonite will be used as buffer material surrounding the canisters in each deposition drift (Figure 5-1). In KBS-3H, the buffer includes the following components: (1) The buffer inside the supercontainer shell, composed of both cylindrical and ring-shaped blocks, as shown in Figure 5-2, and (2) the buffer in distance blocks, shown in brown in Figure 5-1, composed of cylindrical slices (the dimensions of one are shown in Figure 5-3).

The **void spaces** between the bentonite blocks, the gaps between the bentonite blocks and the rock, and between the bentonite and the canister are also considered as a physical subcomponent of the buffer.

Initially the void spaces will contain air but, as artificial watering is used (see below), they will become filled with swelled bentonite, although with low density at the beginning of the swelling process. After continued saturation with the surrounding groundwater in the near-field rock, the resulting **buffer porewater** is the groundwater that has equilibrated with the montmorillonite and accessory minerals in the bentonite.

The reference material for the bentonite blocks is a sodium bentonite (MX-80) that is a natural material from Wyoming, United States. The average bulk mineralogical composition of MX-80 is dominated by montmorillonite (average 90 %) with smaller amounts of accessory minerals such as quartz, mica, feldspar, carbonate, gypsum and pyrite.

![Figure 5-1. The deposition drift and its main components. The deposition drift is excavated from the niche with a slight inclination upwards facilitating drainage during installation. Figure by Saanio & Riekkola Oy.](image-url)
Figure 5-2. Dimensions (mm) and geometry of solid and ring-shaped bentonite blocks inside the supercontainer.

Figure 5-3. Dimensions (mm) and geometry of a 500 mm slice of a distance block. The diameter of distance block is 1765 mm and the length depends on the canister type and the required canister spacing.
After emplacement, water fed through the DAWE system (Posiva 2013a, Section 4.3.4) will begin to be absorbed by the buffer bentonite, and initiate its swelling. The process will continue fed by inflowing groundwater from the surrounding rock, although it may take hundreds to thousands of years until the desired swelling and saturation state is reached. When the bentonite is completely water-saturated and swollen, its hydraulic conductivity will be so low that groundwater and any radionuclides that are eventually released from the canister will only be able to migrate through it by diffusion. The clay mineral structure of the bentonite also provides a high sorption capacity that will retard radionuclide migration.

The initial physical properties of the bentonite blocks, rings and pellets, and their properties after full hydraulic saturation, are shown in Table 5-1.

The hydraulic and physical properties of the buffer after water uptake are controlled by the swelling pressure generated by montmorillonite. The chemical properties of the buffer are, however, largely controlled by the assemblage of accessory minerals, together with the exchangeable cation reactions of the clay and the interactions with the surrounding groundwater.

5.1.1 Long-term safety and performance

The long-term safety principles of the buffer surrounding the canisters and the buffer in the distance blocks are to protect the canisters and to separate hydraulically the supercontainers from each other and from any filling components that are located near sections of high groundwater inflow in the deposition drift, as long as containment of radionuclides is needed, and thus the safety functions assigned to the buffer are to:

- Contribute to mechanical, geochemical and hydrogeological conditions that are predictable and favourable to the canister,
- Protect canisters from external processes that could compromise the safety function of complete containment of the spent nuclear fuel and associated radionuclides,
- Limit and retard radionuclide releases in the event of canister failure.

In addition, the buffer in the distance blocks shall

- Hydraulically and thermally separate the supercontainers from each other.

The buffer shall retain its favourable properties over hundreds of thousands of years (Posiva 2016c).

Table 5-1. Properties of buffer as assumed in this KBS-3H safety case.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gap between the canister and the buffer</td>
<td>~5 mm</td>
</tr>
<tr>
<td>Gap between the distance blocks and rock wall</td>
<td>42.5−45.0 mm</td>
</tr>
<tr>
<td>Initial water content of supercontainer buffer, solid blocks</td>
<td>17 ± 1 %</td>
</tr>
<tr>
<td>Initial water content of supercontainer buffer, ring blocks</td>
<td>11 ± 1 %</td>
</tr>
<tr>
<td>Initial water content of distance blocks</td>
<td>21 ± 1 %</td>
</tr>
<tr>
<td>Final saturated density of the buffer</td>
<td>1950–2050 kg/m³</td>
</tr>
</tbody>
</table>
The ability of the buffer to provide the safety functions, as part of the engineered barrier system, strongly depends on its initial state, which by complying with design specifications, will lead to achieving and maintaining a high swelling pressure after saturation for a long period. In the immediate short-term period following emplacement of the canister and the buffer in the deposition drift, the main processes that will affect swelling are heat transfer and water uptake. Over the long term, chemical processes (e.g. montmorillonite transformation, chemical erosion) may reduce the swelling pressure of the buffer and affect its performance.

5.1.2 Overview of the potentially significant FEPs

There are a number of processes that are considered to be significant for the long-term safety performance of the buffer that relate to system evolution and to the migration of radionuclides and other substances.

Processes related to system evolution are:

5.2.1 Heat transfer
5.2.2 Water uptake and swelling
5.2.3 Mechanical erosion
5.2.4 Chemical erosion
5.2.5 Radiolysis of porewater
5.2.6 Montmorillonite transformation
5.2.7 Alteration of accessory minerals
5.2.8 Microbial activity
5.2.9 Freezing and thawing
5.7.10 Desiccation, formation of cracks

Processes related to the migration of radionuclides and other substances are:

5.3.1 Aqueous solubility and speciation
5.3.2 Precipitation and co-precipitation
5.3.3 Sorption
5.3.4 Diffusion
5.3.5 Advection
5.3.6 Colloid transport
5.3.7 Gas transport
These processes are each potentially affected by a number of features of the repository system that can influence the occurrence, rate, activity and potential couplings between the processes. These features relate either to aspects of the design of the repository or to parameters (characteristics) of the buffer that might be time-dependent during the repository lifetime. The most significant features are:

- Radionuclide inventory
- Temperature
- Swelling pressure
- Buffer geometry
- Water content
- Buffer composition
- Porewater composition
- Gas composition.

The possible influences of these features on the processes considered to be significant for the long-term safety of the buffer are described in each FEP description, and are summarised in Table 5-2.

Many of the processes occurring within the buffer are interdependent and directly coupled to each other. For example, mineralogical transformation of montmorillonite [5.2.6] will directly affect water uptake and swelling [5.2.2]. The direct couplings are listed in each FEP description, and are summarised in the matrix shown in Table 5-3.

Similarly, due to the complex interactions between the various components of the disposal system, the evolution of the buffer can influence (or be influenced by) processes occurring in other parts of the repository through the interactions between various processes. For example, water uptake by the buffer [5.2.2] interacts with groundwater flow and advective transport in the geosphere [10.3.5]. The interactions between the buffer and other components of the disposal system are summarised in Table 5-4.

References


Table 5-2. Possible influences of features of the disposal system on the processes considered to be significant for the long-term performance of the buffer (marked with Y). These influences and couplings are discussed in more detail in each FEP description.

<table>
<thead>
<tr>
<th>Processes related to system evolution:</th>
<th>Features</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Radionuclide inventory</td>
</tr>
<tr>
<td>5.2.1 Heat transfer</td>
<td>Y</td>
</tr>
<tr>
<td>5.2.2 Water uptake and swelling</td>
<td>Y</td>
</tr>
<tr>
<td>5.2.3 Mechanical erosion</td>
<td>Y</td>
</tr>
<tr>
<td>5.2.4 Chemical erosion</td>
<td>Y</td>
</tr>
<tr>
<td>5.2.5 Radiolysis of porewater</td>
<td>Y</td>
</tr>
<tr>
<td>5.2.6 Montmorillonite transformation</td>
<td>Y</td>
</tr>
<tr>
<td>5.2.7 Alteration of accessory minerals</td>
<td>Y</td>
</tr>
<tr>
<td>5.2.8 Microbial activity</td>
<td>Y</td>
</tr>
<tr>
<td>5.2.9 Freezing and thawing</td>
<td>Y</td>
</tr>
<tr>
<td>5.2.10 Desiccation, formation of cracks</td>
<td>Y</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Processes related to the migration of radionuclides and other substances:</th>
<th>Features</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Radionuclide inventory</td>
</tr>
<tr>
<td>5.3.1 Aqueous solubility and speciation</td>
<td>Y</td>
</tr>
<tr>
<td>5.3.2 Precipitation and co-precipitation</td>
<td>Y</td>
</tr>
<tr>
<td>5.3.3 Sorption</td>
<td>Y</td>
</tr>
<tr>
<td>5.3.4 Diffusion</td>
<td>Y</td>
</tr>
<tr>
<td>5.3.5 Advection</td>
<td>Y</td>
</tr>
<tr>
<td>5.3.6 Colloid transport</td>
<td>Y</td>
</tr>
<tr>
<td>5.3.7 Gas transport</td>
<td>Y</td>
</tr>
</tbody>
</table>
Table 5-3. Possible couplings between FEPs within the buffer considered significant for the long-term performance of the disposal system. The numbers on the leading diagonal refer to the FEPs listed in Section 6.1.2. As an example of how to read this table, the blue coloured square means that “Montmorillonite transformation” [5.2.6] directly affects “Water uptake and swelling” [5.2.2].

|      | 5.2.1 |     | 5.2.2 |     | 5.2.3 |     | 5.2.4 |     | 5.2.5 |     | 5.2.6 |     | 5.2.7 |     | 5.2.8 |     | 5.2.9 |     | 5.2.10 |     | 5.3.1 |     | 5.3.2 |     | 5.3.3 |     | 5.3.4 |     | 5.3.5 |     | 5.3.6 |     | 5.3.7 |
|------|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|
| 5.2.1| X     |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |
| X    |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |
| X    |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |
| X    |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |
| X    |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |
| X    |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |
| X    |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |
| X    |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |
| X    |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |
| X    |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |
| X    |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |
| X    |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |
| X    |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |     |       |

157
Table 5-4. Interaction matrix for the buffer. FEPs in italics are addressed in other chapters. A short name for some of the FEPs is used in the table: IRF (Release of the labile fraction of the inventory).

<table>
<thead>
<tr>
<th>Canister</th>
<th>Heat transfer</th>
<th>Gas transport</th>
<th>Advection; Colloid transport; Diffusion; Heat transfer; IRF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sorption</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Bentonite</strong></td>
<td></td>
<td></td>
<td>Heat transfer; Heat transfer; Heat transfer</td>
</tr>
<tr>
<td><strong>Void spaces</strong></td>
<td></td>
<td></td>
<td>Exposure from radiation sources</td>
</tr>
<tr>
<td>Diffusion</td>
<td>Diffusion Sorption</td>
<td>Precipitation and co-precipitation</td>
<td>Pore water</td>
</tr>
<tr>
<td>Advection</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sorption, Diffusion</td>
<td>Water uptake and swelling</td>
<td></td>
<td>Supercontainer shell</td>
</tr>
<tr>
<td>Diffusion Sorption</td>
<td>Water uptake and swelling</td>
<td>Diffusion Sorption</td>
<td>Filling components</td>
</tr>
<tr>
<td>Mechanical erosion, Chemical erosion</td>
<td>Advection Water uptake and swelling</td>
<td></td>
<td>Geosphere</td>
</tr>
<tr>
<td>Inadvertent human intrusion</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>Surface environment</strong></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>External</td>
</tr>
</tbody>
</table>
5.2 System evolution FEPs

To achieve its long-term safety functions, the bentonite has to swell due to absorption of water. This and other processes (radiation, thermal, chemical, hydraulic and mechanical, and their couplings) will affect the evolution of the buffer. The behaviour of the buffer and the achievement of its safety functions will depend on the time and rate at which these processes occur. The couplings of these FEPs with other FEPs are also indicated, but the consequences of interactions or combinations of these are discussed in Posiva (2016b).

References

Posiva 2016b. Safety evaluation for a KBS-3H spent nuclear fuel repository at Olkiluoto – Performance Assessment. Eurajoki, Finland: Posiva Oy. POSIVA 2016-02 (in prep.).

<table>
<thead>
<tr>
<th>5.2.1 Heat transfer</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Type:</strong></td>
</tr>
<tr>
<td><strong>Class:</strong></td>
</tr>
<tr>
<td><strong>Alternative names:</strong></td>
</tr>
<tr>
<td><strong>Section in 2007-09:</strong></td>
</tr>
</tbody>
</table>

**General description:**
Radiogenic heat generation occurs within the spent nuclear fuel [3.2.2] and heat is transferred to the buffer through the canister [4.2.2].

The efficiency of heat transfer through the buffer is essential for the performance of the repository system, since it directly affects the temperature at the canister surface and in the buffer itself. Within the initially unsaturated buffer, heat will be transferred by conduction through the solid clay particles, and by convection through the water-filled pore spaces and voids and, to a lesser extent, by radiation through any remaining air-filled voids. Before complete saturation, conduction through, first water, and gradually bentonite gel, and then a completely saturated and expanded buffer that has filled all the gaps and voids in and around the supercontainer and distance blocks will transfer heat transfer in the water-filled gap between the supercontainer and the rock. The rate of heat transfer during saturation will thus depend on the time at which the buffer reaches complete saturation. Due to the very low permeability of the bentonite, the contribution to heat transfer from convection is minor (Ikonen & Raiko 2015).

In the thermal analysis for KBS-3H, the gaps between the supercontainer shell and rock (47 mm gap) and between the shell and the buffer (5.5 mm gap) are conservatively assumed to be air-filled (Ikonen & Raiko 2015, Section 2.5). There is a gap between the canister lid and the solid buffer blocks, which will result in axial swelling of the buffer during saturation. There is also a gap between the cylindrical wall of the canister and the buffer ring blocks, which is on average 5.1 mm (on the top 10.2 mm and on the bottom 0 mm). According to the geometry of the reference design of KBS-3H, the gap between the canister lid and the solid blocks is 8 mm (Posiva 2013a, Section 4.5.6). This gap will have a high heat transfer resistance due to the low emissivity of the copper
surface and the associated low radiant heat transfer, but the use of the artificial wetting will contribute to a relatively fast establishment of a direct contact between the canister and the buffer (in the time range of several months). Water uptake by bentonite and the development of swelling pressure [5.2.2] will serve to dissipate the decay heat, increase the thermal conductivity and eliminate the gaps and joints around and within the buffer, causing heat transfer to take place only by conduction through the water-saturated bentonite.

During the initial post-emplacement period (days), heat transfer through the buffer will be largely independent of its heat capacity. Instead, the thermal conductivity, \( \lambda \), of the different parts of the system will be the most important controlling parameter. Several laboratory measurements on the thermal conductivity of different bentonites have been made. They show that the thermal conductivity of compacted bentonites depends primarily on density, water saturation, and mineralogical composition, and that the water content, the hysteresis of wetting and drying, and the volumetric fractions of constituents also exert an influence also exert an influence (Tang et al. 2008). According to laboratory experiments (Börgesson et al. 1994), the thermal conductivity of water-saturated MX-80 bentonite at a density of 2000 kg/m\(^3\) is about 1.3 W/(m\(\cdot\)K), whereas, in normal atmospheric conditions, the conductivity is lower at around 0.75 W/(m\(\cdot\)K). In fully dry conditions, the conductivity can be as low as 0.3 W/(m\(\cdot\)K). In the thermal dimensioning report for a KBS-3H repository at Olkiluoto (Ikonen & Raiko 2015, Table 2), a value of 1.0 W/(m\(\cdot\)K) has been used, assuming that the buffer saturation is lowered in the buffer heat-up phase from the initial 0.8 down to 0.5−0.6. The thermal conductivity of the water-filled gaps is 0.6 W/(m\(\cdot\)K), whereas that of air-filled gaps is about 0.03 W/(m\(\cdot\)K) (Ikonen & Raiko 2015, Figure 13), and this applies also to the gaps on both sides of the supercontainer shell (Ikonen & Raiko 2015, Section 2.5). For the average 5.1 mm wide canister/buffer gap, the effective conductivity is 0.044 W/(m\(\cdot\)K), which takes into account the contribution from radiant heat transfer in addition to air conductivity (Ikonen & Raiko 2015, Equation 18). These thermal parameters also depend slightly on the temperature, but a larger effect is that the thermal properties of the buffer and the degree of saturation are coupled.

In KBS-3H, the temperature of the canister surface 5000 years after disposal will be about 20 °C, which is about 9 °C higher than the natural ambient temperature at repository depth. If the buffer saturates before the maximum temperature is reached (during the operational phase or in the early post-closure period), the gaps around the canister close due to bentonite swelling, causing a decrease of up to 12 °C in the maximum canister surface temperature as the heat is transferred more effectively through the buffer to the rock. For details see Ikonen & Raiko (2015, Figures 39 and 42).

There are three important periods for understanding heat transfer in the buffer. The first and most critical period is until the maximum temperature is reached, i.e. the first decade or two. The second is the time it takes to achieve full water saturation, which is estimated to be from tens of years to hundreds or a few thousands of years. After that, heat transfer takes place by conduction under well-defined conditions. The third occurs after a few thousand years when the radiogenic heat production and, thus, heat transfer through the buffer have been reduced to a few percent of their maximum values (Ikonen & Raiko 2015).
Overall, the rate of heat transfer through the buffer is influenced by the following features of the repository system.

− Temperature: temperature differences between the inner and outer surface of the buffer lead to heat transfer.
− Water content (through saturation rate): the saturation influences the bulk thermal conductivity of the buffer. Saturation rate is the major factor in altering the buffer thermal conductivity.
− Swelling pressure: Swelling of the buffer closes the gaps around the buffer and makes the effective thermal conductivity higher.
− Buffer geometry: the dimensions of the buffer influence heat transfer.
− Buffer composition: the mineral composition influences the bulk thermal conductivity of the buffer, although the difference in thermal conductivity of different bentonite types is likely to be a second-order effect.

Uncertainties in the understanding of the FEP:

Heat transfer from the canister via the buffer to the geosphere is, in principle, a simple process that can be described with basic laws of physics. Reliable data on the thermal properties of the engineered barrier materials used in **KBS-3H** are available (Ikonen & Raiko 2015, Table 2). Although the available thermal conductivity data do not uniformly cover the entire range of expected material conditions, the selected low values are conservative.

**Couplings to other FEPs:**

Heat transfer in the buffer is directly affected by the following FEPs:

− Heat transfer (in the canister) [4.2.2]
− Water uptake and swelling [5.2.2]
− Freezing and thawing [5.2.9]
− Heat transfer (in the geosphere) [10.2.1]

Heat transfer (because of temperature evolution) in the buffer directly affects the following FEPs:

− Water uptake and swelling [5.2.2]
− Montmorillonite transformation [5.2.6]
− Alteration of accessory minerals [5.2.7]
− Microbial activity [5.2.8]
− Freezing and thawing [5.2.9]
− Desiccation, formation of cracks [5.2.10]
− Aqueous solubility and speciation [5.3.1]
− Precipitation and co-precipitation [5.3.2]
− Sorption [5.3.3]
− Diffusion [5.3.4]
− Advection [5.3.5]
− Gas transport [5.3.7]
− Heat transfer (in the geosphere) [10.2.1]
5.2.2 Water uptake and swelling

**Type:** Process  
**Class:** System evolution

**Alternative names:**  
Water uptake; Swelling and mass distribution; Homogenisation

**Section in 2007-09:** 4.6.1

**General description:**

Bentonite is used as the buffer material because of its ability to swell when it absorbs water. Swelling in the confined space of the deposition drift will result in a swelling pressure that causes such a low hydraulic conductivity in the buffer that migration of radionuclides and other substances through it will only be able to occur by slow diffusion [5.3.4]. Swelling will also allow redistribution of buffer mass and help to diminish any possible differences in the density of the buffer component, (i.e. will lead to homogenization). Other consequences of swelling are that a high swelling pressure and density, associated with a low water content and a small pore size will be reached as is needed for filtering of colloids potentially formed within the canister [5.3.6] and preventing microbial activity [5.2.8]. To ensure the effectiveness of the buffer, therefore, an adequate swelling pressure should be maintained for a very long period. The process of swelling of buffer through the perforation holes of the supercontainer shell and the reaching of the required density and swelling pressure in the gap is still under study. The modelling of the process is challenging and there is a need to rely also on results from experimental studies.

The main mineral component in bentonite is montmorillonite (75–90 wt.%) and it is this mineral that gives bentonite its swelling properties. The degree of swelling is a function of the mineralogical characteristics of the montmorillonite, specifically:

- the osmotic pressure between the charged double layers at the external surfaces of the stacks of montmorillonite flakes;
- the stored elastic energy within compressed mineral grains; and
- the hydration of the interlamellar cations and surfaces of the montmorillonite mineral grains.
The first of these controls swelling pressure at low bulk densities, whereas the latter two control swelling pressures at high bulk densities, which are relevant to repository conditions. The degree of swelling is also a function of the groundwater composition (salinity), which controls the thickness of the charged double layer on the external surfaces of the montmorillonite flakes and, thus, the osmotic pressure.

The buffer will be emplaced in the KBS-3H deposition drift as shaped, compressed blocks or as rings around the canister. The canister, the ring blocks and two disk blocks on each side of the canister will be enclosed in a perforated titanium shell with end plates without perforations. All these components together form a structure called a supercontainer. Distance blocks located at both ends of the supercontainer form part of the buffer. The initial water content is around 11 % in ring blocks and 17 % in disk blocks inside the supercontainer and in distance blocks (Table 5-1) but, after emplacement, artificial watering (DAWE) will feed water that will begin to be taken up by the buffer due to suction by the bentonite. All components in the drift, such as the supercontainer and the distance blocks will be standing on feet. These facilitate the installation and prevent mechanical erosion of bentonite caused by water flowing along the floor.

Groundwater ingress into the KBS-3H drift is of importance as it finally saturates the buffer after the water fed by the DAWE system has been absorbed (the water introduced by DAWE is not enough for complete buffer saturation). The groundwater entering the deposition drift will transport solutes to the buffer and redistribute solutes in the buffer porewater, it can also dissolve accessory minerals in the bentonite [5.2.7], and possibly release bentonite in colloidal form [5.3.6]. These processes depend largely on the inflow rate and the chemistry of the groundwater entering into the deposition drift.

Water uptake will continue until the buffer has become fully saturated. Calculations show that the wetting time for the buffer depends strongly on the hydraulic conductivity of the rock surrounding the KBS-3H deposition drift/KBS-3V deposition hole (Pintado & Rautioaho 2012). If the hydraulic conductivity is relatively high (exceeding 10⁻¹² m/s), the buffer will become saturated within a few to some hundreds of years. It is considered that the bentonite behaviour will exert a primary control on the wetting time for deposition drifts with relatively high inflows, and that the hydraulic conductivity of the near-field rock will be the primary control on wetting times for deposition drifts with relatively low inflows (Hökmark 2004, Pintado & Rautioaho 2012). Model results indicate that the wetting time could extend from about 30 to 40 years up to hundreds of years or longer, depending on the hydraulic boundary conditions (Pintado & Rautioaho 2012).

After complete saturation, the final swelling pressure that will be achieved is dependent, in part, on the initial dry density and on factors such as the temperature and the salinity of the water being absorbed.

The hydraulic conductivity of the bentonite in its initial compressed state is a function of its density and degree of saturation, but also of the ambient temperature. The viscosity of water decreases as temperature increases, which means that the hydraulic conductivity increases with increasing temperature. Similarly, high ionic strength groundwaters limit the swelling capacity of the bentonite thus also limiting the degree to which hydraulic conductivity decreases during saturation. In the repository, temperatures in the buffer during the initial saturation period will be high (≤ 100 °C) due to radiogenic heat generation [3.2.2]. No changes in the salinity of inflowing groundwater are expected at the same time as the occurrence of the thermal peak.
Overall, fully-saturated bentonite swelling pressures increase with increasing dry density and decreasing salt concentration (Figure 5-4), although the effect of groundwater salinity is relatively small at the high densities found in the repository buffer and will not significantly affect its swelling pressure (see Figure 5-4).

The distribution of hydraulically active fractures in the near-field rock will, however, be heterogeneous and, consequently, the wetting process of the bentonite in the KBS-3H deposition drifts may be non-uniform and vary from one drift to another and in the same drift. This could cause a relatively uneven swelling of the bentonite and localised mechanical stresses on the canister, resulting in movement of the canister, though due to the use of the DAWE system, no major movements are expected.

Localised mass redistribution may occur in the buffer if it intrudes into fractures in the near-field rock. This effect will, however, be very limited due to the small aperture of the fractures and the shear resistance caused by the friction between the bentonite and the fracture surface. As no loss of the bentonite due to mechanical erosion is expected, the effect will be positive because it will result in sealing of the fracture.

The couplings between the forces that control bentonite swelling are complex and there is no general consensus concerning the detailed mechanisms responsible and the way they may be determined or calculated (Karnland & Birgersson 2006, Martikainen & Schatz 2011). In any case, it is clear that the main swelling mechanism is the hydration of the clay minerals and their expansion because of the presence of water (e.g. Pusch et al. 1990, Cases et al. 1992, Quirk 1994).

Overall, water uptake and swelling of the buffer is influenced by the following features of the repository system.

- Temperature: the rate of water uptake by the buffer during saturation will depend on this variable.
- Swelling pressure: affects the pore geometry and distribution, hence affecting also hydraulic conductivity and water uptake.
- Buffer geometry: influences the rate of water uptake and swelling.
- Water content: the evolving water content during saturation is a primary control on water uptake, and mass redistribution (and thus homogenisation).
- Buffer composition: the mineralogy of the buffer material affects pore geometry, final swelling pressure and hydraulic conductivity.
- Porewater composition: the ionic concentration of the porewater may affect the swelling capacity of the buffer.
Figure 5-4. Swelling pressure vs. dry density for a Na-bentonite (above) and for a Ca-bentonite (below). Diamonds are data from Martikainen & Schatz (2011), Kiviranta & Kumpulainen (2011) and Kumpulainen & Kiviranta (2011). Squares are data from Karnland & Birgesson (2006): CT stands for measurements of salinity (TDS) at Clay Technology and DI for deionized water.
**Uncertainties in the understanding of the FEP:**

Water uptake and swelling of the buffer under a temperature gradient is a complex process that is determined by many coupled sub-processes and influenced by parameters of the buffer and the near-field rock.

There is uncertainty in the fracture density distribution in the rock and the capacity of the fractures to maintain a constant water flow. These uncertainties are taken into account in selecting the data for the modelling of buffer performance.

**Couplings to other FEPs:**

Water uptake and swelling of the buffer is directly affected by the following FEPs:
- Heat transfer [5.2.1]
- Montmorillonite transformation [5.2.6]
- Alteration of accessory minerals [5.2.7]
- Freezing and thawing [5.2.9]
- Groundwater flow and advective transport (in the geosphere) [10.3.5]

Water uptake and swelling of the buffer directly affects the following FEPs:
- Deformation (of the canister) [4.2.3]
- Corrosion of the copper overpack [4.2.5]
- Stress corrosion cracking (of the canister) [4.2.7]
- Heat transfer [5.2.1]
- Montmorillonite transformation [5.2.6]
- Alteration of accessory minerals [5.2.7]
- Microbial activity [5.2.8]
- Freezing and thawing [5.2.9]
- Diffusion [5.3.4]
- Advection [5.3.5]
- Colloid transport [5.3.6]
- Gas transport [5.3.7]
- Corrosion (of the supercontainer shell) [6.2.2]
- Deformation (of the supercontainer shell) [6.2.2]
- Stress redistribution (in the geosphere) [10.2.2]
- Rock mass damage (in the geosphere) [10.2.4]

**References:**


5.2.3 Mechanical erosion

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
<tr>
<td>Alternative names:</td>
<td></td>
</tr>
<tr>
<td>Piping and erosion</td>
<td></td>
</tr>
</tbody>
</table>

**General description:**

Piping flow in channels is observed in the laboratory in systems containing compacted non-saturated bentonite when inflow comes from a point-like source into an available, macroscopic void volume (Börgesson et al. 2005, Sandén & Börgesson 2010, Sane et al. 2013, Pintado et al. 2013). Piping flow develops when swelling of the bentonite starts due to inflow from a single source (piping flow) that creates a channel in the bentonite that the swelling is not sufficient to seal. The observed limiting conditions for the piping flow to persist are a pressure head in the order of 100 kPa and a flow rate in the order of $10^4$ L/min. If either the flow rate or the pressure head is below these limits, the swelling of bentonite blocks has been observed to seal the piping flow (Sandén & Börgesson 2010). The process of sealing is complex and stochastic, and thus the limits for sealing cannot be given accurately. Therefore, piping flow and related mechanical erosion is expected while a flow path from a groundwater inflow location (at 4 MPa) to an (air-filled) cavity at atmospheric pressure is available.

In the case of natural water filling of a KBS-3H deposition drift, the process of groundwater inflow from a fracture intersecting the drift, and the consequent piping and erosion, is not expected to be drastically different from that of KBS-3V buffer in a deposition hole despite the differences identified. These are, first, that the gap between the rock and the supercontainer is not filled with pellets; but laboratory tests of the 3V buffer concept with initially empty gaps between blocks and deposition hole walls show similar erosion to those where the gaps are filled with pellets (Pintado et al. 2013). Second, that piping flow in a horizontal drift is expected to occur in the horizontal direction; but erosion tests to compare the effect of direction have been done to a limited degree (Posiva 2013a), with the results showing no major difference. Third, the geometry and volumes are different; in the 3H design, due to efficient plug sealing, the
eroding mass is assumed to remain in the drift and the piping channels end within the drift whereas in the 3V case eroding mass can be transported from the deposition hole to potential empty spaces in the deposition tunnel.

Finally, a minor difference is due to the KBS-3H supercontainer shell hindering the buffer block swelling to some degree, although the buffer will swell through the perforation holes and eventually fill the gap between the shell and rock. This effect is not well quantified, but not expected to be drastic due to the expected overall tightness of the drift or compartment. Therefore, similar erosion rates could be expected in both the KBS-3V and 3H designs. Posiva has estimated piping erosion through a 3V deposition hole to be no more than 0.1 - 1 grammes of clay carried by 1 litre of discharging groundwater for each metre of piping channel the groundwater traverses (Pintado et al. 2013).

Piping flow and erosion will stop once the flow path from a groundwater inflow location (at 4 MPa) to an (air-filled) cavity at atmospheric pressure is no longer available, i.e. the accessible void volume is filled. At this stage, porewater in the bentonite components near inflow locations reaches pressure parity with the surrounding groundwater and imparts a backpressure to the intersecting fractures and inflow rates are significantly reduced. In the assumed evolution of the KBS-3H drift this occurs when the supercontainer shell-rock gap is filled with water and swelling bentonite, effectively sealing the drift to further inflow. Therefore, in a KBS-3H drift, with artificial water filling, piping and related erosion is considered to be virtually non-existent, because the stopping criterion for piping flow is met upon installation of the drift plug and water filling of the gap.

In KBS-3H, the fast initial wetting may cause some initial mechanical erosion, the extent of which has not been directly tested. As the wetting is designed to be performed fast enough that the supercontainer shell/drift wall gap might not have time to fill with bentonite in the short term, the flow during artificial watering will take place through the entire gap and not in piping channels. If artificial watering flow causes some mechanical erosion (or other disruption), the process is expected to be different from piping erosion and therefore piping erosion tests cannot be used to estimate the amount.

The bentonite material that initially swells out of the perforation holes in the KBS-3H supercontainer shell will presumably be of relatively low density and potentially prone to detachment, particularly at the bottom of the supercontainer, during drift filling. Bentonite that is detached from the periphery of the buffer blocks during artificial watering may be drawn along the drift floor towards the drift mouth due to the 2% downwards tilt in the drift. The overall amount of bentonite that can detach during the 8 hours of artificial watering is not known, but is expected to be low.

Aggregation and sedimentation of entrained bentonite will hinder the ability of the artificial water to transport any material along the KBS-3H drift. The flow velocity during the artificial watering is low compared with that in piping channels, due to the flow having the entire supercontainer-rock gap to go through. Therefore, the overall ability of the artificial water flow to carry entrained solids is expected to be limited, and bentonite lost from the buffer during the artificial watering is expected to predominantly fall to the bottom of the drift, and not to move along the drift.
Uncertainties in the understanding of the FEP:

Mechanical erosion is a complicated coupled process that is highly dependent on the hydraulic behaviour of the rock, and especially of the drift-intersecting fractures connected to the central tunnels, and the properties of the bentonite. The specific dependencies of the rate of erosion on features of the repository system such as flow rate, salinity, initial water content and initial dry density are further specified in the Performance Assessment report for KBS-3H (Posiva 2016b).

Couplings to other FEPs:

Mechanical erosion in the buffer is directly affected by the following FEPs:
- Water uptake and swelling [5.2.2]
- Advection [5.3.5]
- Groundwater flow and advective transport (in the geosphere) [10.3.5]

Mechanical erosion in the buffer directly affects the following FEPs:
- Water uptake and swelling [5.2.2]
- Diffusion [5.3.4]
- Advection [5.3.5]
- Colloid transport [5.3.6]
- Gas transport [5.3.7]
- Erosion and sedimentation in fractures (in the geosphere) [10.2.6]
- Colloid transport (in the geosphere) [10.3.6]

References:


Posiva 2016b. Safety evaluation for a KBS-3H spent nuclear fuel repository at Olkiluoto – Performance Assessment. Eurajoki, Finland: Posiva Oy. POSIVA 2016-02 (in prep.).


### 5.2.4 Chemical erosion

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th>Process</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Class:</strong></td>
<td>System evolution</td>
</tr>
<tr>
<td><strong>Alternative names:</strong></td>
<td>Colloid release/erosion</td>
</tr>
<tr>
<td><strong>Section in 2007-09:</strong></td>
<td>4.7.3</td>
</tr>
</tbody>
</table>

**General description:**

The emplacement of compacted bentonite blocks as buffer material surrounding copper canisters containing spent fuel assemblies will be a central feature of the repository at Olkiluoto in either the KBS-3V reference design or the KBS-3H alternative design concept. Bentonites consist primarily of the clay mineral montmorillonite, which lends to the materials their substantial swelling ability when in contact with aqueous solutions. Although bentonites can absorb water and swell to several times their original size, in KBS-3 type repositories the volumes of the deposition holes (-3V) and drifts (-3H) are fixed and the bentonite masses balanced, which leads to the development of suitable swelling pressures. However, the possibility of hydraulically active fractures intersecting deposition holes or drifts implies that volume-constrained conditions may not be ubiquitous and such features may provide pathways for the continued, localized quasi-free swelling of bentonite buffer until an equilibrium or, in the case of erosion, a steady-state is reached. The loss of buffer material due to interaction with dilute groundwater through intersecting, transmissive fractures is referred to as chemical erosion due to its strong dependence on groundwater chemistry (particularly ionic strength).

It is well established experimentally that, given access to free volumes, buffer clay material will swell into such spaces and, if sufficiently low ionic strength conditions are encountered, form a colloidal sol which can be easily transported away in flowing groundwater (Birgersson et al. 2009, Schatz et al. 2013). These studies also indicated that an erosion stability limit of between 4 to 8 mM cation charge equivalents could be identified. Loss of buffer mass by erosion will naturally lead to a reduction in buffer density. If sufficiently extensive, such mass loss could result in advective transport being established in an eroded buffer zone between the canister and the surrounding bedrock. Advective conditions adjacent to the canister would give rise to increased transfer of corrosive agents to the canister surface. If the canister subsequently failed, the degraded buffer would have a reduced radionuclide retention capacity and eroding buffer material could itself serve as a source of colloidal material mediating radionuclide transport.

Recent safety assessments of a KBS-3V repository by Posiva and SKB (Posiva 2012a, SKB 2011) considered the possibility of chemical erosion of the buffer and backfill occurring due to dilute groundwater penetrating to repository depth in association with glacial retreat. In these analyses, mass loss due to chemical erosion was, experimentally and theoretically, largely confined to consideration of interaction with horizontal fractures. In fact, the model used to estimate erosion rates was explicitly defined in terms of a single, parallel-walled fracture intersecting a deposition hole with its plane normal to the deposition hole axis.

By contrast, in a KBS-3H repository it is expected that the deposition drifts will be most frequently intersected by fractures with inclinations from 30° to 60° (Smith et al. 2015). The effect of gravity on buffer erosion has not been fully explored and the model used to estimate erosion rates in the safety assessments mentioned above does not take...
such effects into account. The KBS-3H repository design is potentially more sensitive to chemical erosion, in that if buffer loss through one intersecting fracture is substantial enough, it could lead to multiple canister positions being put at risk along the drift. This scenario has been termed the “domino effect.”

In artificial fracture tests conducted at steep slope angles (≥ 45°), clay mass appears to be lost from the extruded source material via a predominantly sedimentary process (Schatz & Akhanoba 2016). This behaviour is in sharp contrast to that observed in horizontal fractures where the mass release is interpreted as being dispersive in nature (Schatz et al. 2013). Moreover, average mass loss rates in the sloping fractures were always larger than those in the corresponding horizontal cases with larger slope angles generally resulting in increased mass loss rates. Additional, limited evidence is available showing increased mass loss rates over horizontal fractures even at much shallower slope angles (3–15°) (Jansson 2009, Vilks & Miller 2010).

Detachment of mass and sedimentation of the mass loss was observed in sloped fractures under stagnant (no flow) as well as flow-through conditions (Schatz & Akhanoba 2015). An increase in flow velocity down the fracture from zero (stagnant) to ~10^{-6} m/s produced a three-fold increase in mass loss, whereas a further increase in flow velocity by roughly two orders of magnitude yielded only a 15% additional increase in mass loss. In contrast, a similar two order of magnitude flow velocity increase in a horizontal fracture system resulted in an 80% increase in mass loss. Lastly, similar to earlier observations in horizontal fractures, a clear erosion stability limit at an electrolyte concentration of no less than 0.5 g/L NaCl could be identified in the sloped fracture environments (Schatz & Akhanoba 2016).

Sloped fracture tests also show that average erosion rates for purified montmorillonites and as-received bentonites are comparable [ibid]. Such results differ substantially from those observed in horizontal fracture tests and provide further evidence that gravity strongly influences mass loss in sloped fracture environments (Schatz & Akhanoba 2016). Given that there is no suitable model of erosion available to explain the experimental observations outlined above, erosion data from artificial fracture tests can be applied to determine bounding estimates of buffer mass loss during presumed periods of exposure to sufficiently dilute groundwater in sloped fractures intersecting KBS-3H deposition drifts. Potential process mitigating factors to chemical erosion such as surface roughness and fracture clogging may also need to be taken into account for safety assessment purposes as well as the role of the accessory minerals (detritus) in the clogging of fractures.

Overall, chemical erosion is influenced by the following features of the repository system.

- **Swelling pressure**: this is a primary parameter that will control chemical erosion.
- **Buffer geometry**: influences chemical erosion with respect to the position of water-conductive fractures intersecting the KBS-3H deposition drift.
- **Water content**: the initial water content in the bentonite controls the rate of swelling and also the forces attaching bentonite particles to the buffer.
- **Groundwater pressure and volumetric flow rate**: affect the detachment rate of bentonite particles at the buffer/groundwater interface.
- **Buffer composition**: affects pore geometry, swelling pressure and hydraulic conductivity.
- **Porewater and groundwater composition**: in terms of cation content affects the generation and stability of bentonite colloids.
**Uncertainties in the understanding of the FEP:**

Chemical erosion of the buffer in an intersecting, transmissive fracture environment carrying dilute groundwater is a highly complex, coupled transport process involving buffer material evolution, groundwater composition evolution, and bedrock hydrogeology and, as such, uncertainties remain that can, however, be bounded by appropriate design and material selection.

There is a possibility that, due to erosion, accessory mineral particles in buffer will build up and form a ‘filter cake’ limiting further loss of buffer mass. Experimental results indicate that mass loss can slow down or possibly stop due to filtration effects (Birgersson et al. 2009, Richards & Neretnieks 2010).

Uncertainties also relate to the understanding of the nature and effectiveness of the process due to the fact that the experimental information available relates to very simplified systems. In the natural environment, a more complex system will be present. Current understanding from natural smectite occurrences would suggest that montmorillonite could be stable in dilute environments (< 4mM) (e.g. Gehör et al. 1997). However, the mechanisms affecting this are not fully understood.

**Couplings to other FEPs:**

Chemical erosion in the buffer is directly affected by the following FEPs:
- Water uptake and swelling [5.2.2]
- Advection [5.3.5]
- Groundwater flow and advective transport (in the geosphere) [10.3.5]

Chemical erosion in the buffer directly affects the following FEPs:
- Water uptake and swelling [5.2.2]
- Diffusion [5.3.4]
- Advection [5.3.5]
- Colloid transport [5.3.6]
- Gas transport [5.3.7]
- Erosion and sedimentation in fractures (in the geosphere) [10.2.6]
- Colloid transport (in the geosphere) [10.3.6]

**References:**


## 5.2.5 Radiolysis of porewater

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Alternative names:</th>
<th>Section in 2007-09:</th>
</tr>
</thead>
<tbody>
<tr>
<td>None</td>
<td>4.3</td>
</tr>
</tbody>
</table>

### General description:

Radiolysis can potentially occur anywhere in the repository system where water is exposed to radiation. Radiolysis is, however, of most concern within the canister [3.2.5], where dose rates are highest.

Radiolysis of porewater in the buffer may affect corrosion of the copper overpack of the canister [4.2.5] but its significance is very strongly dependent on the dose and dose rate within the buffer.

For as long as the canister remains intact, alpha and beta radiations are shielded by the canister’s internal structures and only gamma radiation and neutrons can penetrate through the walls of the canister and cause radiolysis of the bentonite porewater. The gamma and neutron dose rates at the outer canister surface have been estimated based on the different fuel characteristics and canister designs (Ranta-aho 2008). These estimates have shown that the neutron contribution to the dose is less than 20% of the total dose (Anttila 2005, p. 17). The resulting dose rates are well below the dose rate limit of 1 Gy/h set as a design criterion for the canister and are mostly due to gamma radiation (Raiko 2013).

The gamma dose rate outside the canister will rapidly decrease with time due to radioactive decay of the spent nuclear fuel and become insignificant within the first 1000 years following emplacement, after which radiolysis of the bentonite porewater will become negligible.

Radiolysis of the bentonite porewater may lead to the formation of stable molecular species, such as O$_2$, H$_2$O$_2$ and H$_2$ although this has been shown to be a threshold process depending on the type of radiation, the dose rate, water content and composition [3.2.5].
The composition of the buffer porewater is important for controlling the accumulation of reactive radiolysis products that could potentially corrode the canister. For example, Fe\(^{2+}\) in the buffer porewater is an effective scavenger for oxidising species:

\[
\begin{align*}
&\text{Fe}^{2+} + \text{OH}^{-} \rightarrow \text{Fe}^{3+} + \text{OH}^- \\
&\text{Fe}^{2+} + \text{H}_2\text{O}_2 \rightarrow \text{Fe}^{3+} + \text{OH}^- + \text{OH} \\\n&\text{Fe}^{3+} + \text{H}_2\text{O}_2 \rightarrow \text{Fe}^{2+} + \text{HO}_2 + \text{H}^+
\end{align*}
\]

Other important scavenging species that may alter the concentration of radiolytic products are Cl\(^{-}\) and HCO\(_3\)\(^{-}\) present in the buffer porewater in equilibrium with groundwater. If air is present in the buffer porewater (e.g. before complete hydraulic resaturation), nitrogen oxides and possibly nitric acid will be produced by radiolysis of aerated water/vapour. The very limited extent of formation of nitric acid possible due to the low dose rate will, however, mean that it will have a negligible effect on copper corrosion.

The consequence of the radiolysis of bentonite porewater for corrosion of the canister by the accumulation of reactive radiolysis products has been modelled (Christensen & Bjergbakke 1982) taking into account the presence of 5 ppm Fe\(^{2+}\), which is consistent with calculated iron concentrations in the buffer porewater during repository evolution (Wersin et al. 2014). The radiolytic modelling results show that at the expected dose rates there is net water decomposition by water radiolysis with formation of O\(_2\), H\(_2\)O\(_2\) and H\(_2\). The hydrogen production rate decreases over time and stabilises after about 1000 years (Christensen & Bjergbakke 1982, Figure 4). A literature review (King et al. 2012) of copper corrosion under the effect of radiation concluded that there is no enhanced rate of copper corrosion under the expected dose rates and repository conditions [4.2.5]. Pusch et al. (1992) exposed MX-80 bentonite to gamma radiation at high (130 °C) temperature and observed alteration of accessory minerals and a slight cementation. However, the conditions in this experiment are very far from those expected in the repository, in particular the gamma dose rates exceed those expected at the surface of the canister by 3 orders of magnitude.

In the case of early canister failure, radionuclides that migrate from the canister into the buffer could cause higher rates of radiolysis of porewater by alpha and beta radiation as well as enhanced rates of O\(_2\) and H\(_2\)O\(_2\) formation (due to higher radiolytic yields). It is expected that these radiolysis products would be reduced by rapid reaction with the accessory minerals in the buffer or react with the internal structures of the canister, and would not result in any significant change to the composition (redox conditions) in the buffer porewater. Enhanced corrosion of the canister in this scenario would not be an issue because the canister has already failed.

There are no KBS-3H-specific considerations related to the radiolysis of buffer porewater (Gribi et al. 2007, Section 4.3). For the buffer in the supercontainer, the situation is basically identical to that in KBS-3V buffer, and for the distance blocks, the process is even less important due to the greater distance from the canister.

Overall, radiolysis of the buffer porewater is influenced by the following features of the repository system.

- Radionuclide inventory: this is the primary control on the type of radiation affecting the buffer porewater and the dose rate.
- Water content: controls the absorbed dose in the buffer porewater.
- Buffer composition: controls the reactions involving radiolytic species that occur.
- Porewater composition: controls the radiation chemistry and the formation of radiolytic species.
**Uncertainties in the understanding of the FEP:**
The radiolysis of water is well understood and there are no uncertainties regarding the understanding of the processes at the low dose rates expected at the surface of the canister.

**Couplings to other FEPs:**
Radiolysis of the buffer porewater is directly affected by the following FEPs:
- Radioactive decay (and in-growth) [3.2.1]
- Radiation attenuation (in the canister) [4.2.1]
- Water uptake and swelling [5.2.2]

Radiolysis of the buffer porewater directly affects the following FEPs:
- Corrosion of the copper overpack [4.2.5]
- Aqueous solubility and speciation [5.3.1]
- Gas transport [5.3.7]
- Corrosion (of the supercontainer shell) [6.2.1]

**References:**
5.2.6 Montmorillonite transformation

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:**
Mineral (montmorillonite) transformation

**Section in 2007-09:**
4.7.1

**General description:**
The main mineral component in bentonite is montmorillonite (> 75 wt.%) and it is this mineral that provides bentonite with its swelling properties [5.2.2]. Montmorillonite can be altered by a number of different reactions and transformations and, in most cases, the altered mineral form has a much reduced swelling capability compared with the unaltered montmorillonite. Thus, montmorillonite reactions and transformations, if they occurred in the repository, could compromise the safety functions of the buffer. These reactions and transformations can be divided into:

- Cation-exchange reactions,
- protonation-deprotonation of mineral surfaces,
- alterations to the structural composition and layer charge,
- cementation, and
- reactions with other repository materials (e.g. titanium, cementitious leachates).

The nature of the exchangeable cations (proportions of mono- and divalent cations) may affect the swelling pressure and hydraulic conductivity of the buffer. Cation exchange from a sodium bentonite to a calcium bentonite may thus cause degradation of the buffer, but this effect is insignificant at buffer densities greater than 1500 kg/m³ (Karnland & Birgersson 2006). Under acidic (pH<4) and alkaline conditions (pH>10), montmorillonite becomes thermodynamically unstable and dissolution occurs. This dissolution is proton-promoted at low pH and OH-promoted at high pH.

Alterations to the structural composition (i.e. changes in the interlayer cations) and increase in layer charge often precede the actual mineral transformation, but they do not necessarily compromise the buffer performance because their effect on swelling pressure, hydraulic conductivity and thermal stability is usually minor. The (irreversible) mineral transformation reactions pose the greatest risk to the safety functions of the buffer and are generally coupled with cementation effects. In general, these montmorillonite transformations in the buffer are most significant during the immediate post-emplacement period and for the first 1000 years when repository temperatures are at their maximum (Pastina & Hellä 2006).

**Cation-exchange reactions**
The main cation-exchange reactions (based on sodium bentonite MX-80) are:

\[
\text{NaX} + \text{K}^+ \leftrightarrow \text{KX} + \text{Na}^+
\]

\[
2\text{NaX} + \text{Ca}^{2+} \leftrightarrow \text{CaX}_2 + 2\text{Na}^+
\]

\[
2\text{NaX} + \text{Mg}^{2+} \leftrightarrow \text{MgX}_2 + 2\text{Na}^+
\]

The control exerted by this process on the calcium and magnesium concentrations in the porewater also directly affects the dissolution-precipitation of accessory Mg and Ca minerals in the buffer [5.2.7].
Protonation-deprotonation of mineral surfaces
This process contributes to the pH buffering capacity of the bentonite according to the following reactions on the smectite edge surfaces (≡S):

≡SOH + H⁺ ↔ ≡SOH⁺
≡SOH ↔ ≡SO⁻ + H⁺

Surface complexation reactions influence the chemistry of the bentonite porewater, especially at high bentonite/water ratios (Bradbury & Baeyens 2002).

Alterations to the structural composition and layer charge
The ideal tetrahedral layer structure of montmorillonite contains only silicon as the central cation, and the octahedral layer contains aluminium with some magnesium substituting the aluminium (Figure 5-5). Substitution of aluminium for silicon in the tetrahedral layer results in an increase in the tetrahedral layer charge, which is balanced by interlayer cations. The net negative layer charge of montmorillonites varies from 0.4 to 1.2 per O₂₀(OH)₄.

Several investigations at the Äspö HRL in the LOT and Alternative Buffer Materials projects have observed a slight increase in the cation exchange capacity (CEC) of bentonites in sample profiles with increasing temperature (Karnland et al. 2009; Muurinen 2010, p. 32, Appendix B). These observations may be the result of structural changes in montmorillonite (e.g. beidellitisation) but this remains to be established. Beidellites are swelling dioctahedral smectites like montmorillonites, but due to aluminium substitutions in the tetrahedral layer they tend to have higher net negative charges than montmorillonites. An increase in the layer charge is often found to be a precursor process for illitisation. In the absence of potassium, an increase in the layer charge, above a critical limit, which depends on the interlayer cation, may result in the collapse of the montmorillonite structure and fixation of interlayer cations to form non-swelling, paragonite-type minerals (Karnland & Birgersson 2006). These minerals are, however, much less commonly found in natural sediments than are illites.

![Figure 5-5. The mineralogical structure of montmorillonite.](image)
Mineral transformations

Illitisation: illite has a crystalline structure that is similar to that of montmorillonite but with a higher layer charge (1.2 to 1.8 per O$_2$(OH)$_4$) due to partial replacement of tetrahedral silicon by aluminium. The interlamellar space of illite is collapsed due to replacement of the hydrated cations by non-hydrated potassium, which makes illite a non-swelling mineral. Illite is a common transformation product of smectite and is frequently found interstratified with smectite layers, and potentially could occur in the buffer at temperatures > 100 °C (Wersin et al. 2007). Illitisation is a well-known process that has been observed in many different geological environments (Laine & Karttunen 2010, p. 65-109) and has been reproduced in laboratory conditions. During illitisation, silica is released, which may precipitate and induce cementation:

\[
\text{Ca}^{2+}/\text{Na}^+\text{-montmorillonite} + \text{K}^+ + (\text{Al}^{3+}) \rightarrow \text{Illite} + \text{Silica} + \text{Ca}^{2+}/\text{Na}^+
\]

The transformation is kinetically controlled and dependent mainly on temperature and the availability of potassium in the porewater, but is also influenced by the pressure, smectite composition and layer charge, and the porewater aluminium and silica concentrations. Various models of smectite-to-illite transformation have been developed (e.g. Huang et al. 1993, Cuadros & Linares 1996) and a kinetic model (Huang et al. 1993) is considered as the most generally applicable. This model has been used to calculate the amount of illitisation that might occur under the thermal (T < 50 °C after 1000 years) and geochemical conditions ([K$^+$] < 1 mM) expected for a KBS-3 repository at Olkiluoto and this showed the process will be insignificant (Karnland & Birgersson 2006).

Chloritisation: chlorite has the same basic 2:1 structure as montmorillonite but the octahedral Al concentration relative to Mg and Fe is often low. The layer charge is higher than in montmorillonite and balanced by positively charged octahedrally coordinated hydroxide sheets of Mg, Fe$_2^{2+}$, Fe$_3^{3+}$ and Al instead of exchangeable cations as in montmorillonite. Iron is a common constituent of many chlorites and, thus, chloritisation may be relevant in the repository where montmorillonite–iron interactions are thermodynamically possible (Karnland & Birgersson 2006). There is some early reported work on the formation of hydroxyl interlayers (chloritisation) in smectites at low temperatures (Rich 1968, Carstea 1968, Carstea et al. 1970), but generally under oxic conditions. The kinetic rates for the process are, however, very low and only significant at high pH and temperatures > 200 °C, which is considerably in excess of the maximum temperature that is expected to occur at the surface of the canister [4.2.2] (Wersin et al. 2008).

Kaolinitisation and pyrophyllitisation: kaolinite and pyrophyllite are non-swelling clays that may form from montmorillonite in the absence of potassium at temperatures greater than 200 °C and in the presence of brines with salinities in excess of those found in Olkiluoto groundwaters. These processes are not, therefore, considered to be relevant for the repository (Laine & Karttunen 2010, p. 35).

Cementation

Montmorillonite dissolution and transformation reactions may cause the release of tetrahedral silica from the mineral structure. The temperature gradient that forms across the buffer during the thermal peak [5.2.1] may then induce a silica concentration gradient within the buffer. The silica released from the montmorillonite may then be transported towards the outer part of the buffer where it can precipitate due to the lower temperature.
Precipitated silica will form in the pore spaces and cement together the bentonite grains, causing a loss of plasticity that may compromise the integrity of the buffer. Observations from the Swedish Kinnekulle natural analogue study support this mechanism (Pusch et al. 1998), but the extent of the dissolution-precipitation processes that might take place under repository conditions is estimated to be small (Arthur & Zhou 2005).

Besides silica, other precipitates (iron oxides, carbonates, sulphates etc.) may cause cementation of the buffer but these reactions are generally not coupled with montmorillonite transformations and tend to be localised (e.g. adjacent to the canister or rock depending on the temperature gradient) and rather short-lived (e.g. related to the immediate post-emplacement period). Therefore, their significance for buffer performance is less than that of cementation by silica precipitation.

Reactions with other materials

Reaction with alkaline leachates from cement degradation: the hyperalkaline leachates from cement degradation [9.2.8] may cause dissolution of montmorillonite when the tetrahedral silica in the montmorillonite structure becomes available for dissociation reactions. At neutral pH, the solubility of silica is negligibly low, but starts to become significant above pH 9 and is 16 times higher at pH 11 than under neutral conditions (Karnland & Birgersson 2006). Leachates from degradation of cementitious materials such as plugs and seals [9.2.8] may dissolve montmorillonite and liberate silica, which would precipitate and induce cementation. This would lead to a decrease in the swelling pressure and an increase in the hydraulic conductivity (Posiva 2009, p. 356). It should be noted that no cement plugs will be located in the KBS-3H deposition drifts, so this process is less relevant for the buffer in 3H than in 3V, where the deposition tunnel plugs are made of concrete and are located rather close to the buffer of the first deposition holes in a tunnel.

Reaction with iron materials and iron corrosion products: Corrosion of iron components, such as the iron insert, will lead to the release of hydrogen and Fe(II), and the formation of iron corrosion products (e.g. magnetite). The solubility of corrosion products is low and in a similar range as the iron concentration in the groundwater in contact with the buffer. However, Fe released by corrosion can also react with the clay contacting the steel component. Under the expected conditions the amount of iron components in contact with the buffer during repository lifetime is small to negligible.”

Over a long period, interaction of iron with the clay could transform montmorillonite into a non-swelling clay mineral (e.g. serpentine minerals such as berthierine) or induce cementation via precipitation of secondary iron minerals or silica liberated from montmorillonite transformation. In each case, the result would be a reduction in the swelling pressure and chemical stability of the buffer. Experimental studies performed at room temperatures show no clear evidence of montmorillonite transformation into non-swelling minerals, but they do indicate iron incorporation into the montmorillonite structure, an increase in CEC and a decrease in swelling pressure (Kumpulainen et al. 2010, p. 63-64). There are also experiments showing transformation of montmorillonite into non-swelling minerals, mostly at higher temperatures (above 200 °C) but also at lower temperatures down to 80 °C (e.g. as summarised in Wersin & Snellman 2008). There are uncertainties in the thermodynamic data for these newly formed phases and in the transformation kinetics.
Reaction with titanium (Ti) from the KBS-3H supercontainer shell and titanium corrosion products: natural bentonites contain Ti, either as small TiO$_2$ particles or incorporated in the clay structure (Wersin et al. 2011, Posiva 2013a). Differences in Ti concentration or speciation do not appear to affect the bulk properties of natural bentonites, as indicated from the study of Karnland et al. (2006). The corrosion rate of the Ti shell is expected to be very low. Preliminary data on Ti-clay interaction suggest that Ti released from corrosion is transferred to the clay (Wersin et al. 2011, Posiva 2013a). A more detailed study was performed in 2011–2015 on the identification of the nature of the Ti species transferred to the clay from a corroding metal source (Wersin et al. 2015). The recently completed studies show that the Ti corrosion rate is low (nm/year) and the Ti released by corrosion reacts with the clay leading to the incorporation of the Ti metal in a neo-formed clay-like structure. Thus, the Ti released by corrosion is immobilised. The combination of these two phenomena results in an effective restriction of the diffusion of Ti through the clay and the process is expected to be “interfacial” and affect only a thin buffer layer. Overall, montmorillonite transformation processes are influenced by the following features of the repository system.

- Temperature: controls the rate of the reactions that induce the transformations and temperature gradients can lead to migration and precipitation of solutes.
- Swelling pressure: influences the availability of chemical components that may react with the bentonite.
- Water content: any reactions would occur at the mineral-water interface and no reactions are expected under dry conditions.
- Buffer composition: the mineralogy and bulk composition of the buffer is significant for all chemical reactions in the buffer.
- Porewater composition: is a significant control for all chemical reactions in the buffer.
- Gas composition: if gas is present, it will be significant for some chemical reactions.

Uncertainties in the understanding of the FEP:

Transformation rates of montmorillonite under repository conditions will be very slow. This holds despite the fact that the exact effective reaction rates are still not well known due to uncertainties in the thermodynamic properties of smectites. The composition of the bentonite porewater and the near-field groundwater will vary during the evolution of the repository (especially in respect of salinity and abundance of exchangeable cations such as Ca and Na). The effects of these variations have been studied in a recent work on bentonite porewater chemistry, which has led to an improved geochemical database and updated radionuclide solubility limits (Wersin et al. 2014).

Couplings to other FEPs:

Montmorillonite transformation is directly affected by the following FEPs:

- Heat transfer [5.2.1]
- Water uptake and swelling [5.2.2]
- Alteration of accessory minerals [5.2.7]
- Corrosion (of the supercontainer shell) [6.2.1]
- Chemical degradation of cement [9.2.8]
- Rock-water interaction [10.2.7]
Montmorillonite transformation directly affects the following FEPs:
- Water uptake and swelling [5.2.2]
- Alteration of accessory minerals [5.2.7]
- Aqueous solubility and speciation [5.3.1]
- Precipitation and co-precipitation [5.3.2]
- Sorption [5.3.3]
- Diffusion [5.3.4]
- Advection [5.3.5]
- Colloid transport [5.3.6]
- Gas transport [5.3.7]

References:


5.2.7 Alteration of accessory minerals

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:**
Alterations of impurities

**Section in 2007-09:**
4.7

**General description:**

The bentonite material used for the buffer will predominantly contain montmorillonite (e.g. 75–90 wt.% in MX-80) but also a range of accessory minerals including feldspars, quartz, cristobalite, gypsum, calcite, dolomite, siderite and pyrite, Fe(III)(hydr)oxides as well as minor amounts of organic impurities. The type and amount of accessory minerals vary quite substantially between the different commercial bentonite products, principally depending on the mining site and its geological environment (Kumpulainen & Kiviranta 2010).

The swelling pressure of the buffer required for long-term performance is governed by the abundance of montmorillonite [5.2.2]. This mineral has a low solubility under the conditions expected in the repository near field [5.2.6] and, consequently, the bentonite porewater composition is largely controlled by the assemblage of more soluble accessory minerals, together with the exchangeable cation reactions of the clay and the interactions with the surrounding groundwater. The composition of the porewater and the temperature determines the alteration of accessory minerals. Figure 5-6 gives a schematic illustration of the geochemical equilibrium processes considered most important in bentonite. The reactions between the porewater with the accessory minerals can be:

- fast, as in the case of precipitation/dissolution of carbonates and sulphates; or
- slow, kinetically controlled chemical reactions, as in the case of aluminosilicate dissolution.

![Figure 5-6. Schematic illustration of geochemical equilibrium processes in bentonite. The montmorillonite layer and interlayer sites are seen on the left, the mineral equilibria on the right and the entrapped gases at the top. From Luukkonen (2004).](image)
Some reactions, such as primary silicate dissolution, are irreversible under repository conditions. In general, accessory mineral transformations in the buffer are most significant during the immediate post-emplacement period and for the first 1000 years when repository temperatures are at their maximum. The relevant reactions are discussed below and listed according to their reaction kinetics.

**Sulphate dissolution and precipitation**

This reaction controls the calcium ion concentration in the bentonite porewater leading to indirect buffering of the carbonate dissolution/precipitation reaction:

\[ \text{CaSO}_4(s) \leftrightarrow \text{Ca}^{2+} + \text{SO}_4^{2-} \]

The precipitation of gypsum (CaSO₄·2H₂O) and anhydrite (CaSO₄) is dependent on the temperature such that this process strongly depends on the thermal gradient across the buffer during the initial thermal period of repository evolution. Accumulation of sulphates in the hottest parts of the buffer and depletion of sulphates in peripheral parts has been confirmed in the LOT and ABM field experiments at Åspö (Karnland et al. 2009; Muurinen 2010, Appendix A). As temperatures and temperature gradients decrease, it is likely that the sulphate precipitates will redissolve, and disperse within the buffer by diffusion.

**Dissolution-precipitation of carbonates**

The carbonate minerals of importance are calcite (CaCO₃), dolomite (CaMg(CO₃)₂) and siderite (FeCO₃), which can dissolve or precipitate according to the following reactions:

\[ \text{CaCO}_3(s) + \text{H}^+ \leftrightarrow \text{Ca}^{2+} + \text{HCO}_3^- \]

\[ \text{CaMg(CO}_3)_2(s) + 2\text{H}^+ \leftrightarrow \text{Ca}^{2+} + \text{Mg}^{2+} + 2\text{HCO}_3^- \]

\[ \text{FeCO}_3(s) + \text{H}^+ \leftrightarrow \text{Fe}^{2+} + \text{HCO}_3^- \]

These reactions are important for controlling the pH of the bentonite porewater and the last (iron) reaction is also important for controlling the redox conditions. Generally, the solubility of all carbonates is strongly temperature dependent. Observations from field tests show that the carbonate content of bentonite decreases with increasing temperature (Karnland et al. 2009) which suggests that dissolution of carbonates in the buffer closest to the canister can be expected during the post-emplacement thermal period. Precipitation of calcium carbonates (aragonite, CaCO₃) has been observed at the interfaces between bentonite and corroding iron (Milodowski et al. 2009; Kumpulainen et al. 2010, p. 29). Carbonate reactions that are coupled with iron corrosion are expected to be localised in the repository near field.

Modelling calculations show that the intrusion of the high-salinity Laxemar water (similar to high-salinity Olkiluoto groundwater, even if not at repository depth, but much deeper) into a buffer comprised of MX-80 bentonite has no significant effect on the pH evolution of the buffer porewater, which is predicted to stay close to 7.0. More significant changes to pH would occur if dilute and alkaline glacial meltwater were to intrude into the buffer, causing dissolution of the carbonate minerals and a consequent increase in pH to around 8.3–9.6, depending on the groundwater composition (Arcos et al. 2008, Wersin et al. 2014).

**Equilibrium with CO₂ (gas)**

The partial pressure of CO₂ controls calcite equilibrium and thus alkalinity according to the following reaction:

\[ \text{CaCO}_3(s) + \text{CO}_2(g) + \text{H}_2\text{O} \leftrightarrow \text{Ca}^{2+} + 2\text{HCO}_3^- \]

This reaction is important for controlling the pH of the porewater.
Oxidation-reduction processes in bentonite

The redox conditions in the buffer will be controlled by the redox active components in bentonite, such as O₂, Fe, S and organic carbon. If pyrite (FeS₂) and O₂ are present in the early phase after emplacement, oxidation can occur through the following reaction:

\[ \text{FeS}_2(s) + 3.75\text{O}_2(g) + 3.5\text{H}_2\text{O} \rightarrow \text{Fe(OH)}_3(s) + 2\text{SO}_4^{2-} + 4\text{H}^+ \]

Siderite oxidation is another redox buffering reaction that might occur in presence of oxygen:

\[ \text{FeCO}_3(s) + 2.5\text{H}_2\text{O} + 0.25\text{O}_2(g) \leftrightarrow \text{Fe(OH)}_3(s) + \text{H}^+ + \text{HCO}_3^- \]

Reduction of sulphate is irreversible under repository conditions if sulphate-reducing microbes are active. In addition, reduction of ferric minerals (e.g. goethite FeOOH) and precipitation of Fe monosulphides (FeS) may take place in the presence of dissolved sulphide. Also, silicates that contain Fe in the silicate matrices may participate in reduction/oxidation reactions, although their kinetic rates are very slow.

Silica dissolution/precipitation

Other geochemical processes that can involve accessory minerals in the buffer include dissolution/precipitation of silica phases (quartz, cristobalite and amorphous SiO₂), especially in the presence of a thermal gradient:

\[ \text{SiO}_2(s) \leftrightarrow \text{SiO}_2 \]

Quartz is stable under repository conditions but its solubility increases with increasing temperature; consequently, silica may dissolve at the higher temperature close to the canister and be transported by diffusion outwards into the cooler parts where precipitation may take place. In the Buffer Mass Test study at Stripa, the buffer was analysed with respect to the distribution of silica but no definite conclusion could be drawn regarding possible enrichment in the coldest part (Pusch 1985).

Dissolution of aluminosilicates

The dissolution of accessory aluminosilicate minerals in the bentonite, such as plagioclase (anorthite CaAl₂Si₂O₈, albite Na₂Al₂Si₂O₈) or K-feldspar (KAlSi₃O₈) may occur:

\[ \text{CaAl}_2\text{Si}_2\text{O}_8 + 8\text{H}_2\text{O} \rightarrow \text{Ca}^{2+} + 2\text{Al(OH)}_4^- + 2\text{Si(OH)}_4 \]
\[ \text{Na}_2\text{Al}_2\text{Si}_2\text{O}_8 + 8\text{H}_2\text{O} \rightarrow 2\text{Na}^+ + 2\text{Al(OH)}_4^- + 2\text{Si(OH)}_4 \]
\[ \text{KAl}_3\text{Si}_3\text{O}_8 + 8\text{H}_2\text{O} \rightarrow \text{K}^+ + \text{Al(OH)}_4^- + 3\text{Si(OH)}_4 \]

The rate of aluminosilicate dissolution is very slow and irreversible under repository conditions. Apart from dissolution, incongruent dissolution of primary aluminosilicate minerals and formation of secondary aluminosilicate minerals (e.g. kaolinite Al₂Si₂O₅(OH)₄) may be possible in the very long term:

\[ \text{CaAl}_2\text{Si}_2\text{O}_8 + 2\text{H}^+ + \text{H}_2\text{O} \rightarrow \text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4 + \text{Ca}^{2+} \]

All dissolution and alteration reactions involving aluminosilicates are dependent on pH and, thus, have an impact on the pH buffering capacity of the bentonite. Aluminosilicate dissolution becomes significant when bentonite porewater interacts with the high pH leachates from cement degradation [9.2.8].
Overall, the alteration of accessory minerals (and impurities) is influenced by the following features of the repository system.

- Temperature: controls the rate of the reactions that cause the transformations and temperature gradients can lead to silica migration.
- Swelling pressure: influences the availability of chemical components that may react with the bentonite.
- Water content: the reactions would occur at the mineral-water interface and no reactions are expected under dry conditions.
- Buffer composition: the mineralogy and bulk composition of the buffer is significant for all chemical reactions in the buffer involving the accessory minerals.
- Porewater composition: is a significant control for all chemical reactions in the buffer.
- Gas composition: if gas is present, it will be significant for some chemical reactions.

Uncertainties in the understanding of the FEP:

There are analytical uncertainties in determining the nature and quantity of accessory mineral phases. Given that the amount and type of accessory minerals such as sulphides and carbonates are important for controlling the buffer porewater chemistry, especially redox and pH buffering reactions, uncertainties exist in predicting the porewater evolution. More information on natural variations in the mineralogy of available buffer materials has been recently acquired to reduce this uncertainty (Kiviranta & Kumpulainen 2011).

Couplings to other FEPs:

Alteration of accessory minerals is directly affected by the following FEPs:

- Corrosion (of cast iron insert) [4.2.6]
- Heat transfer [5.2.1]
- Water uptake and swelling [5.2.2]
- Montmorillonite transformation [5.2.6]
- Microbial activity [5.2.8]
- Chemical degradation of cement [9.2.8]
- Rock-water interaction [10.2.7]

Alteration of accessory minerals directly affects the following FEPs:

- Corrosion of the copper overpack [4.2.5]
- Water uptake and swelling [5.2.2]
- Montmorillonite transformation [5.2.6]
- Aqueous solubility and speciation [5.3.1]
- Precipitation and co-precipitation [5.3.2]
- Sorption [5.3.3]
- Diffusion [5.3.4]
- Advection [5.3.5]
- Corrosion (of supercontainer shell) [6.2.1]
**References:**


<table>
<thead>
<tr>
<th>5.2.8 Microbial activity</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Type:</strong> Process</td>
</tr>
<tr>
<td><strong>Alternative names:</strong> Microbial processes</td>
</tr>
<tr>
<td><strong>Section in 2007-09:</strong> 4.1.1, 4.7.1</td>
</tr>
</tbody>
</table>

**General description:**

Microbial activity and production of certain microbial metabolites may cause potential detrimental effects with respect to container corrosion and effectiveness of the multi-barrier system employed in the KBS-3 method for nuclear fuel waste disposal. Hence the process of microbial activity in buffer materials needs to be considered.
Sources of microbes in bentonite

Bentonite deposits naturally contain microbes (e.g., Fukunaga et al. 2005) of which some survive processing (heating, grinding, etc.) into the commercial product. Microbes exist naturally in deep rock at fracture surfaces and in groundwater. In a repository environment these species may migrate into the bentonite during water uptake and swelling [5.2.2], although it has been found that gram-negative groundwater microorganisms were poorly represented in highly compacted saturated bentonite from large in situ experiments conducted at Åspö (Fru & Athar 2008). Microbes will also likely be introduced directly into the underground disposal facility from the surface with the bentonite blocks and other engineering and stray materials (Hallbeck 2010). These microbes from different origins may potentially affect the geochemical system in the bentonite provided they maintain viable and in situ active populations under repository conditions. Generally, many of the introduced microbes will be adapted to near-surface aerobic environments and may not remain active or even viable in the anaerobic conditions that will prevail post-closure within the buffer. The microbial species that may persist under anaerobic repository conditions include methanogenic bacteria, sulphate-reducing bacteria (SRB), acetogens, iron-reducing bacteria, etc. (a large variety of bacteria has been found in bentonite materials, e.g., Svensson et al. 2011), although viable populations would require access to available water, energy, nutrients and space for in situ activity.

Investigations of several commercially available bentonites show a positive correlation between microbial activity and the concentration of organic carbon in the bentonite (Svensson et al. 2011). Many of these bentonites also contain natural populations of thermophilic sulphate-reducing bacteria (SRB) that are active at temperatures > 50 °C under enrichment conditions in growth media (Masurat et al. 2010a, Svensson et al. 2011). It is, thus, evident that many of the bentonites that may be used as buffer material include SRB that can withstand high temperatures and can utilise organic carbon as a nutrient. These SRB species could, under favourable conditions and at certain locations such as interfaces within a repository, be active in situ and produce sulphide.

Pertinent physiological microbial processes

Active microbes can produce carbon dioxide gas if organic carbon is available for metabolism. Anaerobic methane oxidation has been identified as an important microbial process that produces sulphide when methane is oxidised with sulphate. Therefore, the presence of methane may imply sulphide production at locations where microbial activity is possible in the buffer. Similarly, microbes may also use naturally occurring hydrogen or hydrogen from anaerobic iron corrosion in sulphate reduction resulting in sulphide production. The accumulation of sulphide is of particular interest because it could potentially cause corrosion of the copper canister [4.2.5]. This process is mitigated by the fact that sulphide is commonly precipitated with ferrous iron (when present). Sulphide concentrations in deep groundwaters are typically too low to chemically buffer copper corrosion reactions (Pedersen 2010). However, if ferrous iron sources are limited (e.g., if dissolution of iron silicate is kinetically constrained), notably higher sulphide levels can be observed locally. Such is the case in Olkiluoto borehole KR13 where sulphide concentrations up to 12 mg/L have been measured (Pedersen 2008).

Iron-reducing bacteria have been demonstrated to dissolve iron-rich smectite through reduction of structural Fe(III) to Fe(II) at room temperature and atmospheric pressure within weeks under good growth conditions (Kim et al. 2004). Other studies have also suggested mineral dissolution and clay weathering as a result of microbial activity (e.g.,...
Perdrial et al. 2009, Mulligan et al. 2009). Microbial processes may consequently have an influence on the stability of Fe(III)-containing montmorillonites if they maintain viable, active populations under repository conditions. The reduction process has been observed in different clay minerals and the amount of iron reduced has been at most 25–30 % (Pentrakova et al. 2013) and is dependent on the total amount of Fe in the clay and the distribution of iron in the octahedral position.

Other potentially negative effects of microbial activity on the integrity of the bentonite material itself are also of concern. For instance, Perdrial et al. (2009) studied the interaction between bentonite (MX-80 and nontronite) and introduced bacteria (Shewanella putrefaciens) at a dry density of 1300 kg/m³. The presence of bacteria appeared to cause an increase in water content and pore space (in MX-80) or a partial dissolution of clay minerals (in nontronite), which could affect swelling ability. Several other studies also have suggested the enhanced occurrence of processes such as smectite-to-illite transformation, mineral dissolution and clay weathering in bentonite, as a result of bacterial activity (e.g. Kim et al. 2004, Mulligan et al. 2009). Such possible microbial effects could jeopardize aspects of the intended functions of compacted bentonite buffer in a repository. However, Nakano & Kawamura (2010) estimated the extent of corrosion of compacted bentonite (i.e., dissolution of smectite) by a conceptual model based on microbial growth dynamics. The model used energy conservation between the Gibbs free energy of formation of products from the elements of smectite and the energy required for growth and maintenance of micro-organisms. This model predicted a mean population of micro-organisms of $10^6–10^7$ cells/cm³ on the bentonite surface, with a biofilm thickness of 5–10 µm. The microbial corrosion depth was estimated to be in the range of less than 0.2–5.3 mm per 100,000 years in nature, provided the smectite density was 1600 kg/m³. The corrosion depth varied inversely with the smectite density.

**Pertinent physical constraints on microbial sulphide production**

All microbes have a temperature range within which they are active. Within this range, increasing temperatures will generally result in increased microbial activity and, thus, the microbial populations may be higher during the thermal period compared with the ambient temperature period in a repository. There is a limit to temperature resistance, however, and the highest recorded temperatures for active microbial life are 113 °C (Stetter 1996) and, more recently, 121 °C for the single cell microbe Strain 121 (Kashefi & Lovley 2003) and 122 °C for a hyperthermophilic methanogen (Takai et al. 2008).

Microbes are generally tolerant of radiation, but their resistance varies between species. Increasing radiation doses generally will decrease the number of active microbes (e.g., Stroes-Gascoyne 2010).

Most microbes tolerate large variations in hydrostatic pressure and flow (Pedersen et al. 2000a, 2000b). Masurat et al. (2010b) put forward the hypothesis that cell integrity below swelling pressures of 2 MPa is possible though limited because of a reported upper limit for internal cell turgor pressure of 2.02 MPa. A maximum internal cell turgor pressure of about 2 MPa could help explain the sharp decrease in aerobic culturability in compacted bentonite at swelling pressures higher than 2 MPa (e.g., Stroes-Gascoyne et al. 2010).

A combination of low energy availability and low water content is detrimental to many microbes. Decreasing water availability reduces the activity and diversity of microbes.
because water is needed for active life. Some microbes can compensate for low water contents by using metabolic, energy-consuming processes.

Most of the pore diameters in highly compacted bentonite were measured around 0.02 μm (with a range from ~0.005 to 0.1 μm), with a very small population of macropores in the range of 5–100 μm (Stroes-Gascoyne et al. 2010), using mercury intrusion porosimetry. Dixon et al. (1999) reported a large component of micro pores at about 0.02 μm in highly compacted Wyoming MX-80 bentonite with a much smaller population of macropores in the range of 10–200 μm. In comparison, the size range for most vegetative microbes is 0.5 to 10 μm, while the size-range of starved or ultramicrobacteria is 0.2–0.4 μm (Krumholtz et al. 1997). Fredrickson et al. (1997) have shown that subsurface bacteria require interconnected pore throats larger than 0.2 μm for sustained metabolic activity to continue, but that viable bacteria can be maintained at such small pore throat sizes.

Measurements of sulphide production in compacted bentonites

The activity of SRB has been investigated in compacted bentonites with a range of densities at full water saturation using stainless steel oedometers and $^{35}$SO$_4^{2-}$ as an oxidised sulphur source for the SRB respiratory processes (Masurat et al. 2010b). These investigations were performed at the Åspö Hard Rock Laboratory using natural SRB populations from the groundwater at a depth of 450 m. The results (Figure 5-7) showed that SRB can be active and generate hydrogen sulphide during the initial phase of bentonite swelling in a repository.

![Figure 5-7. Graphic representation of the mean copper sulphide production rates on copper plates that were exposed (ex) and embedded (em) at different saturated bentonite densities (1.5, 1.8 and 2.0 g/L, corresponding to 1500, 1800 and 2000 kg/m$^3$). The treatments were unfiltered (uf) or filtered (f) in experiment G and exposed to 25 °C (25) and 120 °C (120) for 15 h. From Masurat et al. (2010b).]
In this experiment, copper plates were placed in oedometers either in direct contact with the groundwater (exposed) or separated from the groundwater by a 3–4 mm thick layer of the compacted bentonite (embedded). The gap that is present in the repository between the bentonite and the rock was simulated in the experiment by introducing a space between the water inlet filter and the compacted bentonite layer. Groundwater was introduced to the oedometers and the bentonite swelled and homogenised. Corrosion of the copper caused by the SRB was identified by the generation of radioactive hydrogen sulphide. Control experiments were run using filter-sterilised groundwater (0.2 µm) and heat-treated bentonite (120 °C for 12 h).

Overall, it was concluded that the rate of copper corrosion was inversely proportional to the final density of the water-saturated bentonite. The experiments with sterile groundwater and those with sterile groundwater plus heat treatment of the bentonite confirmed that SRB can be present in a dormant state in the commercial bentonite. By addition of water, these dormant SRB may become active and produce hydrogen sulphide until the full swelling pressure is achieved. Pedersen (2010) expanded on this study and concluded that microbial activity will be very limited in highly compacted bentonite (i.e. density of 2000 kg/m³ or a dry density of 1600 kg/m³).

Microbial activity has been demonstrated to decrease exponentially with increasing buffer densities and approach nil at wet densities above 2000 kg/m³ (Masurat et al. 2010b, Pedersen 2010), which is the expected density of the buffer after complete swelling. Stroes-Gascoyne et al. (2010) showed that culturability in fully saturated highly compacted bentonite was reduced to background levels (in dry bentonite) around dry densities of 1600 kg/m³ (i.e., wet densities of around 2000 kg/m³). However, phospholipid fatty acid (PLFA; an integral part of microbial cell walls) profiles in bentonites with dry densities ranging from 800 to 1800 kg/m³ revealed only a reduction by a factor of three in PLFA concentrations between bentonite with densities of 800 and 1600 kg/m³, whereas culturability was reduced by several orders of magnitude, suggesting that microbes were inactivated but not dead. Stroes-Gascoyne et al. (2011) also showed that culturability could be restored when the dry density was reduced from 1600 to 1000 kg/m³.

The results obtained on the survival and activity of microbes in compacted bentonite can be summarised in a conceptual model, as depicted in Figure 5-8 (Pedersen et al. 2000a).
Overall, microbial activity is influenced by the following features of the repository system.

- Radionuclide inventory: this controls the radiation intensity and, therefore, dose rate to the microbes that may affect their viability.
- Temperature: temperature increase may enhance microbial activity up to some optimal temperature.
- Swelling pressure: may constrain activity by limiting pore size.
- Buffer geometry: the size and shape of the pores may constrain microbial activity.
- Water content: water activity (relative humidity) is important because microbes need water to develop activity.
- Buffer composition: particularly the content of organic carbon is important as a nutrient.
- Porewater and groundwater composition: controls the availability of nutrients for microbial activity.
- Gas composition: gas content and composition is significant for microbial processes, particularly availability of methane and hydrogen as nutrients and products of microbial activity.
Uncertainties in the understanding of the FEP:

There are a number of uncertainties related to the understanding of microbial activity in the buffer. Importantly, the rate of microbial sulphide production (if any) at the final swelling pressure, especially at the rock-buffer interface is not well known. The lower limit of dry density of compacted bentonite to attain insignificant microbial activity is being investigated (Pedersen & Hallbeck 2013), and may be between 1400 and 1550 kg/m\(^3\) (Stroes-Gascoyne et al. 2010, Stroes-Gascoyne 2011).

The migration of microbes through compacted bentonite has not been studied extensively. Some studies indicate that microbes may clog the porosity of bentonite (Francisca & Glatsein 2010) and, consequently, the restrictions due to a small pore size and the narrow throat size between the pores may need to be experimentally defined. Stroes-Gascoyne et al. (1999) showed that microbes did not migrate into compacted bentonite-sand mixtures to any distance beyond the smallest distance sampled (5 mm). Fukunaga et al. (2001) reached similar conclusions.

The formation of biofilms on the canister surface has also been proposed. This may be the case during the initial swelling phase, but the viability of these microbes will be constrained by the same factors as microbes in any other part of the buffer. Furthermore, the stress from heat and radiation will be more severe at the canister surface than anywhere else in the buffer, certainly during the initial phase in which water is driven away from the canister surface which will be hot soon after deposition.

The mechanisms for survival of microbes in the buffer are not fully understood. Evidence for the presence of viable microbes in commercial MX-80 bentonite suggests that SRB and other species can withstand the very dry conditions (water content 10 %) in commercial bentonite. The present hypothesis is that microbes are both naturally present in the bentonite source as well as introduced to the clay during mining, processing and deposition. Processing of the bentonite includes heating which may select for the survival of (thermophilic) harder organisms and sporeformers. Furthermore, the clay causes dehydration, which will gently remove water from the microbial cells. The cells will be inactive, but viable. This process is similar to freeze drying of cells, which also results in inactive but viable cells (e.g., freeze-dried baker’s yeast). Adding water revives the microbes to activity, if conditions are favourable with respect to temperature, nutrients and space available for the microbial cells (e.g., Stroes-Gascoyne et al. 2011).

The observed suppression and disappearance of microbial activity and viability in highly compacted bentonite under repository conditions is hypothesised to be a combined effect from desiccation and mechanical pressure and other stress factors. The sum of the stress factors, radiation, heat, low water activity and a high swelling pressure after saturation of the buffer may ultimately result in death of the microbes. However, the timescale of actual cell death is uncertain and many inactivated but still viable cells may survive for long periods of time in the buffer material and provide a potential for increased microbial activity should buffer density decrease due to loss of bentonite near active fractures.

There are large uncertainties with respect to the conditions where the structural Fe(III) reduction process occurs in different clays. In each case, the result would be a change in physical and chemical properties of the clay, such as a reduction in the swelling pressure and chemical stability of the buffer. However, as long as the required swelling pressure and high density are fulfilled for the buffer, the limited microbial activity will likely limit the iron reduction process.
For the horizontal **KBS-3H** emplacement concept, a (temporary) reduction in density may occur outside the perforated titanium shell where water uptake by, and swelling of, the bentonite through the perforation is expected to occur. Microbial activity and microbial production of sulphide is most likely to occur outside the perforated titanium shell in the gap between the titanium shell and the rock prior to and during water uptake, swelling and ultimately homogenization of the bentonite density. Modelling efforts are underway to quantify the likelihood of increased MIC of the copper canister because of this expected activity, using sulphide production rates and sulphide diffusion coefficients provided in the work by Masurat (2010b) and Pedersen (2010).

**Couplings to other FEPs:**

Microbial activity in the buffer is directly affected by the following FEPs:
- Heat transfer [5.2.1]
- Water uptake and swelling [5.2.2]
- Diffusion [5.3.4]
- Advection [5.3.5]
- Microbial activity (in the filling components) [7.2.7]
- Microbial activity (in the geosphere) [10.2.10]

Microbial activity in the buffer directly affects the following FEPs:
- Corrosion of the copper overpack [4.2.5]
- Alteration of accessory minerals [5.2.7]
- Aqueous solubility and speciation [5.3.1]
- Precipitation and co-precipitation [5.3.2]
- Corrosion (of the supercontainer shell) [6.2.1]

**References:**


5.2.9 Freezing and thawing

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:** Freezing

**Section in 2007-09:** 4.4.2

**General description:**

The freezing and thawing process is discussed in this report based on the feedback received from STUK on the FEP report POSIVA 2007-12 (Miller & Marcos 2007), although this process would normally be screened out as being ‘unlikely’ based on modelling work that suggests permafrost cannot extend to repository depths, as discussed below.

Repeated glaciation and deglaciation events related to climate evolution [see 10.2.1 in Posiva 2012d] are expected to occur at Olkiluoto in the future. An estimate of Pimenoff et al. (2011) suggests that the present interglacial period will last for at least another 50,000 years, though a wide range of glacial inceptions are being proposed, depending on internal variabilities in the climate system, alternative carbon-emissions scenarios and geoengineering proposals (Ganopolski et al. 2016). After the current interglacial, cold periods leading to glacial conditions [see 10.2.2 in Posiva 2012d] and the formation of permafrost [see 10.2.3 in Posiva 2012d] are expected to occur.

Numerical simulations of ground temperature using pessimistic conservative boundary conditions indicate a maximum penetration depth of permafrost of between 275 and 300 m (Hartikainen 2012). As a consequence, freezing of the access tunnel backfill may occur in the upper parts of the disposal system [9.2.7] but permafrost is unlikely to penetrate down to repository depths and, consequently, is not expected to affect the buffer. If, however, permafrost did extend to repository depths, the porewater in the buffer may still not freeze because radiogenic heat will be generated within the spent nuclear fuel and transferred through the canister to the buffer [5.2.1] for up to 50,000 years after disposal [4.2.2].

The freezing point of porewater in the buffer is not precisely known, but will be lower than 0 °C because of the high hydrostatic pressure at repository depth and the salinity of the porewater, and because of confining water in small pores due to the Gibbs-Thomson effect. For buffer material with a dry density of 1.6 g/cm³, experimental evidence indicates porewater would freeze at temperatures between –5 and –10 °C (Schatz & Martikainen 2010). Independent experiments on backfill materials at swelling pressures close to 2 MPa indicated freezing points of between –2 and –3 °C (Schatz & Martikainen 2012). These freezing temperatures agree with estimates based on observations for unfrozen water in porous soils (Anderson & Tice 1972). For such low temperatures to be achieved at repository depth, would require sustained annual mean air temperatures of approximately –15 °C (Hartikainen 2012). Such long-lasting air temperatures are not, however, supported by evidence from the past glacial period (Weichselian climate data).

Two sets of independent experiments have investigated the effect of freezing and thawing on fully-saturated buffer and backfill materials (Birgersson et al. 2010, Schatz & Martikainen 2012). The main conclusions from these studies were that exposure to freezing temperatures initially results in a loss of swelling pressure until a critical
temperature is reached, at which point an increase in pressure occurs due to the formation of ice in the material. Increases in pressure, due to ice formation, have been observed at temperatures below the freezing point (Schatz & Martikainen 2010, Birgersson et al. 2010). Consequently, if the porewater in the buffer material did freeze, the increase in pressure would increase the stress on the canister but is unlikely to result in any deformation [4.2.3]. The impact of buffer freezing on canister integrity has been studied in the canister design (Raiko 2013, Section 8.4.4). Importantly, the effects of freezing on the buffer have been shown to be entirely reversible because both its swelling pressure and hydraulic conductivity essentially return to the pre-freezing levels upon thawing, even after multiple freezing and thawing cycles (Schatz & Martikainen 2010, 2012, Birgersson et al. 2010).

If freezing of the buffer porewater occurs after failure of the canister, this would reduce the rate at which any radionuclides could migrate through the buffer and in the groundwater because both would be frozen.

Overall, freezing and thawing of the buffer is considered very unlikely because permafrost is not expected to reach repository depths based on climate data used in modelling studies. If the buffer did freeze, however, its main function of protecting the canister would be temporarily lost because of the changes in its rheological properties. During this time, the groundwater in the geosphere up to the surface would be frozen with limited or no flow. There would be no long-term reduction in the buffer’s barrier properties because the effects of freezing are fully restored when thawing occurs.

Freezing and thawing of the buffer is influenced by the following features of the repository system.

− Temperature: the geothermal gradient and radiogenic heat generation in the fuel control the temperature in the buffer.
− Swelling pressure: affects the temperature at which freezing of porewater will occur.
− Buffer geometry: the size and geometry of the deposition tunnels exposed to permafrost will affect the mass of buffer that can freeze.
− Water content: the water content of the buffer affects the amount of expansion and stress increase due to freezing and the freezing point.
− Buffer composition and density: the freezing point is affected by the material density, the higher the density the lower the freezing point.
− Porewater composition: significant because the composition of the porewater affects the temperature at which it freezes, the higher the salinity the lower the freezing point.

Uncertainties in the understanding of the FEP:

The exact depth to which permafrost will penetrate into the geosphere and the duration of freezing are uncertain but modelling based on Weichselian climate data and on the Olkiluoto site conditions (e.g. thermal conductivity in rocks) suggests it is unlikely that permafrost will extend to repository depths.

If the permafrost did extend to the buffer, it is uncertain at what temperature the buffer porewater would freeze due to variations in radiogenic heat generation, ambient pressure and porewater composition, but it is likely to be below 0 °C. If the buffer did freeze, the hydraulic conductivity and swelling pressure in the buffer would be affected
but, at that time, the entire geosphere up to the surface will be frozen with little or no groundwater flow. Therefore, the uncertainties related to freezing and thawing of the buffer, and the consequences for radionuclide transport, are negligible. The consequences of buffer freezing on the canister strength have been considered in the canister design and are also considered to be small and not result in deformation.

**Couplings to other FEPs:**

Freezing and thawing in the buffer is directly affected by the following FEPs:
- Heat transfer [5.2.1]
- Water uptake and swelling [5.2.2]
- Permafrost formation [see 10.2.3 in Posiva 2012d]

Freezing and thawing in the buffer directly affects the following FEPs:
- Heat transfer [5.2.1]
- Water uptake and swelling [5.2.2]
- Diffusion [5.3.4]
- Advection [5.3.5]
- Colloid transport [5.3.6]
- Gas transport [5.3.7]

**References:**


5.2.10 Desiccation, formation of cracks

<table>
<thead>
<tr>
<th>Type:</th>
<th>Process</th>
</tr>
</thead>
<tbody>
<tr>
<td>Class:</td>
<td>Evolution</td>
</tr>
</tbody>
</table>

**Alternative names:** Shrinkage & cracking

**Section in 2007-09:** -

**General description:**

The temperature at the canister-buffer interface will increase up to around 95 °C and will then decay exponentially. During the heating process, the bentonite buffer in contact with the canister will dry and the vapour will move to the cooler parts. This drying (desiccation) process has associated a shrinkage process and cracks could appear in the inner part of the blocks at early stages, and, in case of **KBS-3H**, after the artificial wetting, if no more water were available. These cracks will however close when the bentonite hydrates and swells, as has been observed in the works of e.g. Burghignoli et al. (2000), Cekerevac & Laloui (2004), Lloret et al. (2004), Villar & Lloret (2004), Villar & Gómez-Espina (2007) and Villar et al. (2010, 2012).

Overall, desiccation and formation of cracks is influenced by the following features of the repository system.

- **Temperature:** cracks will form if temperature remains relatively high and no water is available.
- **Water content:** initial water content will determine the time it takes to form cracks if no other water source is available.
- **Buffer composition:** controls the uptake of water, if available.

**Uncertainties in the understanding of the FEP:**

No uncertainties are associated with this process, except for the extent at which could occur.

**Couplings to other FEPs:**

Crack formation is directly affected by the following FEPs:

- Heat transfer [5.2.1]

Crack formation in the buffer directly affects the following FEPs:

- Diffusion [5.3.4]
- Advection [5.3.5]

**References:**


5.3 Migration FEPs

The primary safety function provided by the buffer, with regard to migration, is to limit and retard radionuclide releases in the event of canister failure (i.e. by ensuring diffusive transport and providing sorption capacity). The ability of the buffer to provide this function, as part of the engineered barrier system, strongly depends on it achieving a high swelling pressure after complete hydraulic saturation, and maintaining that pressure over very long periods of time. If a canister fails, radionuclides will be released from the fuel and canister (Chapters 3 and 4), and will migrate through the buffer. A number of processes will then affect the migration of radionuclides and other species and their migration rate.

5.3.1 Aqueous solubility and speciation

<table>
<thead>
<tr>
<th>Type: Process</th>
<th>Class: Migration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alternative names:</td>
<td>Section in 2007-09: 4.8</td>
</tr>
<tr>
<td>Dissolution and speciation; Solubility and speciation; Porewater speciation; Speciation of radionuclides</td>
<td></td>
</tr>
</tbody>
</table>

General description:
Some radionuclides released from the canister will diffuse into the buffer [5.3.4] and be available for transport in the geosphere. Waste-derived radionuclides may only occur in the buffer after the canister has been breached. This is not expected to occur until several hundred thousands of years after disposal by which time the buffer will have reached its full swelling pressure, except for the case of canisters with an initial penetrating defect.

The majority of the radionuclides released to the buffer will be present either in the aqueous phase or sorbed to the bentonite mineral surfaces [5.3.3]. Smaller fractions of the inventory may also be associated with colloids [5.3.6] or the gas phase [5.3.7].

In this context, solubility refers to the total aqueous concentration of an element in all dissolved chemical forms in the buffer porewater, which are in equilibrium with each
other and the minerals in contact with the groundwater. The chemical form (speciation) that a radionuclide will take once in the aqueous phase will depend on the presence of other dissolved inorganic and organic compounds in the groundwater with which it can bond.

The composition of the buffer porewater will be controlled by a combination of the processes of montmorillonite transformation [5.2.6] and alteration of accessory minerals [5.2.7]. It is anticipated that the buffer porewater will be chemically reducing and mildly alkaline once chemical equilibrium has been reached.

The speciation depends on the chemical nature of the radionuclide and the composition of the bentonite porewater. Under the expected geochemical conditions at Olkiluoto, the most relevant ligands are hydroxide, carbonate, sulphate, chloride and sulphide. The solubility and sorption of radionuclides are strongly affected by their speciation. In general, radionuclides that may form free anions or cations and anionic complexes show higher solubility and lower sorption values than those that form cationic and neutral complexes. Temperature may have an effect on the release of the radionuclides and their solubility and speciation, but only in the case of an initial canister failure when the ambient temperatures are high.

The aqueous solubility and speciation of radionuclides in the canister and bentonite porewater has been assessed (Wersin et al. 2014) based on reference and bounding groundwater compositions during different time periods at Olkiluoto (Hellä et al. 2014). The solubility and speciation was calculated using the ThermoChimie thermodynamic database (Andra 2009). This database contains all the critically reviewed and recommended thermodynamic data from the NEA. For most of the safety relevant radionuclides, good or at least relatively good thermodynamic data and corresponding uncertainties are included in the database. For some elements, such as Pa or Mo, the data are rather poor and the uncertainties related to speciation are large. For actinides and lanthanides, carbonate complexation is important, especially under the more dilute and carbonate-rich conditions that might occur due to the intrusion of dilute water from an ice sheet during climatic evolution. The sorption of radionuclides forming free cations (e.g. Cs\(^+\), Sr\(^{2+}\), Ra\(^{2+}\)) will be affected by the salinity of the groundwater due to competition for interlayer exchange sites with Na\(^+\), Ca\(^{2+}\) and Mg\(^{2+}\) in the groundwater.

Overall, aqueous solubility and speciation in the near field are influenced by the following features of the repository system.

- Radionuclide inventory: controls the type and amount of radionuclides that may be available for transport.
- Temperature: a first-order control on the solubility of radionuclides.
- Swelling pressure: will influence solubility and speciation, but is a second-order control in the repository environment.
- Water content: with low water content in the buffer, radionuclide transport is strongly restricted; therefore, relevant conditions are those close to saturation.
- Buffer composition: the mineralogical properties of montmorillonite and of accessory minerals affect porewater composition by dissolution/precipitation and surface reactions (cation exchange and surface complexation).
− Porewater composition: is a first-order control on the solubility and speciation of radionuclides, particularly the pH, Eh plus the type and concentration of complex-forming dissolved species in the porewater.
− Gas composition: will affect the porewater composition (redox) if a two-phase system develops.

**Uncertainties in the understanding of the FEP:**

The solubility and speciation of radionuclides in the buffer is constrained by the porewater composition, which has been assessed by modelling (Wersin et al. 2014). The porewater composition will change over time as the near-field system evolves, but the exact composition through time is uncertain. This uncertainty has been bounded in a robust way, by defining reference and bounding bentonite porewaters (Hellä et al. 2014). Thus, a large span of pH, Eh, carbonate and salinity values are considered for radionuclide speciation to account for the uncertainty in porewater composition.

There is also some uncertainty related to the thermodynamic data used for modelling solubility and speciation. For many radionuclides, the uncertainty related to the porewater composition has a more significant effect on solubility and speciation than that related to the thermodynamic data.

**Couplings to other FEPs:**

Aqueous solubility and speciation in the buffer is directly affected by the following FEPs:
− Heat transfer [5.2.1]
− Radiolysis of porewater [5.2.5]
− Montmorillonite transformation [5.2.6]
− Alteration of accessory minerals [5.2.7]
− Microbial activity [5.2.8]
− Chemical degradation of cement [9.2.8]

Aqueous solubility and speciation directly affects the following FEPs:
− Precipitation and co-precipitation [5.3.2]
− Sorption [5.3.3]
− Diffusion [5.3.4]

**References:**


5.3.2 Precipitation and co-precipitation

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Alternative names:</th>
<th>Section in 2007-09:</th>
</tr>
</thead>
<tbody>
<tr>
<td>None</td>
<td>4.8</td>
</tr>
</tbody>
</table>

**General description:**

Precipitation and co-precipitation are two chemical mechanisms that may retard radionuclide transport. Bentonite is an effective sorbent and many radionuclides are retarded by the mineral grain surfaces due to surface sorption or surface complexation [5.3.3].

If the concentration of a radionuclide exceeds its solubility limit, it will precipitate as a solid phase. In the buffer, however, the radionuclide concentrations are expected to be very low (below saturation) and, therefore, the primary retardation mechanism will be sorption rather than precipitation.

Co-precipitation of a radionuclide with a major element to form a solid solution may also occur in the buffer. This process is strongly influenced by the porewater composition, which at any time depends on bentonite-groundwater interactions, and thus is site-specific. One important and well-established case of solid solution is the co-precipitation of Ra-226 with Ba, which has been investigated in detail (Bosbach et al. 2010). This process is considered for the derivation of radium solubility limits. Other than this case, there are few reliable thermodynamic data for solid solutions. Consequently, co-precipitation is not generally accounted for in performance assessments, which is generally a conservative assumption (Bruno et al. 2007).

A special case of solid solution is isotopic exchange between a radionuclide in solution and a stable nuclide of the same element included in a mineral. This retention process is considered for inorganic C-14 which is incorporated in calcite via the isotopic exchange process (Bradbury & Baeyens 2003, Wersin et al. 2014).

Precipitation and co-precipitation of radionuclides in naturally occurring bentonite and other clays have been reported in connection with many natural analogue studies and also in laboratory experiments (e.g. Cramer & Smellie 1994, Marcos et al. 2000).

Precipitation and co-precipitation are most relevant for defective canister scenarios, when temperatures are high and the radionuclide concentrations that may arise in the buffer could exceed solubility limits.

Precipitation and co-precipitation, if it occurred on solid surfaces such as the mineral grains, would retard radionuclide transport. The mechanism is considered to be irreversible unless a change in geochemical conditions causes the precipitated mineral phases to redissolve. It is possible that precipitation could cause the formation of suspended colloids directly from solution and, if this were to occur, it might enhance radionuclide transport, although colloids are not expected to be mobile in the buffer [5.3.6].
Overall, precipitation and co-precipitation are influenced by the following features of the repository system.

- Radionuclide inventory: controls the availability of radionuclides that could be included in precipitates.
- Temperature: a first-order control on the solubility of radionuclides.
- Swelling pressure: can influence solubility limits and, thus, precipitation, but is a second-order control in the repository environment.
- Buffer geometry: the sizes and shapes of the pores, as well as the electrical and chemical surface properties are significant for the nucleation and formation of precipitates.
- Water content: controls the availability of water needed for chemical reactions.
- Buffer composition: the mineralogical properties of montmorillonite and of accessory minerals affect porewater composition and, thus, radionuclide speciation and solubility.
- Porewater composition: is a first-order control on the solubility limits and the presence of other dissolved elements controls the potential for co-precipitation to occur.
- Gas composition: will affect the porewater composition (redox) if a two-phase system develops.

### Uncertainties in the understanding of the FEP:

Although the precipitation-dissolution of solid phases including radionuclides can be derived in a straightforward way from thermodynamic data, kinetic constraints may inhibit the formation of a given solid phase. There is a lack of kinetic data under relevant conditions for many radionuclides. Co-precipitation and solid solution formation has been studied only for specific systems, such as for pure carbonate and sulphate systems. The uncertainty for repository conditions is large and, therefore, this process is usually not considered in radionuclide transport modelling, which is generally a conservative approach. However, co-precipitation of Ra-226 with Ba has been considered as a bounding case in TURVA-2012 (Wersin et al. 2014).

### Couplings to other FEPs:

Precipitation and co-precipitation in the buffer is directly affected by the following FEPs:

- Heat transfer [5.2.1]
- Montmorillonite transformation [5.2.6]
- Alteration of accessory minerals [5.2.7]
- Microbial activity [5.2.8]
- Aqueous solubility and speciation [5.3.1]
- Sorption [5.3.3]
- Diffusion [5.3.4]
- Chemical degradation of cement [9.2.8]

Precipitation and co-precipitation in the buffer directly affects the following FEPs:

- Criticality (if it were to occur) [3.2.11]
- Sorption [5.3.3]
- Diffusion [5.3.4]
- Advection [5.3.5]
- Colloid transport [5.3.6]
References:

5.3.3 Sorption

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
</tr>
</tbody>
</table>

Alternative names:
- Ion exchange;
- Physical adsorption

Section in 2007-09: 4.8

General description:
Sorption is a general term describing the attachment of dissolved species to mineral surfaces. It includes ion exchange, physical adsorption and surface complexation. Sorption can also be considered as the precursor to precipitation.
Sorption is element specific and depends on the speciation (valency state, hydrolysis, complexation), and on porewater ionic strength and the solid phase surface characteristics. Radionuclides may be sorbed on clays either by surface complexation or by ion exchange.
Surface complexation is a mechanism involving a covalent or electrostatic bond between the hydrated surface of the solid and a radionuclide. This mechanism is most efficient for cations that are strongly hydrolysed and is very important for radionuclides with a high positive charge and high electronegativity (Bradbury & Baeyens 2009a, 2009b). Surface complexation is also the main sorption mechanism of oxyanions.
Ion exchange is a process in which an ion in solution is interchanged with another one accumulated at the surface of a solid with a permanent surface charge. This occurs
strongly on smectite and mica minerals due to the presence of exchangeable cations that compensate for the negative charge in the mineral structure. This mechanism is normally more efficient for the less hydrolysable radionuclide species.

In the buffer, the principal sorbing component is montmorillonite, which has two distinctly different types of surfaces, where two different types of sorption can take place (e.g. Sposito 1984, Stumm & Morgan 1996).

First, the surfaces of montmorillonite clay platelets carry a permanent negative charge arising from isomorphic substitution of lattice cations by cations of a lower valence. Charge neutrality is maintained by the presence of an excess of cations in solution held electrostatically in close proximity around the outside of the Al-Si-Al clay units. The electrostatically bound cations can undergo stoichiometric exchange with the cations in solution. Sorption by this mechanism strongly depends on ionic strength/solution composition with weak dependency on pH. Cation exchange reactions are commonly described by selectivity coefficients defined over mass action equations (Gaines & Thomas 1953). The total permanent negative charge of a clay mineral is defined as the cation exchange capacity (CEC). Ion exchange is the typical sorption mechanism for alkali and alkaline-earth elements, as well as transition metals at all pH values where positively charged solution species are predominant. In MX-80, the major exchangeable cation is Na⁺. The cation exchange capacity is about 800 meq/kg (Dohrmann et al. 2012).

Second, the surface hydroxyl groups (=S–OH) form reactive sites associated with montmorillonite. These groups are situated along the edges of the clay platelets. The CEC capacity of these sites in bentonite is about 80 meq/kg (Bradbury & Baeyens 2002). They can protonate or deprotonate so that the concentrations of neutral, protonated and deprotonated edge sites (=S–OH, =S–OH⁺, =S–O⁻) change as a function of pH. These sites can form complexes with cations and ligands in the solution. Many radionuclides can be taken up on the amphoteric hydroxyl surface groups and this process, modelled by surface complexation, is probably the most important sorption mechanism for heavy metals, transition metals, lanthanides and actinides in bentonite systems. The surface complexation of metals at =S–OH type sites is normally characterised by a strong dependency on pH, a weak dependency on ionic strength and a strong dependency on concentration (Bradbury & Baeyens 2003).

The supply of calcium from the deep groundwater into the buffer and the dissolution of calcium-bearing accessory minerals [5.2.7] may convert the Na-clay to the calcium form through cation exchange. The exchange process depends strongly on the groundwater chemistry and flow at the buffer-rock boundary. Despite the fact that this conversion is accelerated in the presence of a Ca-rich groundwater, the maximum conversion to the Ca-form will occur slowly due to the slow diffusion in compacted bentonite and the limited groundwater supply from the adjacent host rock. Considering saline water and a high groundwater flow rate, only a few percent of the Na-bentonite is calculated to alter to Ca-bentonite over the first 10,000 years (Liu & Neretnieks 1997, Bruno et al. 1999). If flow rates were much higher due to a hydraulic conductive feature intersecting a deposition hole in KBS-3V, then 20 % Na by Ca replacement has been calculated after 1000 years, and 47 % after 60,000 years (Arcos et al. 2006). The same results apply to KBS-3H if the boundary conditions are the same.

The sorption of radionuclides on the buffer is quantified by the distribution coefficient (Kd) between the sorbed concentration as mass per unit mass of solid material and the concentration in solution. The Kd value is strongly dependent on the chemical
conditions and is valid only for the particular experimental conditions studied. $K_d$ values of different radionuclides on bentonite have been thoroughly studied by many different laboratories and different databases have been compiled by the various waste management agencies (Bradbury & Baeyens 2003, Ochs & Talerico 2004).

Determinations of $K_d$ values in disperse systems cannot be easily extrapolated to compacted systems due to the fact that $K_d$ is an aggregated parameter that depends on the conditions of the experiment. Mechanistic models and descriptions have been developed in recent years that allow a deeper understanding of the sorption processes, and facilitate the definition of uncertainty ranges for this parameter (Bradbury & Baeyens 2003, Ochs & Talerico 2004, Wersin et al. 2014).

Overall, sorption is influenced by the following features of the repository system.

- Radionuclide inventory: controls the radionuclides that are available for sorption.
- Temperature: sorption ($K_d$) and availability of sites is controlled by the temperature.
- Buffer geometry: may affect the availability of sorption sites.
- Water content: controls sorption in terms of the availability of the solute species.
- Buffer composition: controls the nature of sorption sites and their availability.
- Porewater composition: is a control for all chemical processes in the buffer.

**Uncertainties in the understanding of the FEP:**

Conceptual understanding and a large quantity of measurement data exist for cation exchange and sorption of many radionuclides in simplified systems. There is, however, a lack of data for understanding and predicting the influence of some important variables, such as dissolved carbonate concentration or competition between major cations, on radionuclide sorption. This has been taken into account in evaluating uncertainties in $K_d$ values (Ochs & Talerico 2004).

It is clear that $K_d$ is a highly conditional parameter in terms of chemical conditions (pH, ionic strength, etc.) and has to be derived for each set of conditions. Also, the range of potential changes in groundwater composition during the long-term evolution of the repository is a source of uncertainty, though bounded by selecting a wide range of groundwater compositions (Hellä et al. 2014).

**Couplings to other FEPs:**

Sorption in the buffer is directly affected by the following FEPs:

- Heat transfer [5.2.1]
- Montmorillonite transformation [5.2.6]
- Alteration of accessory minerals [5.2.7]
- Aqueous solubility and speciation [5.3.1]
- Precipitation and co-precipitation [5.3.2]
- Diffusion [5.3.4]

Sorption in the buffer directly affects the following FEPs:

- Criticality (if it were to occur) [3.2.11]
- Precipitation and co-precipitation [5.3.2]
- Diffusion [5.3.4]
- Advection [5.3.5]
- Colloid transport [5.3.6]
References:
### 5.3.4 Diffusion

<table>
<thead>
<tr>
<th>Type:</th>
<th>Process</th>
</tr>
</thead>
<tbody>
<tr>
<td>Class:</td>
<td>Migration</td>
</tr>
</tbody>
</table>

**Alternative names:** Advection-diffusion

**Section in 2007-09:** 4.8

**General description:**
Diffusion is the process whereby chemical species move under the influence of a chemical potential gradient (usually a concentration gradient). In the buffer, diffusion of dissolved species will be the dominant transport process to the geosphere for radionuclides released after the canister has failed. Diffusion in the buffer is also an important process for:

- mineral transformation of the bentonite [5.2.6] and the accessory minerals [5.2.7] in the buffer, and the development of porewater composition; and
- the transport of corrosive substances (e.g. sulphide, oxygen) to the surface of the copper overpack [4.2.5].

The final swelling pressure that is achieved after water uptake [5.2.2] and the consequent modification of the bentonite large fraction of interlayer porosity is the dominant control on the rate of diffusion. Buffer geometry determines the diffusion lengths. The influence of pore geometry is included in tortuosity and constrictivity, and its effect is seen in the values of the diffusion coefficients.

The composition of montmorillonite, accessory minerals and the porewater also affect the diffusion coefficients. Diffusion in bentonite has been thoroughly studied in conjunction with radionuclide transport. Diffusion equations for radionuclides have been described in detail (Yu & Neretnieks 1997, SKB 2006).

Diffusivity data for radionuclides through compacted bentonite have been compiled by different authors and are summarised in Wersin et al. (2014). There may be differences in the diffusion behaviour of anions, cations and neutral species through the buffer. Anions are excluded from the smallest micropores due to their repulsion from negatively charged mineral surfaces. Diffusion within the electrical double layer next to the mineral surfaces (surface diffusion) may occur for cations (e.g. Cs⁺), and contribute to the overall diffusion coefficient.

Whether a diffusive barrier can be maintained will depend on the physical and chemical processes that affect the buffer over time. Loss of swelling pressure can occur due to mechanical [5.2.3] and chemical erosion [5.2.4] or alteration of the montmorillonite [5.2.6]. If, however, there was substantial loss in swelling pressure (e.g. by gradual chemical erosion of the buffer in contact with dilute groundwater), advection might become significant for radionuclide transport [5.3.5].

A semi-permeable boundary will form at the buffer-rock interface after swelling of the buffer in the deposition drift. This boundary results in Donnan equilibrium (i.e. the distribution of ions in the vicinity of a charged surface separating two solutions) and osmotic pressure (i.e. the result of osmosis at a semipermeable membrane).

Donnan equilibrium may arise from the distribution of ions between an ionic and colloidal solution (like montmorillonite) that are separated by a semi-permeable
membrane or boundary (Karnland 1998, Ståhlberg 1999). The ions and solvent can pass across the boundary but the colloidal particles cannot. The boundary maintains an unequal distribution of ionic solute concentration by acting as a selective barrier to ionic diffusion. The condition for equilibrium is that the chemical potentials are equal on both sides of the membrane for all components that can permeate.

Osmotic flow is the net movement of a solvent across a semi-permeable membrane from a region of high solvent potential to a region of low solvent potential when the membrane is permeable to the solvent but not the solute. The movement of the solvent can be counteracted by increasing the pressure of the more-concentrated solution (low solvent potential) with respect to the less-concentrated one (high solvent potential). The osmotic pressure is defined to be the pressure required to maintain the equilibrium, with no net movement of solvent. Osmotic pressure depends on the concentration of the solute but not on its identity. The total osmotic pressure is the sum of the partial pressures caused by each solute type.

In the buffer, swelling pressure develops as a result of both the osmotic effect and the hydration of interlayer cations, when in contact with groundwater.

Overall, diffusion is influenced by the following features of the repository system.

- Radionuclide inventory: controls the radionuclides that are available for diffusion.
- Temperature: controls the rate of diffusion, although this is of secondary importance.
- Swelling pressure: controls whether advection or diffusion is the dominant transport mechanism in the buffer.
- Buffer geometry: affects the pathways for diffusion.
- Water content: affects the swelling pressure and bulk diffusivity.
- Porewater composition: affects the final swelling pressure that is achieved.
- Gas composition: if gas is present, it affects the diffusion rate and process.

**Uncertainties in the understanding of the FEP:**

There is a good conceptual understanding of the diffusion process that will occur in water-saturated, swollen bentonite. There are also good parameter data available for radionuclide diffusivities in buffer material that has reached its intended swelling pressure and density under expected repository conditions (Wersin et al. 2014). There is, however, some uncertainty about the diffusion rates and processes that may occur in a buffer that has a reduced swelling pressure caused, for example, by chemical erosion. This uncertainty is bounded in the selection of scenarios and the values of parameters used to analyse them.
**Couplings to other FEPs:**

Diffusion in the buffer is directly affected by the following FEPs:

- Heat transfer [5.2.1]
- Water uptake and swelling [5.2.2]
- Mechanical erosion [5.2.3]
- Chemical erosion [5.2.4]
- Montmorillonite transformation [5.2.6]
- Alteration of accessory minerals [5.2.7]
- Freezing and thawing [5.2.9]
- Desiccation, formation of cracks [5.2.10]
- Aqueous solubility and speciation [5.3.1]
- Precipitation and co-precipitation [5.3.2]
- Sorption [5.3.3]
- Colloid transport [5.3.6]
- Corrosion (of the supercontainer shell) [6.2.1]

Diffusion in the buffer directly affects the following FEPs:

- Criticality (if it were to occur) [3.2.11]
- Corrosion of the copper overpack [4.2.5]
- Stress corrosion cracking (of the canister) [4.2.7]
- Diffusion (in the canister) [4.3.4]
- Microbial activity [5.2.8]
- Precipitation and co-precipitation [5.3.2]
- Sorption [5.3.3]
- Gas transport [5.3.7]
- Corrosion (of the supercontainer shell) [6.2.1]

**References:**


5.3.5 Advection

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
</tr>
</tbody>
</table>

**Alternative names:**
Advection-diffusion

**Section in 2007-09:**
4.8

**General description:**

Advection is transport of a substance by the bulk movement of groundwater (i.e. flow) due to a hydraulic (head) gradient. This process is important during the period soon after the emplacement of the dry, compacted bentonite blocks.

During the initial hydraulic saturation phase, groundwater may flow into KBS-3H deposition drifts through intersecting hydraulically active fractures. If the rate of inflow exceeds the rate of water uptake in the bentonite [5.2.2] then active flow channels or ‘pipes’ may develop in the buffer.

Advection will continue until a sufficient swelling pressure has been achieved so that the hydraulic conductivity of the bentonite becomes too low to allow advective flow.

Complete swelling of the buffer should occur long before the canister fails and, therefore, advection in the buffer is not considered a significant process for radionuclide transport, though it will be taken into account in scenario analysis.

Maintaining a diffusive barrier is dependent on the physical and chemical processes that affect the buffer over time. Loss of swelling pressure can occur due to mechanical erosion [5.2.3] and chemical erosion [5.2.4] or alteration of the montmorillonite [5.2.6]. Slow loss of swelling, and an increase in diffusion rates, is anticipated but it is not expected to be significant for safety over the time scales of interest. If, however, there was substantial loss in swelling pressure, advection might become significant for radionuclide transport.

If advection through the buffer did occur, it would suggest that colloidal transport might also take place [5.3.6] because open pathways might be created.

Overall, advection is influenced by the following features of the repository system.

- Temperature: a temperature gradient will cause thermal convection if water flow is possible.
- Swelling pressure: controls whether advection or diffusion is the dominant transport mechanism.
- Buffer geometry: affects the pathways for advection, such as through ‘pipes’.
- Water content: the initial water content in bentonite will control the wetting time and period over which advection could take place.

**Uncertainties in the understanding of the FEP:**

Water uptake and advection in the buffer under unsaturated conditions and in the presence of a temperature gradient is a complex process that is determined by many coupled sub-processes and influenced by parameters of the buffer and the near-field rock.

Advection through the buffer after complete swelling is not anticipated, although it could occur if physical or chemical processes caused the swelling pressure to drop substantially. The conditions under which this may occur are considered unlikely. This uncertainty is then bounded in the selection of scenarios and the values of parameters used to analyse them.
**Couplings to other FEPs:**

Advection in the buffer is directly affected by the following FEPs:
- Criticality (if it were to occur) [3.2.11]
- Heat transfer [5.2.1]
- Water uptake and swelling [5.2.2]
- Mechanical erosion [5.2.3]
- Chemical erosion [5.2.4]
- Montmorillonite transformation [5.2.6]
- Alteration of accessory minerals [5.2.7]
- Freezing and thawing [5.2.9]
- Desiccation, formation of cracks [5.2.10]
- Precipitation and co-precipitation [5.3.2]
- Sorption [5.3.3]
- Gas transport [5.3.7]

Advection in the buffer directly affects the following FEPs:
- Advection (in the canister) [4.3.5]
- Gas transport (in the canister) [4.3.7]
- Mechanical erosion [5.2.3]
- Chemical erosion [5.2.4]
- Microbial activity [5.2.8]
- Colloid transport [5.3.6]
- Gas transport [5.3.7]

**Related bibliography not cited in the text:**


### 5.3.6 Colloid transport

<table>
<thead>
<tr>
<th>Type: Process</th>
<th>Class: Migration</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Alternative names:</strong></td>
<td><strong>Section in 2007-09:</strong></td>
</tr>
<tr>
<td>Colloid formation and colloid facilitated transport, colloid release/erosion</td>
<td>4.7.3, 4.8</td>
</tr>
</tbody>
</table>

**General description:**

In general, any particle that has a linear dimension between $10^{-9}$ and $10^{-6}$ m (i.e. nm to µm size) is considered to be colloidal (Hiemenz & Rajagopalan 1997). Larger solids are often termed ‘suspended particles’ and anything smaller is considered to be in solution.
Most colloidal phases are effective sorbents because of their high surface/volume ratio. This is particularly true for inorganic colloids such as clay minerals, metal oxides and carbonates that are effective at adsorbing radionuclides and metals through ion exchange and surface complexation reactions (Ryan & Elimelech 1996).

Colloid formation and colloidal radionuclide transport are relevant to the defective canister scenarios. For the entire time the canister remains intact, no colloid-mediated radionuclide transport can occur in the buffer.

In the repository system, a variety of inorganic and organic colloids may serve as source material for colloid-mediated transport. It is possible also, under repository pH conditions, that hydrolysed radionuclide species may form intrinsic colloids through aggregation. For colloid-mediated transport of radionuclides to be considered significant for repository safety, a number of conditions must be satisfied at the same time (Wold 2010). The colloids should:

- be present at sufficient concentration;
- have sufficient affinity for radionuclide binding;
- be stable at prevailing conditions for sufficient duration; and
- be sufficiently mobile.

It is generally considered that the buffer, once it has reached its full swelling pressure [5.2.2], will serve as an efficient filter of all but the smallest colloids, and thus also filter effectively the radiocolloids formed and released from the canister. This view has been supported by numerous laboratory experiments. For example, column-type transport experiments using 15 nm gold colloids in compacted Kunigel bentonite with a relatively low dry density of 1000 kg/m³ showed that the colloidal particles were effectively filtered (Kurosawa et al. 1997). Filtration would be expected to be even more effective at higher dry densities, which would ensure a small pore size for the buffer bentonite.

Studies with added organic colloids to compacted MX-80 bentonite have shown that these may be able to diffuse through bentonite compacted to dry densities between 600–1800 kg/m³ at a solution ionic strength ≥ 0.01 M. Given the broad size distribution of the starting organic material and the extremely low amounts of diffusing mass, however, a significant filtration effect cannot be ruled out (Wold & Eriksen 2003). In more recent studies evaluating the diffusion of negatively charged 2, 5 and 15 nm gold colloids in MX-80 bentonite compacted to dry densities of between 600 and 2000 kg/m³, colloid diffusion was observed only for the smallest particles at the lowest dry density (Holmboe et al. 2010).

In the case of a buffer system in contact with an intersecting, transmissive fracture, chemical erosion of the bentonite involving colloidal transport cannot be ruled out [5.2.3]. In this case, radionuclide sorption onto the eroded bentonite mineral grains could lead to colloid-mediated radionuclide transport (Alonso et al. 2006).

The sorption properties of actinides, fission products and activation products on bentonite and other minerals have been well studied (Wold 2010). There are, however, few reliable data regarding desorption and even fewer for adsorption/desorption to the colloidal fraction, particularly with respect to the longer time scales more relevant for transport processes through the geosphere. Such information could help determine whether sorption onto colloids should be treated as a reversible or irreversible process
in radionuclide transport models. Nonetheless, bounding assessment calculations can be carried out with conservative assumptions.

Overall, colloidal formation and colloid transport are influenced by the following features of the repository system.

- Radionuclide inventory: controls the radionuclides that may be available for association with colloids.
- Temperature: the stability of colloids may be temperature dependent, although this is only a second-order control.
- Swelling pressure: a higher swelling pressure and density leads to more effective colloid filtration because it reduces the size and shape of pores.
- Buffer geometry: the size and shape of the pore spaces is important for determining the efficiency of filtration of colloids.
- Water content: the primary control on the swelling pressure and, thus, the ability of the buffer to filter colloids.
- Buffer composition: influences the composition of colloids formed from bentonite.
- Porewater composition: is an important control for the formation and stability of colloids.

**Uncertainties in the understanding of the FEP:**

Given the observed diffusivity of lignosulfate colloids through compacted bentonite, the issue of organic-colloid-mediated radionuclide transport may warrant further examination.

The uncertainties regarding chemical erosion of the buffer apply here, with special emphasis on bentonite colloids as source material for colloid-mediated radionuclide transport.

There is a lack of accurate data regarding radionuclide sorption on colloids, in particular montmorillonite colloids (Wold 2010). Forms of uncertainty include experimental error, the conditional nature of experimentally determined distribution coefficients, not only on geochemical conditions but also on the specific characteristics of the colloid, and effects due to colloid-size distributions.

**Couplings to other FEPs:**

Colloid transport in the buffer is directly affected by the following FEPs:

- Colloid transport (in the canister) [4.3.6]
- Water uptake and swelling [5.2.2]
- Mechanical erosion [5.2.3]
- Chemical erosion [5.2.4]
- Montmorillonite transformation [5.2.6]
- Freezing and thawing [5.2.9]
- Precipitation and co-precipitation [5.3.2]
- Sorption [5.3.3]
- Advection [5.3.5]
- Gas transport [5.3.7]

Colloid transport in the buffer directly affects the following FEPs:

- Diffusion [5.3.4]
- Colloid transport (in the geosphere) [10.3.6]
References:

5.3.7 Gas transport

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
</tr>
</tbody>
</table>

**Alternative names:**
Two-phase flow; Gas transport/dissolution; Transport of radionuclides in gas phase

**Section in 2007-09:**
4.5, 4.7, 4.8

**General description:**
Gas in the buffer can originate from air incorporated in the bentonite at the time of emplacement or introduced by the groundwater. If the initial quantity of air in the buffer is small or the rate of new gas generation is low, the gas (air) will be dissolved by the groundwater and will be transported out of the repository by diffusion.
During the initial post-emplacement period, before complete saturation of the buffer, the thermal gradient across the bentonite will cause the bentonite closest to the canister to become drier [5.2.1] and there will be a vapour flux towards the outer, cooler parts of the bentonite where it will condense. This vapour flux is governed mainly by Fick’s law in the absence of a gas pressure gradient. As the bentonite closest to the canister
dries out due to the vapour flux, its thermal conductivity reduces and the temperature increases (Toprak et al. 2013, Pintado et al. 2012).

Additional gas can be generated in the repository by corrosion of the cast iron insert [4.2.6], radiolysis of water [3.2.5, 5.2.5], microbial activity [5.2.8], corrosion of copper [4.2.5] or corrosion of the titanium shell of the supercontainer [6.2.1] and Ti plugs [8.2.1]. Of these, corrosion of the cast iron insert is likely to be the primary source of gas, but this cannot occur until after the canister has failed. Consequently, gas transport is particularly relevant to the defective canister scenarios.

If the rate of gas generation exceeds the capacity of the groundwater to dissolve the gas, then a free gas phase may be formed in the deposition drift and gas pressure will develop. If the gas pressure increases and exceeds the confining pressure imposed by the buffer, it will open a flow path and ‘break through’ the buffer. The pore geometry, swelling pressure, smectite composition, porewater composition and bentonite composition are all relevant factors determining the break-through pressure. After breaking through, the gas pressure will drop again to a point where the gas transport pathway closes (the ‘shut-in pressure’).

Several gas migration experiments and modelling studies have been performed in compacted bentonite over the last 20 years, and these have considerably improved the understanding of this process (Harrington & Horseman 2003, SKB 2006, Rodwell 2005, Olivella & Alonso 2008). These studies provide strong evidence that free gas is able to be transported through bentonite via a network of pressure-induced pathways.

The main gas transport process is an advective flux, which is controlled by the pressure gradient and is determined by Darcy’s law. There is also a non-advective flux which is controlled by the concentration gradient and is determined by Fick’s law.

The gas pressure depends on the temperature and gas permeability through the buffer, which in turn depend strongly on the water content of the clay because this determines the swelling pressure [5.2.4]. Since the gas pressure depends on the temperature, gas expulsion and formation of pathways in the buffer is most relevant during the initial thermal phase. The intrinsic permeability for gas is orders of magnitude higher than for water. In unsaturated conditions, macropores are present in the clay and the gas flows easily. When the clay becomes saturated, the pores are much smaller and the buffer material is less permeable.

Radionuclides can be transported directly in the gas phase (e.g. C-14 in methane or H-3 as hydrogen gas), although H-3 is of little relevance to post-closure safety due to its short half-life. Radionuclides may also be transported in the aqueous phase within water expelled from the buffer by the gas as it breaks through and is transported through the gas pathways. The creation of gas pathways and the movement of a free-gas phase through them are not, however, expected to displace a significant amount of porewater or dissolved radionuclides (Harrington & Horseman 2003).

Gas expulsion and formation of pathways are most relevant during the initial thermal phase when water may contact the cast iron insert in a defective canister scenario. If sufficient gas pressure is produced in the canister due to corrosion of the cast iron insert, transport pathways may be forced open through the buffer allowing rapid gas outflow. If, however, the breakthrough pressures are not exceeded, gaseous species would migrate only by diffusion when dissolved in the aqueous phase.
Overall, gas transport is influenced by the following features of the repository system.

- Radionuclide inventory: controls the radionuclides that may be available for gas transport.
- Temperature: significant for the reaction rates leading to gas production and controls gas pressure and transport.
- Swelling pressure: controls the breakthrough pressure required to form gas pathways.
- Buffer geometry: influences the formation of paths for gas transport.
- Water content: may control the amount of gas in solution and the transport of gas.
- Porewater composition: controls the solubility of gas and whether a separate gas phase can form.
- Gas composition: the nature of the gas will control whether it is dissolved or in a gas phase.

**Uncertainties in the understanding of the FEP:**

The hydro-mechanical behaviour of the water/vapour/gas system in a defective canister is governed by several coupled processes and parameters. Significant advances in the understanding of gas transport in bentonite buffer have been recently achieved during the FORGE EU project. In this project, uncertainties related to the persistence of gas-bearing fractures in bentonite have been notably reduced, showing that gas-bearing fractures close soon after the gas has been released.

**Couplings to other FEPs:**

Gas transport in the buffer is directly affected by the following FEPs:

- Heat transfer [5.2.1]
- Water uptake and swelling [5.2.2]
- Mechanical erosion [5.2.3]
- Chemical erosion [5.2.4]
- Radiolysis of porewater [5.2.5]
- Montmorillonite transformation [5.2.6]
- Freezing and thawing [5.2.9]
- Diffusion [5.3.4]
- Advection [5.3.5]

Gas transport in the buffer directly affects the following FEPs:

- Gas transport (in the canister) [4.3.7]
- Advection [5.3.5]
- Colloid transport [5.3.6]
- Gas transport (in the geosphere) [10.3.7]

**References:**


6 SUPERCONTAINER SHELL AND MINOR TITANIUM COMPONENTS

6.1 Description

This chapter discusses the KBS-3H titanium components other than the compartment and drift plugs (which are discussed in Chapter 7). These other components comprise:

- supercontainer shell
- spray and drip shields
- DAWE (Drainage, Artificial Watering and air Evacuation) pipes (only the short air evacuation pipes in the rear part of both compartments remain in the drift)
- feet of various drift components.

In the KBS-3H alternative, the canister, surrounded by bentonite buffer, will be deposited in the deposition drift in a prefabricated package, the supercontainer, the outer part of which is a metal shell (see Figure 1-2). Titanium alloy (Grade 12) has been selected as the shell material. The supercontainer shell will be perforated to allow the bentonite inside the supercontainer to become wetted, to swell and extrude through the holes. The supercontainer design is described in Posiva (2013a).

Previously to the selection of titanium as the shell material, several copper and steel alloys were also considered. Titanium turned out to be clearly the best choice in terms of long-term safety due to its inert nature and low corrosion rate, having also the lowest hydrogen production rate. For more details on the comparison between the shell materials, see Posiva (2013a, Chapter 7).

Spray and drip shields will also be made of titanium alloy (Grade 12), but their proportion of the total quantity of titanium in the repository is very small.

The artificial watering and air evacuation system (DAWE) contains short watering pipes (to be removed completely) and one long air evacuation pipe in both compartments of a drift, which is designed to be removed after its use (although the short end part of the pipe will remain). The air evacuation system will consist of 6 m long pipes that are connected using a screw type coupling. The pipes will also be made of titanium alloy (Grade 12) – the tensile strength of titanium is sufficiently high for this application and the consequences for long-term safety are expected to be limited if the pipe becomes stuck when removing it and has to be left in the drift. The air evacuation pipe will be installed in the lower part of the drift, but in order to function properly the end of the pipe in the rear section of the compartment will need to be turned upwards towards the top of the drift, where the air will accumulate. This will be achieved using a separate pipe (diameter 17.2 mm), which will be fixed on the end face of the compartment (Posiva 2013a, Section 4.10.3).

All clay components to be emplaced in the drift will be equipped with titanium feet to enable their emplacement.
6.1.1 Long-term safety and performance

These other titanium alloy (Grade 12) components do not have long-term safety functions, but, naturally, they are not allowed to impair the safety functions of the actual barriers. They are only required to perform during the operational phase. In the long term, any processes that might affect the titanium components are mainly relevant from the point of view of their possible effect on the performance of the buffer and other components made of bentonite. The long-term safety and performance of the buffer is discussed in Section 5.1.1.

6.1.2 Overview of the potentially significant FEPs

There are a number of processes related to these other titanium components that are considered to be significant for the long-term safety of the KBS-3H repository. Processes directly related to the performance of the buffer (such as titanium-bentonite interactions) are discussed in Chapter 5 (Buffer, see processes 5.2.6 and 5.2.7). The processes discussed in this chapter are:

6.2.1 Corrosion
6.2.2 Deformation

Both processes are related to system evolution. There are no processes relevant to the migration of radionuclides and other substances that might affect this and the other titanium components, because, in common with the supercontainer shell, they have neither containment nor a retardation function. The titanium corrosion products may have some effect on the mass transport behaviour at the buffer/rock interface, and these are discussed in 5.2.6 (titanium-bentonite interactions within montmorillonite transformation) and in more detail in Posiva (2016b).

Of the Ti components in the drift, the supercontainer shell is closest to the radiation and heat from the canister. The temperature of the shell is at maximum around 60 °C (Ikonen & Raiko 2015) and it is not expected to have an impact on the Ti shell and the feet below the shell. The other titanium components are farther away from the radiation and heat source and thus, the possible effect of radiation-related and thermal processes on these titanium components are expected to be no significant and are not discussed. Gas generation, if any, is discussed under 6.2.1 Corrosion.

Both corrosion and deformation are potentially affected by a number of features of the repository system that could influence the occurrence, rate, activity and potential couplings between the processes. These features relate either to aspects of the design of the repository or to characteristics of the buffer that might be time-dependent during the repository lifetime. The most significant features are:

- Radionuclide inventory
- Temperature
- Pressure
- Supercontainer shell geometry
- Mechanical stresses
- Material composition
- Water composition
- Gas composition.
The possible influences of these features on the processes considered to be significant for the long-term safety of the repository are described in each FEP description, and are summarised in Table 6-1.

The interactions between the titanium components and other components of the KBS-3H disposal system are summarised in Chapters 5, 7 and 9 (see e.g. processes [5.2.6], [7.2.5] and [9.2.4]).

References


Posiva 2016b. Safety evaluation for a KBS-3H spent nuclear fuel repository at Olkiluoto – Performance Assessment. Eurajoki, Finland: Posiva Oy. POSIVA 2016-02 (in prep.).

Table 6-1. Possible influences of features of the disposal system on the processes considered to be significant for the long-term performance of other titanium components (marked with Y). These influences and couplings are discussed in more detail in each FEP description.

<table>
<thead>
<tr>
<th>Processes related to system evolution:</th>
<th>Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radionuclide inventory</td>
<td>Temperature</td>
</tr>
<tr>
<td>6.2.1 Corrosion</td>
<td>-</td>
</tr>
<tr>
<td>6.2.2 Deformation</td>
<td>-</td>
</tr>
</tbody>
</table>

1. This is excluded because the dose rate affecting the supercontainer shell and the other Ti components will not be above the background radiation levels.

2. Some corrosion processes are pressure dependent but the effect on the corrosion of titanium alloys in the repository environment is likely to be minimal.
6.2 System evolution FEPs

The processes in the supercontainer shell, drip shields, DAWE pipes and titanium feet (corrosion and deformation, and their couplings) may have an impact on the evolution in the drift and the near-field rock. The behaviour of these titanium components and their effect on the near field will depend on the time and rate at which these processes occur. The couplings of these FEPs with other FEPs are also indicated, but the consequences of interactions or combinations of these are discussed in Posiva (2016b).

The term “KBS-3H” is not shown in **bold** in this chapter, because the components (supercontainer shell and minor titanium components) are completely KBS-3H-specific and the description of the FEPs apply to these. Thus, there is no need to highlight the sections that have been updated for 3H.

References

Posiva 2016b. Safety evaluation for a KBS-3H spent nuclear fuel repository at Olkiluoto – Performance Assessment. Eurajoki, Finland: Posiva Oy. POSIVA 2016-02 (in prep.).

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:**

None

**Section in 2007-09:**

5.7.1 and 5.5.1

**General description:**

The supercontainer shell and the feet under the supercontainer are currently planned to be made of titanium alloy (Grade 12). The surfaces of these titanium components will be exposed to the groundwater environment or bentonite; initially the conditions will be aerated and at low temperature, but will soon be anoxic as oxygen is consumed. The temperature will increase due to radiogenic heating from the spent fuel, and a maximum temperature of about 60 °C is expected at the supercontainer shell within less than 100 years after closure (Raiko & Ikonen 2015).

**Uniform corrosion**

Titanium alloys have a high corrosion resistance (e.g. Cotton 1994, King 2010) over a wide range of environmental conditions. It has a superior corrosion resistance to that of carbon steel, which was previously selected as the KBS-3H plug material (the previous “drift end plug” included both a steel plug and a concrete plug). The hydrogen production rate due to the anaerobic corrosion of titanium alloys is also lower than that of carbon steel (the passive film on titanium is highly stable in water). This means that titanium alloys are more favourable for the long-term safety of a KBS-3H repository (the aspects of Ti-clay interaction and any possible impact of Ti on the clay performance are discussed under FEP 5.2.6) than carbon steel. A large body of literature exists on the corrosion behaviour of Ti and Ti alloys. Comprehensive reviews on this topic are given for example by Schutz (2005), Hua et al. (2004, 2005) and King...
et al. (2010). Wersin et al. (2010, Table 2-1) give representative data on general Ti corrosion rates for unalloyed titanium and titanium grades 2 and 7, under a variety of conditions. Titanium alloys exhibit a range of corrosion and physical properties that make them suitable for numerous applications and they have been considered as radioactive waste container materials by a number of waste management organisations (e.g. King 2010).

All commercially available grades of titanium alloys exhibit excellent corrosion resistance to a wide range of environments. The corrosion behaviour of titanium is governed by the low solubility of a stable tetravalent TiO₂ passive surface corrosion layer under both oxic and reducing conditions, over a wide pH range. TiO₂ or rutile, is an insoluble, thermodynamically stable, naturally occurring mineral (Wersin et al. 2010). The dependence of the composition and properties of the oxide film on electrochemical potential has been extensively studied and the main features of the passive film behaviour and corrosion of titanium are summarised in Figure 6-1. The different factors controlling film growth are reasonably well understood, as are the associated corrosion processes (Hua 2004, 2005, Shoesmith 2006). The oxide is reported to be an n-type semiconductor (Zeng et al. 2010) and the composition and structure of the passive film formed on titanium have been investigated using a range of electrochemical techniques, in particular electrochemical impedance spectroscopy (e.g. by Pan et al. 1996). Equivalent electrical circuits for the oxide film derived from these investigations suggest that the oxide film has a bi-layer structure, with a thin compact barrier-type inner layer and a porous outer layer.

**Figure 6-1.** Summary of the passive properties and localized corrosion behaviour of α-titanium alloys: \( E_{oc} \) – open circuit corrosion potential; \( E_{FB} \) — flatband potential; \( N_D \) - density of defects; HFIC - high field ion conduction (Shoesmith 2006).
As revealed from previous studies (Mattsson & Olefjord 1984), the long-term corrosion rate of titanium in compacted bentonite is very low; studies of oxide growth rate showed that it follows a logarithmic law, so that after 10,000 years an overall uniform corrosion rate of \(< 1 \text{ nm/a}\) is predicted (Mattsson & Olefjord 1984). The uniform corrosion rate is not strongly affected by the chemical conditions (pH, Eh, salt content) (Hua et al. 2004, 2005). Passivity will be maintained during the evolution of the repository environment in the absence of localised corrosion. Thus, a titanium plug will corrode and release titanium slowly (cf. Posiva 2013a, Sections 7.2.3, 7.5.3). Titanium plugs are likely to have a much longer lifetime than the thinner and perforated titanium supercontainer shells because of their greater thickness.

Electrochemical corrosion studies on Ti in solution and bentonite suspensions have been conducted by a Japanese group (Azumi et al. 2000). From experiments carried out under neutral anoxic and weakly alkaline conditions at two different temperatures for up to 20 weeks exposure, it was deduced that an oxide film formed on all samples, which however was “unstable” at high temperature (80 °C), especially in the bentonite suspension (Azumi et al. 2000).

The low content of other metals in the Ti alloys restricts any possible impact on the surrounding bentonite, for example the recommended Ti Grade 12 alloy has such a low content of other metals in the alloy (0.3% Fe, 0.2-0.4% Mo, 0.6-0.9% Ni) that the possible impact of these on the surrounding bentonite will be negligible (Posiva 2013a, Section 7.2.3).

In very tight drift sections (i.e. sections with low water permeability), corrosion may be limited by the supply of liquid water and water vapour and the corrosion rate may decrease (Gribi et al. 2007, Section 5.7.1).

Due to its very low corrosion rate, titanium will release H₂ at a low rate, which will dissipate via diffusion. The risk of formation of a separate gas phase is approximately three orders of magnitude less than if steel were used instead (Posiva 2013a, Section 7.4 and Table 7-12).

According to Little et al. (1991, 2007), Ti alloys are probably the only common engineering materials that are immune to microbially influenced corrosion, MIC.

*Localised corrosion*

Titanium alloys can be susceptible to localised corrosion under some critical conditions (e.g. crevice corrosion in acids). Crevice-corrosion resistant titanium alloys have been developed through the addition of Pd (ASTM grades 6, 11, 16 and 17) (Schutz 2005) and Mo and Ni (Grade 12 has 0.3% Mo and 0.8% Ni, for improved crevice corrosion resistance).

The crevice corrosion susceptibility of titanium alloys has been investigated by Schutz (1992a, b) who established the domains of corrosion for several grades of titanium alloy, including Grade 12, which is the alloy proposed for the Finnish repository (see Figure 6-2). It can be seen that although Grade 12 is affected by crevice corrosion in acidic conditions and at high temperatures, the operating and long-term conditions for the repository will be well away from the region of crevice corrosion susceptibility for this grade. Furthermore, the data shown in Figure 6-2 refer to the behaviour in aerated conditions and as oxygen is consumed by corrosion reactions and microbial activity the driving force for crevice corrosion will decrease, as the corrosion potential will become more negative and therefore the separation between the repassivation potential and the
corrosion potential will increase. Even if crevice corrosion were to occur the metal ions would be confined to the crevice site and not be released in to the surrounding bentonite, as shown in Figure 6-3, so although crevice corrosion could affect the structural integrity of the titanium components it is not expected to have any effect on the local composition of the bentonite.

Figure 6-2. Temperature-pH limits for crevice corrosion of titanium alloys in NaCl brines based on laboratory and field experience, and zones of hydrogen pick-up compared to crevice corrosion susceptibility (Schutz 1992a,b).

Figure 6-3. Schematic showing the mechanism of crevice corrosion for titanium in aqueous chloride media (Schutz 1992a).
Hydrogen embrittlement of titanium

In the presence of hydrogen in the metal lattice, titanium can suffer from hydrogen embrittlement or hydriding, which leads to a reduction in the mechanical properties of the titanium. Many titanium alloys are also susceptible to hydrogen induced cracking in certain circumstances. However, the passive oxide film is an effective barrier to the ingress of hydrogen, and in most applications hydrogen damage is not a problem. The combination of conditions that cause hydrogen embrittlement can be summarised as the following (Timet 2015, Shoesmith 2006):

1. pH <3 or >12
2. impressed potentials more negative than -0.7V
3. temperature >77 °C
4. a source of hydrogen, e.g. corrosion of titanium

On the basis of these threshold values it can be concluded that the titanium components in the repository (i.e. the supercontainer shell and the drift and compartment plugs) will not be susceptible to hydrogen embrittlement because they will not fulfil requirements 1 to 3. In addition, the general corrosion rates will be so low that the quantity of hydrogen produced by anaerobic corrosion will be negligible and any hydriding would be confined to the uppermost surface regions. Shoesmith (2006) has reviewed and modelled the likelihood of failure of titanium alloys by hydrogen induced cracking (HIC) in the Canadian vault environment. Failure will only occur if the hydrogen concentration in the titanium reaches a critical value, which is approximately 500 µg/g. This concentration could only be achieved if active crevice corrosion were occurring and for Grade 12 only uniform corrosion needs to be considered. Based on the film growth data of Mattsson et al. (1984, 1985, 1990a, b) lifetimes based on HIC susceptibility in the range \(1.5 \times 10^5\) to ~\(10^6\) years are predicted.

The interactions between titanium and clay are discussed under FEP 5.2.6.

Overall, the rate of corrosion of the supercontainer shell is influenced by the following features of the repository system.

- Temperature: controls the rate of corrosion reactions.
- Supercontainer shell geometry: the dimensions and shape of the supercontainer have an effect on the exposed surface area for general corrosion.
- Mechanical stresses: the combination of stress and a chemically aggressive groundwater/porewater may promote stress corrosion cracking.
- Material composition: the corrosion processes (especially the rate) and the nature of the corrosion products depend on the composition of the titanium alloy.
- Water composition: is the primary control on the corrosion mechanisms and its rates.

Uncertainties in the understanding of the FEP:

The corrosion behaviour of titanium is well understood (e.g. Posiva 2013a, Table 7-12). A number of uncertainties, however, remain related to process understanding, such as the formation of intermetallic phases and their role in hydrogen induced cracking (Hua 2005), and the possible impact on the physical properties in relevant repository conditions (Posiva 2012b, Section 5.10.7). The uncertainties related to the reactivity of titanium with clay are discussed under FEP 5.2.6.
**Couplings to other FEPs:**

Corrosion of the supercontainer shell is directly affected by the following FEPs:

- Heat transfer [5.2.1]
- Water uptake and swelling (in the buffer) [5.2.2]
- Radiolysis of porrewater (in the buffer) [5.2.5]
- Alteration of accessory minerals (in the buffer) [5.2.7]
- Microbial activity (in the buffer) [5.2.8]
- Deformation [6.2.2]
- Microbial activity (in the host-rock) [10.2.10]
- Diffusion (in the buffer) [5.3.4]
- Diffusion (in the host-rock) [10.3.4]

Corrosion of the supercontainer shell directly affects the following FEPs:

- Deformation [6.2.2]
- Montmorillonite transformation [5.2.6]
- Diffusion (in the buffer) [5.3.4]

**References:**


### 6.2.2 Deformation

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Deformation</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:** None

**Section in 2007-09:** 5.6.1

**General description:**

Deformation is the only relevant mechanical process that could affect the supercontainer shell and may hence affect the outer part of the buffer depending on how the shell deforms and whether it generates heterogeneities (Gribi et al. 2007, Section 5.6). Gribi et al. (2007) considered a steel shell, but the same assessment is considered to be valid also for a titanium shell. Titanium alloy (Grade 12) is a strong material with good mechanical properties, which is the reason for the titanium shell being 2 mm thinner than the steel shell, with acceptable stresses, strains and deformations during emplacement (Posiva 2013a, Section 4.4.2).

The expected difference of swelling pressure between the inside and outside of the supercontainer may lead to considerable forces acting on the perforated titanium shell and to elasto-plastic deformations. Rupturing of the shell may occur, most likely at or near the circular edges of the supercontainer (end-plates), where the stresses are expected to be highest, and as result of the ongoing corrosion and weakening of the titanium, although the weakening will be slight if the overall corrosion rate is <1 nm/a (cf. Gribi et al. 2007, Section 5.6.1).

A quasi-stationary state of stress equilibrium is reached when all forces acting in the system (including the force caused by volume expansion of corrosion products, by gas pressure build-up, hydrostatic pressure and rock stress) are balanced, resulting in a homogenisation of bentonite swelling pressure inside and outside the supercontainer. The formation of corrosion products involves a volume increase (cf. Gribi et al. 2007, Section 5.6.1). For titanium, the volume increase factor is 1.8 (Posiva 2012b, Table 5-4). Thus, corrosion of titanium will lead to a very slight increase in bentonite density and swelling pressure (see FEP 5.2.2).

Due to the transient temperature increase and subsequent decrease (Ikonen & Raiko 2015), the supercontainer will experience thermal expansion and contraction, and hence possibly some structural alterations. These effects may be enhanced by increased temperatures, due to a reduction of the heat transport capacity provided by gaps initially present around the canister, buffer and supercontainer. In permeable drift sections, these gaps are expected to close relatively rapidly due to the swelling of bentonite. However, in drift sections where the surrounding rock is less permeable, they may remain partially open for longer periods, although the artificial watering system will result in buffer swelling, even in very dry sections. Given that the maximum temperatures within the bentonite will remain below 90 °C (i.e. 10 °C below the design basis maximum of 100 °C), thermal expansion/contraction of the supercontainer shell is expected to be insignificant. Likewise, structural alterations in the titanium alloy components induced by thermal gradients are not significant under the expected thermal conditions in the repository (cf. Gribi et al. 2007, Section 5.6.1). The coefficients of thermal expansion are of similar order of magnitude for both titanium...
(8.6×10⁻⁶ m · m⁻¹ · K⁻¹) and steel (11.8×10⁻⁶ m · m⁻¹ · K⁻¹), so the same conclusions apply to both shell materials.

Boundary conditions
The relevant boundary conditions for assessing the mechanical deformation of the supercontainer shell are determined by the stresses exerted by bentonite and by the surface of the rock, by hydraulic forces acting in the system, by temperature gradients and by processes leading to volume changes (bentonite swelling, corrosion) (cf. Gribi et al. 2007, Section 5.6.1).

Model studies/experimental studies
The propensity for swelling of bentonite through the holes of the supercontainer has been analysed both theoretically and experimentally for a steel shell (Börgesson et al. 2005). The theoretical analysis showed that the maximum swelling pressure is reduced when bentonite swells through the holes and reduces further when it swells into the void space between supercontainer and rock. However recent laboratory tests (e.g. Posiva 2013a, Sandén et al. 2008) have demonstrated that bentonite swelling through the perforations in the supercontainer and behind the shell does actually occur and that the measured swelling pressures inside and outside the shell are similar to the swelling pressure expected in the absence of the supercontainer. This is explained by the observed expansion of the perforated shell, leading to stress equilibration. The axial hydraulic conductivity of the buffer in the slot outside the supercontainer was measured and found to be ~10⁻¹² m/s. This value is higher than expected, based on measured density and swelling pressure, but still low enough for the buffer to be sufficiently impermeable. The increase is likely to have been caused by uneven swelling of the bentonite behind the container, as shown by the theoretical calculations.

Overall, the deformation of the supercontainer shell is influenced by the following features of the repository system.

- Temperature: temperature increase and decrease may cause structural deformation.
- Pressure: the internal and external pressures are the primary control on deformation, particularly the external hydrostatic and bentonite swelling pressures.
- Supercontainer geometry: in particular, the dimensions and shape of the supercontainer have a control on its overall strength, stiffness and stress concentrations.
- Mechanical stresses: stresses exerted by bentonite determine the relevant boundary conditions for mechanical deformations of the supercontainer shell.
- Material composition: is a direct control on the mechanical properties of the supercontainer (strength, ductility, thermal expansion).

Uncertainties in the understanding of the FEP:
The data from the reviews considered here suggests that the understanding of the deformation mechanisms (i.e. creep and sustained load cracking) of titanium alloy Grade 12 at low temperature is relatively immature, with marked differences in operating mechanisms being observed and reported. This makes any clear statements on the mechanistic understanding of low temperature titanium creep that are of practical value, difficult to make.

There is an uncertainty about whether oxygen-induced embrittlement of the titanium alloy could occur in the long-term.
Full-scale tests with titanium supercontainer shells have not yet been done, so their mechanical behaviour in repository-like conditions has not been demonstrated. As mentioned above, the various strains that could develop during the early evolution of the supercontainer shells are not well understood (cf. Griibi et al. 2007, Section 5.6.1). Nonetheless, there are no associated long-term safety functions of the supercontainer shell, as it mostly serves to facilitate emplacement of the spent fuel canister and the buffer.

For further knowledge on titanium deformation see FEP [8.2.2]

**Couplings to other FEPs:**

Deformation of the supercontainer shell is directly affected by the following FEPs:

- Corrosion [6.2.1]
- Heat transfer (in the buffer) [5.2.1]
- Water uptake and swelling (in the buffer) [5.2.2]
- Reactivation-displacement along existing fractures (in the geosphere) [10.2.3]
- Creep (in the geosphere) [10.2.5]

Deformation of the supercontainer shell directly affects the following FEPs:

- Corrosion [6.2.1]

**References (most come from FEP [8.2.2]):**


6.3 Migration FEPs

As the supercontainer and minor titanium components have no long-term safety functions, no migration related FEPs are defined. Even if sorption on titanium alloys and titanium oxide was observed, to be conservative/pessimistic, no credit would be given to these components for their sorption properties and they are thus not described.
7 FILLING COMPONENTS

Filling components include filling blocks and transition blocks as well as pellet filling, the latter two components forming the so-called “transition zones” related to the drift plugs and compartment plugs, and also the filling of the pilot hole and drift bottom plus the possible filling of locations of rock breakage in the drift.

7.1 Description

In the KBS-3H conceptual design, there are six types of filling components; the components are shown in Figure 7-1 and listed below:

1. Filling adjacent to drift plug (compartment side), including pellet filling (dark brown in the figure) and transition block (yellow) (together termed transition zone)
2. Filling in an inflow position (termed filling block)
3. Filling on entrance side of compartment plug (pellets in dark brown, transition block in yellow; together termed transition zone)
4. Filling on drift end side of compartment plug (pellets in dark brown, transition block in yellow; together termed transition zone)
5. Filling at the drift end
6. Filling of the pilot hole.

The filling components are planned to be composed of similar clay material to the buffer. The conceptual design of the filling components is based on the use of pellets and cylindrical blocks similar to distance blocks if possible. The blocks can be combined from fixed thickness cylindrical blocks or the thickness can be adjusted to specific requirements, with the choice being based on operational considerations (Posiva 2013a, Section 4.6.2).

7.1.1 Long-term safety and performance

The long-term safety and performance requirements of the filling components are discussed in Posiva (2016c) and summarised below.

![Figure 7-1. KBS-3H drift design with different filling components (Posiva 2012b, Fig. 4-9): a) Filling on the sealed side of the drift plug (and compartment plug), b) Filling blocks in position of inflows, c) Filling on the drift entrance side of the compartment plug, d) Filling at drift bottom end (far end of the drift) and e) Filling of pilot hole. (Buffer & Filling Components PL Report).](image)

The safety functions of the filling components are to:

- contribute to favourable and predictable mechanical, geochemical and hydrogeological conditions for the buffer and canisters and to
- limit and retard radionuclide releases in the possible event of canister failure.
The filling blocks (i.e. filling components at inflow locations) have an additional safety function to:

- separate possible transmissive sections of the drift from the canisters and buffer.

The specific purposes of the filling blocks are (i) to fill void spaces in the drift, contributing to its mechanical stability, and to confine the buffer as it takes up water, such that the buffer’s saturated density remains within the design specifications, (ii) to protect the buffer from the effects of transient water flows (e.g. piping and erosion, that may occur during the operational period for a drift and the following period leading to saturation), and (iii) to separate the canisters and buffer from larger and more transmissive geological features that may detrimentally affect the canisters and buffer in the longer term and provide preferential pathways for radionuclide transport in the event of canister failure.

The purpose of the transition zone on the sealed side of the compartment plug is to fill the empty drift section next to the plug that is needed for mounting the plug in a way that supports the performance of the adjacent distance block. The purpose of the transition zone on the drift entrance side of the compartment plug is to function as backfilling material supporting the performance of adjacent drift components.

The purpose of the transition zone for the drift plug is to fill the empty drift section next to the plug that is needed for mounting the plug in a way that supports the performance of the adjacent distance block.

### 7.1.2 Overview of the potentially significant FEPs

As the filling components are made of bentonite, i.e. the same material used for the buffer, the same FEPs as for the buffer apply, with the exception of radiolysis of porewater, as the filling components are far from the canister, which is the immediate radiation source. These are also far from the heat source and the temperature effects, related to FEPs such as desiccation and formation of cracks or montmorillonite transformation, are expected to be more limited than for the case of the buffer. The filling blocks are planned to be used in drift sections intersected by water-bearing fractures and, thus, these are likely more prone to chemical erosion [FEP 5.2.4] than the buffer positions. The FEPs are listed in the sections below, but for a full description see Sections 5.2 and 5.3 in Chapter 5.

### References


### 7.2 System evolution FEPs

The full descriptions of the FEPs can be found in Section 5.2 in Chapter 5 because the material is the same.

#### 7.2.1 Heat transfer

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

#### 7.2.2 Water uptake and swelling

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

#### 7.2.3 Mechanical erosion

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

#### 7.2.4 Chemical erosion

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

#### 7.2.5 Montmorillonite transformation

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

#### 7.2.6 Alteration of accessory minerals

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

#### 7.2.7 Microbial activity

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

#### 7.2.8 Freezing and thawing

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>
7.2.9 Desiccation, formation of cracks

| Type: Process | Class: Evolution |

7.3 Migration FEPs

The full descriptions of the FEPs can be found in Section 5.3 in Chapter 5.

7.3.1 Aqueous solubility and speciation

| Type: Process | Class: Migration |

7.3.2 Precipitation and co-precipitation

| Type: Process | Class: Migration |

7.3.3 Sorption

| Type: Process | Class: Migration |

7.3.4 Diffusion

| Type: Process | Class: Migration |

7.3.5 Advection

| Type: Process | Class: Migration |

7.3.6 Colloid transport

| Type: Process | Class: Migration |

7.3.7 Gas transport

| Type: Process | Class: Migration |
8 COMPARTMENT AND DRIFT PLUGS

8.1 Description

Two different plug structures (Table 8-1) have been designed for the KBS-3H deposition drift:

- the compartment plug,
- the drift plug.

According to the current design these will be made of Titanium Grade 12 (ASTM) (Posiva 2013a, Section 4.7.1). The compartment plug (CP) is used for hydraulically separating and sealing drift sections (~150 m long at most) and it also enables the water filling procedures of DAWE. The design of the plug is illustrated in Figure 8-1 and elaborated in Anttila et al. (2008). The compartment plug consists of the following three titanium alloy components: the fastening ring, which is cast into a rock notch using low-pH concrete (pH<10), the collar, which is attached to the fastening ring, and finally the cap. The collar is fastened to the fastening ring by welding, as is the cap to the collar. The compartment plug is designed so that the welds do not carry any load and, thus they only function as a seal. Leakage is possible at the boundary between the metal components and the concrete casting that secures the plug to the rock and at the rock-concrete interface.

The drift plug (DP), which will be located at the mouth of each drift, will also be made of titanium alloy (Grade 12). The shape of the DP is very similar to that of the CP (Figure 8-1). The main difference is that the plates will be thicker in the DP. Table 8-1 shows the mass of titanium used in the plugs and the cast cement volumes.

![Figure 8-1. Compartment plug (drift plug will have the same shape) (Nottegar, 2010).](image-url)
Table 8-1. The quantities of titanium (kg) and cement (dm³) in compartment and drift plugs.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Compartment Plug</td>
<td>330</td>
<td>450</td>
<td>280</td>
<td>1 060</td>
<td>200</td>
</tr>
<tr>
<td>Drift Plug</td>
<td>330</td>
<td>550</td>
<td>450</td>
<td>1 330</td>
<td>200</td>
</tr>
</tbody>
</table>

8.1.1 Long-term safety and performance

The long-term safety and performance requirements of the compartment and drift plugs are discussed in Posiva (2016c) and summarised below.

Compartment plugs are used to hydraulically separate sections of the deposition drift. The requirement for hydraulic separation is mainly relevant during the operational phase, but the compartment plug is an important element supporting the function of other drift components, and therefore it is considered to be part of the engineered barrier system of KBS-3H. The artificial watering is expected to contribute significantly to the performance of the other barriers, and would be very difficult to execute in a long drift without sectioning it to two compartments. Therefore, all drifts longer than approximately 150 m will contain a compartment plug.

The function of the drift plug is similar to that of KBS-3V deposition tunnel plugs; it is to avoid significant water flows out of the drift through the cast concrete in the fastening ring, which could give rise to piping and erosion of the buffer. It also keeps the buffer and filling components in place prior to the backfilling and saturation of the adjacent central tunnel (Posiva 2013a, Section 4.8.1).

The safety function of the compartment and drift plugs is to contribute to favourable and predictable mechanical, geochemical and hydrogeological conditions for the filling components, buffer and canisters by keeping the drift components in place.

8.1.2 Overview of the potentially significant FEPs

There are a number of processes related to the compartment and drift plugs that are considered to be significant for the long-term safety of the KBS-3H repository that relate to system evolution and to the migration of radionuclides and other substances. Processes directly related to the performance of the buffer are discussed in Chapter 5 (Buffer).

Processes related to system evolution are:

8.2.1 Corrosion
8.2.2 Deformation
8.2.3 Degradation of the cast concrete of the fastening ring.
Processes related to the migration of radionuclides and other substances through the cast concrete are:

8.3.1 Diffusion
8.3.2 Advection
8.3.3 Gas transport.

No radiation-related processes of importance were identified by Gribi et al. (2007, Section 6-3) for the drift plug, because of the large distance between the plug and the source of radiation (i.e. the nearest canister). For the same reason, radiation-related and thermal processes are also considered irrelevant for the compartment plugs.

Microbial processes were omitted by Gribi et al. (2007, Table 6-3) and they are considered to be even less relevant for titanium plugs compared with the earlier concrete/steel drift end plug, because titanium is considered to be immune to microbially influenced corrosion, MIC (Little & Lee 2007).

The processes relating to the compartment plugs and drift plugs are potentially affected by a number of features of the repository system that can influence the occurrence, rate, activity and potential couplings between the processes. These features relate either to aspects of the design of the repository or to parameters (characteristics) of the components that might be time-dependent during the repository lifetime. The most significant features are:

- Temperature
- Pressure
- Drift geometry
- Mechanical stress
- Material composition
- Water composition
- Gas composition.

The possible influences of these features on the processes considered significant for the long-term safety of the compartment and drift plugs are described in each FEP description below, and are summarised in Table 8-2.
Table 8-2. Possible influences of features of the disposal system on the processes considered to be significant for the long-term performance of the compartment and drift plugs (marked with Y). These influences and couplings are discussed in more detail in each FEP description.

<table>
<thead>
<tr>
<th>Processes</th>
<th>Features</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Radionuclide inventory</td>
</tr>
<tr>
<td>Processes related to system evolution:</td>
<td></td>
</tr>
<tr>
<td>8.2.1 Corrosion</td>
<td></td>
</tr>
<tr>
<td>8.2.2 Deformation</td>
<td></td>
</tr>
<tr>
<td>8.2.3 Degradation of the cast concrete of the fastening ring</td>
<td></td>
</tr>
<tr>
<td>Processes related to the migration of radionuclides and other substances:</td>
<td></td>
</tr>
<tr>
<td>8.3.1 Diffusion</td>
<td></td>
</tr>
<tr>
<td>8.3.2 Advection</td>
<td></td>
</tr>
<tr>
<td>8.3.3 Gas transport</td>
<td></td>
</tr>
</tbody>
</table>

The processes occurring within the compartment and drift plugs can be interdependent and directly coupled to each other. The direct couplings have been listed in each FEP description.

References


8.2 System evolution FEPs

The fulfilment of the long-term safety functions of compartment and drift plugs will depend on the processes occurring in these components, and on the time and rate at which these processes occur. The couplings of these FEPs with other FEPs are also indicated, but the consequences of interactions or combinations of these are discussed in Posiva (2016b).

The term “KBS-3H” is not shown in bold in this chapter, because the components (compartment and drift plugs) are completely KBS-3H-specific and the description of the FEPs apply to these. Thus, there is no need to highlight the sections that have been updated for 3H.

References

Posiva 2016b. Safety evaluation for a KBS-3H spent nuclear fuel repository at Olkiluoto – Performance Assessment. Eurajoki, Finland: Posiva Oy. POSIVA 2016-02 (in prep.).

8.2.1 Corrosion

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th><strong>Class:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:** None

**Section in 2007-09:** Not applicable

**General description:**

The compartment plugs (CP) and drift plugs (DP) are currently planned to be made of titanium alloy (Grade 12). In summary, the surfaces of the CPs and DPs will be exposed to low-pH concrete, the groundwater environment or bentonite; initially the conditions will be aerated and cool but after repository closure the environment will become anoxic as residual oxygen is consumed. The temperature will also increase due to radiogenic heating from the spent fuel but the temperature at the plug surface – which is at a large distance from the canister – will be at most about 50 °C (cf. Ikonen & Raiko 2015, Figure 36).

The corrosion processes are discussed under FEP 6.2.1.

Overall, the rate of corrosion of the compartment and drift plugs is influenced by the following features of the repository system.

- Temperature: controls the rate of corrosion reactions.
- Pressure: might contribute to mechanical stresses, which adding to a chemically aggressive groundwater/porewater composition may promote stress corrosion cracking.
- Mechanical stresses: see also pressure.
- Material composition: the corrosion processes, and especially the rate, depend on the composition of the titanium alloy.
− Groundwater composition: is the primary control on the corrosion mechanism and its rate, and the nature of any solid and gaseous corrosion products that may be formed.
− Gas composition: might affect corrosion, especially if dissolved in water or even as gas.

**Uncertainties in the understanding of the FEP:**
See FEP 6.2.1.

**Couplings to other FEPs:**
Corrosion of the compartment and drift plugs is directly affected by the following FEPs:
− Water uptake and swelling (in the filling components) [7.2.2]
− Alteration of accessory minerals (in the filling components) [7.2.6]
− Microbial activity (in the filling components) [7.2.7]
− Deformation [8.2.2]
− Microbial activity (in the host rock) [10.2.10]
− Diffusion (in the filling components) [7.3.4]
− Diffusion (in the host rock) [10.3.4]

Corrosion of the compartment and drift plugs directly affects the following FEPs:
− Deformation [8.2.2]

**References:**
As in FEP 6.2.1

### 8.2.2 Deformation (of titanium plugs)

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th><strong>Class:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:**
None

**Section in 2007-09:**
Not applicable

**General description:**
The requirements (see Posiva 2016c) regarding the pressure tolerances and durability for the drift plug are considerably higher than those for the compartment plug. This is because the drift plugs must withstand the full hydrostatic pressure and the bentonite swelling pressure, and be sufficiently tightly fitted in the drifts to form a part of the engineered barrier system. The drift plug is required to stay in place under the applied loads (with no significant displacement allowed) until the adjoining central tunnels are backfilled (Posiva 2012b, Section 4.2.4.2).

A Finite Element Method (FEM) analysis has been carried out during the design phase for the drift plug design based on Titanium alloy Grade 12. The analysis of maximum swelling pressure was used to define the design specification of the plug. According to
the analysis, the drift plug will withstand a load of 22 MPa before failure of the components is expected, which indicates that it will accept the design loading with a high degree of confidence (Posiva 2013a, Section 4.8.3; Posiva 2012b, Section 4.2.4.2).

The compartment and drift plugs will be subject to mechanical loading during their planned lifetimes. There is a potential for these titanium components to be loaded by swelling of the bentonite and any movement in the surrounding rock formation. However, there is currently little information to enable any detailed evaluation of the stress state in the components and hence any potential deformation mechanism that might be operative. However, from a general consideration of the component location it would appear that some form of sustained loading might be possible. The other conditions that are relevant to these components are that they are planned for a very long life (i.e. >100,000 years) and it is expected that the temperature on the surface of the plug will be at the highest up to ~50 °C in the early period of higher temperature in the drift. The following issues should be considered from a structural and mechanical behaviour viewpoint:

- Long-term stability of the basic titanium alloy microstructure in the ambient environment
- Creep deformation
- Sustained load cracking

These issues are considered below.

**Stability of Grade 12 titanium microstructure**

The microstructure of Grade 12 titanium can be seen in Figure 8-2. It consists of fine equiaxed α grains with some β phase present. In the view of the longitudinal section (L-ST) the grains can be seen to be elongated in the rolling (or extrusion direction). It would be expected that there will be a relatively low level of β phase present because of the small amount of β stabilising elements present (i.e. Fe, Ni and Mo) but nonetheless this β phase volume fraction will exceed the amount seen in the commercial purity titanium grades (Grades 1-4).

One of the major challenges related to numerous structural components has been the assumption that the material used remains in the same condition throughout service life. This has been particularly true for applications to e.g. electrical power generation stations (conventional – oil/gas or coal, or nuclear), where numerous instances of changing material condition have led to an unexpected structural performance change. It is worth noting that many of these are high temperature applications, which clearly affects the microstructural development of materials much more rapidly than at temperatures in the 20-100°C range. However, it must be also acknowledged the the potential for unexpected developments due to the very long timescales associated with nuclear waste disposal.
The possibility that interstitial oxygen, i.e. oxygen that occupies empty spaces in the titanium lattice, represents a more thermodynamically stable state than does titanium dioxide (TiO$_2$). Hence, the formation of TiO$_2$ at room temperature could be due to kinetic limitations in the dissolution of oxygen in titanium. However, if this thermodynamic stability of interstitial oxygen was found to occur, then this could provide a driving force for a long-term change in any titanium alloy (i.e. to higher oxygen concentration and hence to higher strength but lower ductility levels). It is worth noting that titanium has only a relatively short history of human usage, with the first semi-industrial quantities being isolated in the UK in ~1947. Thus, the earliest titanium has less than 70 years’ exposure to the environment.

**Creep deformation**

Creep is a long-term deformation process, which occurs under sustained loading, usually at high temperatures, but such deformation can also occur at room temperature in some metals, of which titanium is an example. With the possibility of a sustained load being applied to the compartment and drift plugs, this is a deformation mode that should be considered. It is also worth noting that creep may have the potential to be either detrimental, if it leads to complete rupture of a component (requiring high levels of strain usually) or it can also be beneficial because it permits stress relaxation of localised loads, re-distributing and lowering the applied stress.

A typical creep strain versus time plot for a ductile material is shown in Figure 8-3, where an initial increase in strain rapidly diminishes (known as primary behaviour) to a minimum strain rate, prior to eventually accelerating to failure (known as tertiary behaviour). It was originally thought that a secondary (or steady state) creep rate was attained in the central portion of the deformation versus time curve, however, it is now generally believed that all creep deformation behaviour is transitory in nature. Thus, the changes in behaviour as the minimum creep rate is approached may be small but nonetheless real. This distinction is important as a considerable number of the analytical creep models originally used the secondary creep rate as a characteristic for a given temperature and load condition; however, in reality the minimum creep rate has generally been substituted without particular problems.

---

**Figure 8-2.** Microstructure of ASTM Grade 12 titanium alloy bar – ST – short transverse direction and L – longitudinal direction (i.e. extrusion or rolling direction).
The low temperature creep of titanium has been reviewed previously (Ankem 2006, Dutton 1996a) and these reports provide a good summary of the physical deformation mechanisms which are operative in this regime. The deformation mechanisms vary with both temperature and applied stress. At the likely operating temperatures for the drift and compartment plugs (~20-50 °C) the deformation mechanism may be associated with diffusional flow (at the lowest stresses), and obstacle-controlled plasticity and thence drag-controlled plasticity at the higher stresses. However, as noted above, the Grade 12 titanium alloy will contain a small volume fraction of β phase, which may change the deformation behaviour in comparison to the behaviour for commercial purity grade titanium. The scale and direction of these changes is not easy to predict because of the scarcity of supporting information.

Figure 8-3. Typical creep strain versus time curve for a titanium based material (tested at 700°C), along with a curve showing more brittle behaviour (test at 600°C).

Creep deformation is an area where some work on general titanium alloys has been performed but not specifically on titanium alloy Grade 12. Studies focussing on the low temperature regime for creep deformation in titanium alloys are also relatively scarce and this makes assessment of the likely behaviour difficult. Of the materials evaluated and reported, the commercial purity titanium alloys are probably the nearest to Grade 12 but the presence of the β phase complicates the comparisons. However, in experimental studies the following creep deformation mechanisms have been observed for commercial purity titanium alloys (including Grade 7, which includes some Pd):

- Slip and “time dependent” twinning at applied loads near to the yield strength (Ankem, 2006)
- Slip only at lower loads (down to 65% of the yield strength) (Ankem, 2006)
- Thermally-activated dislocation motion overcoming obstacles (interstitial oxygen and nitrogen in particular) (Dutton, 1996a).

It is worth noting that “time dependent” twinning is an unusual proposed mechanism, as twinning is usually thought of as diffusionless, and occurring at very high speeds. It
has been suggested that a diffusion-based mechanism, grain boundary sliding, which is usually associated with high temperatures, is unlikely because of the low application temperature here. However, caution needs to be applied to this statement because of the limited available data, especially at relatively low loads and for prolonged periods of time.

One important finding is the existence of some long-term (>27 year) creep tests on pure titanium (Drefahl et al. 1985) which will be important in supporting any analysis because of the scarcity of other long-term data on any titanium alloy. Alongside the basic mechanisms of creep in titanium alloys, there are also additional factors to consider, for example, the grain size, microstructural morphology, phase distribution and crystallographic texture. These are not well characterised under low temperature creep conditions. Although generally it would be expected that changing from an equiaxed structure in an α/β alloy to a fully transformed, Widmanstätten type structure would lead to an increase in creep resistance (Ankem 2006).

One interesting finding that requires further evaluation has been the observation that creep strain rates for titanium alloys reduce as the deformation temperature is increased from 25°C up to 100-150°C (Ankem 2007). If this effect is found to be real, then it has been suggested that it may be associated with a change from both slip and twinning at 25 °C and 50 °C to only slip at the higher temperatures (Ankem 2007). Caution should be exercised with this data because only a single creep test was performed under each test condition. The level of variability is not at all clear and higher temperature tests of stainless steels suggest that there can be considerable variability in creep strain behaviour for samples taken from an identical source. Thus, the importance of having an understanding of the level of inherent variability with the creep test data is clear.

**Sustained load cracking**

This is a relatively unusual damage mechanism in current applications of titanium, for example in aerospace. However, some applications in the oil and gas industry have shown this problem, in some instances driven by residual stresses created during welding, and here cracks have developed some time after the structure had been produced (Kostrivas et al. 2003). The phenomena is related to the creep deformation noted above and appears to be associated with local creep ductility exhaustion, crack initiation and thence propagation. There are two principal theories for sustained cracking (Kostrivas et al. 2003):

1) Hydrogen (or hydride formation) at grain or α/β boundaries can weaken these locations and fracture under the application of a sustained load.
2) Mismatch of creep strain accumulation in adjacent grains, due to crystallographic orientation differences, could lead to a large accumulation at some grain boundaries and again lead to fracture. This latter mechanism could also be influenced by the presence of hydrogen.

There appears to be a load threshold, below which cracking does not occur, however, it is not clear how much longer term work has been done in this area, with some work terminating investigations after 720 hours without cracking had been achieved (Kostrivas et al. 2005). There is a suggestion that sustained load cracking is particularly associated with high strength alloys, however, this may just be symptomatic of a low creep ductility.
For the present application and chosen titanium alloy, no direct information has been found on the subject of sustained load cracking. However, any environmental or fundamental thermodynamic microstructural changes that reduce creep ductility may lead to an increased susceptibility to this damage mechanism. Again, this is an area where additional experimental work to support a safety case might be needed but this initial evaluation suggests a relatively low likelihood of this being a problem in the near term, because of an expected relatively high creep ductility for the Grade 12 titanium alloy. Overall, the deformation of the compartment and drift plugs is influenced by the following features of the repository system.

- Temperature: many material properties are temperature dependent.
- Pressure: the internal and external pressures are the primary control on deformation, particularly the external hydrostatic and bentonite swelling pressures.
- Drift geometry: in particular, the dimensions and shape of the drift influence those of the plugs and control stress concentrations in the plug.
- Mechanical stresses: the dominant control on the deformation of the plugs.
- Material composition: is a direct control on the mechanical properties of the titanium plugs (strength, ductility, thermal expansion).

Uncertainties in the understanding of the FEP:

The data from the reviews (Ankem 2006, Dutton 1996a, Kostrivas et al. 2003) considered here suggests that the understanding of the deformation mechanisms (i.e. creep and sustained load cracking) of titanium alloy Grade 12 at low temperature is relatively immature, with marked differences in operating mechanisms being observed and reported. This makes any clear statements on the mechanistic understanding of low temperature titanium creep that are of practical value, difficult to make.

There is an uncertainty about whether oxygen-induced embrittlement of the titanium alloy could occur in the long-term.

There is also a lack of detailed stress analysis information for the drift and compartment plugs during the envisaged operational period.

Full-scale tests with titanium plugs have not yet been done, so their mechanical behaviour in repository-like conditions has not been demonstrated, but the overall uncertainty is related to whether this is at all significant.

Couplings to other FEPs:

Deformation of the compartment and drift plugs is directly affected by the following FEPs:

- Corrosion (of titanium plugs) [8.2.1]
- Water uptake and swelling (in the filling components) [7.2.2]
- Reactivation-displacement along existing fractures (in the geosphere) [10.2.3]
- Creep (in the geosphere) [10.2.5]

Deformation of the compartment and drift plugs directly affects the following FEPs:

- Corrosion (of titanium plugs) [8.2.1]
References:


<table>
<thead>
<tr>
<th>Type:</th>
<th>Process</th>
<th>Class:</th>
<th>System evolution</th>
</tr>
</thead>
</table>

8.2.3 Degradation of the cast concrete for the fastening ring

The degradation processes of concrete are discussed in Chapter 9 under Closure [9.2.8, 9.2.9].

8.3 Migration FEPs

Water transport and gas transport/dissolution are the only hydraulic processes relevant to the drift plug (Gribi et al. 2007, Section 6.5). This applies to compartment plugs as well.

The diffusive and advective mass transport as well as gas transport around the plug are sections of the transport paths, which are formed together with the corresponding sections in the drift at both sides of the plug. Thus, the limitation of transport along these have to be viewed all together as resistances in series.

The drift plugs are not specifically required to provide a barrier to radionuclide transport in the long term. This is because in KBS-3H, the main transport resistance along the axis of the deposition drifts is provided by the buffer (Gribi et al. 2007, Section 6.8). A similar conclusion can be made for the compartment plugs. Due to this, a transport path along the axis of the deposition drift past a compartment plug or a drift plug would have a significantly higher transport resistance than that provided by a transport path from a failed canister to rock fractures intersecting the deposition drift. Radionuclide transport around the compartment and drift plugs is, therefore, not considered a significant process (regardless of the transport properties around the plug) (cf. Gribi et al. 2007, Section 6.8).
### 8.3.1 Diffusion

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th><strong>Class:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Alternative names:</strong></th>
<th><strong>Section in 2007-09:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Advection-diffusion</td>
<td>4.8</td>
</tr>
</tbody>
</table>

**General description:**

The plug occupies most part of the tunnel cross-section and diffusive mass transfer can only take place around the plug through the concrete casting that secures the plug to the rock (see Figure 8-1) and at the rock-concrete interface. The transfer rate depends on the diffusion coefficient in concrete, cross-sectional area and path length around the plug.

General description of diffusion is presented in Section 5.3.4. Diffusion around titanium drift or compartment plugs is a relevant process in cases when different evolution on the different sides of a plug causes concentration differences between the sides. In such cases chemical species tend to equalize between the sides. The extent of equalization depends also on the mass transfer rates on each side of the plug. Especially in longer time scales this means diffusion in drifts or tunnels.

The evolution of the pore spaces and potential cracking of concrete are the dominant controls on the rate of diffusion. The concrete geometry in the notch determines the diffusion lengths and the area through which the diffusive mass transfer can take place. The influence of pore geometry is included in tortuosity and constrictivity, and their effects are seen in the values of the diffusion coefficients.

Evolution of diffusivity through concrete with time has been recently studied by Höglund (2014). Diffusion of radionuclides in concrete-bentonite systems has been studied e.g. by Albinsson et al. (1996).

Overall, the diffusive transport around compartment and drift plugs is influenced by the following features of the repository system.

- **Temperature:** is a control on diffusion rates but at the temperatures expected this may not be a significant effect at depth.
- **Pressure (hydrostatic) differences** may affect diffusive transport.
- **Material composition:** the composition of the plug components and their degradation products influences diffusion and sorption processes. Material composition also affects the availability of soluble substances.
- **Groundwater composition:** the composition of the natural groundwater affects the transport processes as well as the solubility of the plug components (particularly the cast cement) and their chemical equilibration processes.

**Uncertainties in the understanding of the FEP:**

There is a good conceptual understanding of the diffusion process and the evolution of concrete that will occur in water-saturated conditions. There are also good parameter data available for radionuclide diffusivities in concrete material (Höglund 2014). There is, however, some uncertainty about the diffusion rates and processes that may occur in concrete, e.g. cracking. This uncertainty is bounded in the selection of the values of parameters used to analyse them.
**Couplings to other FEPs:**

Diffusive transport around compartment and drift plugs is directly affected by the following FEPs:

- Water uptake and swelling (in the plug-related filling components) [7.2.2]
- Physical degradation (of cement) see [9.2.8]
- Chemical degradation (of cement) see [9.2.9]
- Groundwater flow and advective transport (in the geosphere) [10.3.5]

Diffusive transport around compartment and drift plugs directly affects the following FEPs:

- Advection (in the plug-related filling components) [7.3.5]

**References:**


---

**8.3.2 Advection**

| **Type:** | Process |
| **Class:** | Migration |

**Alternative names:** Advection-diffusion

**Section in 2007-09:** 4.8

**General description:**

General description of advection is presented in Section 5.3.5. Flow around a compartment or drift plug can take place if it is not prevented by the swelling of the drift or tunnel materials on either side of the plug. In early phases before proper swelling of the drift or tunnel materials the casted concrete joint can limit the flow rate past the plug to values that do not cause piping [5.3.5].

The plugs are designed to limit the flow rate to less than 0.1 L/min for a 5 MPa pressure difference over the plug (Posiva 2013a, Section 4.7.1). Such pressure differences occur only in early phases before the resaturation has taken place at both sides of a plug. The tightness of the plug depends on the casted concrete joint between the rock and the fastening ring for the plug itself. Degradation of the concrete could increase the hydraulic conductivity of the concrete, which together with the prevailing head difference determines the flow rate around the plug in long term.

The evolution of the pore spaces and potential cracking of concrete are the dominant controls also on the flow rate. The concrete geometry in the notch determines the hydraulic barrier thickness and the area through which the flow can take place. Evolution of hydraulic conductivities with time through concrete have been recently studied by Höglund (2014).
Overall, the advective transport around compartment and drift plugs is influenced by the following features of the repository system.

- Temperature: is a control on advection but at the temperatures expected this may not be a significant effect at depth.
- Pressure (hydrostatic) affects the rate and direction of advective transport.
- Groundwater composition: the composition of the natural groundwater affects the transport processes (due to density differences) as well as the solubility of the plug components (particularly the cast cement) and their chemical equilibration processes.

**Uncertainties in the understanding of the FEP:**

There is a good conceptual understanding of the process of flow in porous media or fractures and the evolution of concrete that will occur in water-saturated conditions. There are also good parameter data available for radionuclide advection in concrete material (Höglund 2014). There is, however, some uncertainty about the flow rates and processes that may occur in concrete, e.g. cracking. This uncertainty is bounded in the selection of the values of parameters used to analyse them.

**Couplings to other FEPs:**

Advective transport around compartment and drift plugs is directly affected by the following FEPs:

- Water uptake and swelling (in the plug-related filling components) [7.2.2]
- Physical degradation (of cement) see [9.2.8]
- Chemical degradation (of cement) see [9.2.9]
- Groundwater flow and advective transport (in the geosphere) [10.3.5]

Advective transport around compartment and drift plugs directly affects the following FEPs:

- Advection (in the plug-related filling components) [7.3.5]
- Groundwater flow and advective transport (in the geosphere) [10.3.5]

**References:**


### 8.3.3 Gas transport

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th><strong>Class:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
</tr>
</tbody>
</table>

**Alternative names:**
- Two-phase flow; Gas transport/dissolution; Transport of radionuclides in gas phase

**Section in 2007-09:**
4.5, 4.7, 4.8

**General description:**

General description of gas transport is presented in Section 5.3.5. Gas transport around a compartment or drift plug can take place if there is gas on either side or both sides of the plug. Potential gas pressure differences between plug sides are equalized quickly because gas conductivity in concrete is relatively high. Without a gas pressure difference potential gaseous concentration differences equalize by diffusion also rather quickly due to large diffusion coefficients. Thus, the casted concrete joint does not alone hinder very effectively flow of gas or transport of gaseous concentrations. Buffer and filling materials have the main role to control transport in gas phase. This is described in Section 5.3.7. As long as there are gaseous conditions at some part of the casted concrete the gas pressures can equalize quite well.

Overall, the gas transport around compartment and drift plugs is influenced by the following features of the repository system.

- Temperature: is a control on gas generation rates, and thus gas volume transport rate.
- Pressure affects gas volume and transport rate.
- Material composition: the material composition affect properties (porosity, connectivity) that allow gas transport.

**Uncertainties in the understanding of the FEP:**

There is a good conceptual understanding of the flow and transport in gas phase processes in porous media. There is, however, some uncertainty about the gaseous diffusion rates and processes that may occur in concrete, e.g. cracking. This uncertainty is bounded in the selection of the values of parameters used to analyse them. The effect of these uncertainties is relatively low because a small resistance for the gaseous transport past the casted concrete joint of the plug is assigned.
9 CLOSURE

9.1 Description

In the context of **KBS-3H**, closure refers to all backfills and plugs in the underground disposal facility (and in the investigation boreholes) outside the deposition drifts (up to the drift plug). It differs from the KBS-3V closure only with respect to the following.

- The backfill of the deposition niches, which is part of the closure backfill. In Posiva’s 3H repository layout, the connecting tunnels between the double central tunnels serve as deposition niches, but their number is larger and their dimensions different from the 3V connecting tunnels. The backfill material is, however, the same.

- The filling material of the first 10 m or so of the deposition drift before the drift plug (shown as a white area in Figure 5-1). This is considered to be part of the closure, as it will be filled at the same time as the central tunnels and the deposition niche. The planned filling material is of the distance block bentonite type.

In this chapter, FEPs related to **closure backfill** and **closure plugs** used at repository depth are discussed, and due to the use of the same materials as in 3V, the discussion is largely based on Chapters 6 and 7 of Posiva (2012). The closure backfill alternatives for the upper part of the disposal facility are not discussed in this report because no selection of materials has yet been done. The processes in the bentonite filling of the first drift section (before the drift plug) may be assumed to be similar to those in the buffer bentonite (Chapter 5), although they are of lesser significance due to the larger distance from the canister. Therefore, the processes in this drift section are not discussed separately in this report.

The latest closure design has been presented in Sievänen et al. (2012). A flexible tool box approach is adopted for closure; requirements can be achieved with a wide range of material choices. Mechanical plugs will be used for example if there is a need to support the installed backfilling material. Hydraulic plugs are used when the backfill type changes or to isolate major hydraulically conductive zones from adjacent tunnel backfill. The closure of the underground disposal facility is finalised with intrusion obstructing plugs, which are to be installed at the mouths of the access tunnel and shafts (not discussed here). Deep investigation boreholes are planned to be closed using a tight backfill material in non-water conductive sections and concrete plugs in the fractured or water conductive borehole sections (Sievänen et al. 2012).

Closure backfill and plugs will mostly be composed of either clay-based or cementitious materials at repository depth.

The reference design for the central tunnels (and deposition niches) is block and pellet backfill installed in a manner similar to that used in the smaller KBS-3V deposition tunnels (Keto et al. 2013). The blocks are currently designed to be composed of 100 % Friedland Clay or other suitable swelling clay and the pellets/granules are produced from high-smectite-content bentonite (Sievänen et al. 2012, Section 3.2).
For plugs at the repository level, a low-pH concrete is planned to be used. The low pH concrete is currently under development and will be based on the formulation given in Table 9-1. In the upper parts of the disposal facility, standard OPC-based cement is planned to be used for plugs. This is reflected in the current FEPs.

Other cementitious components that may be present in the repository system after closure include shotcrete, rock bolt grouts and cementitious injection grouts, although the majority of the shotcrete will be removed before closure (Karvonen 2011). No cementitious grouts are planned to be used in the deposition drifts.

The use of the various closure components in the different parts of the disposal facility (central tunnels, technical rooms, access tunnel, shafts, investigation boreholes) are described in detail in Sievänen et al. (2012).

9.1.1 Long-term safety and performance

The primary requirement of the closure components is to isolate and decouple the repository from the surface environment, including people, animals and plants. Thus, the safety functions assigned to closure are to (Posiva 2016c):

- prevent the underground openings from compromising the long-term isolation of the repository from the surface environment and normal habitats for humans, plants and animals,
- contribute to favourable and predictable geochemical and hydrogeological conditions for the other engineered barriers by preventing the formation of significant water conductive flow paths through the openings, and
- limit and retard inflow to and release of harmful substances from the repository.

Swelling and mechanical erosion of the clay-based closure materials are coupled processes that may affect their performance during the resaturation period, and so are highly dependent on the hydraulic behaviour of the near-field rock. Over both the short and long-term periods, chemical processes (e.g. chemical degradation and leaching of cement) may locally affect the performance of the closure components.

Table 9-1. Reference recipe for the low-pH concrete planned to be used in the closure plugs. Data from Vogt et al. (2009).

<table>
<thead>
<tr>
<th>Design parameter</th>
<th>Material</th>
<th>Composition (kg/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Binder</td>
<td>Cement CEM I 42.5 MH/LA/SR</td>
<td>120</td>
</tr>
<tr>
<td></td>
<td>Densified silica fume</td>
<td>80</td>
</tr>
<tr>
<td>Water</td>
<td>Tap water</td>
<td>165</td>
</tr>
<tr>
<td>Filler</td>
<td>Limestone filler L25</td>
<td>369</td>
</tr>
<tr>
<td></td>
<td>Sand 0-8 mm</td>
<td>1037</td>
</tr>
<tr>
<td></td>
<td>Gravel 8-16 mm</td>
<td>558</td>
</tr>
<tr>
<td>Admixture</td>
<td>Superplasticiser Glenium 51</td>
<td>6.38</td>
</tr>
</tbody>
</table>
9.1.2 Overview of the potentially significant FEPs

There are a number of processes that are considered to be significant for the long-term performance of the closure components at repository level that relate to system evolution and to the migration of radionuclides and other substances. The processes are organised in this chapter so that the backfill-related processes are discussed first, followed by the plug-material-related processes.

Processes related to system evolution are:

9.2.1 Water uptake and swelling
9.2.2 Mechanical erosion
9.2.3 Chemical erosion
9.2.4 Montmorillonite transformation
9.2.5 Alteration of accessory minerals
9.2.6 Microbial activity
9.2.7 Freezing and thawing
9.2.8 Chemical degradation (of closure plugs)
9.2.9 Physical degradation (of closure plugs)
9.2.10 Freezing and thawing (in closure plugs)

Processes related to the migration of radionuclides and other substances are:

9.3.1 Transport through closure backfill and plugs

These processes are each potentially affected by a number of features of the repository system that can influence the occurrence, rate, activity and potential couplings between the processes. These features relate either to aspects of the design of the repository system or to parameters (characteristics) of the closure components that might be time-dependent during the repository lifetime. The most significant features are:

- Radionuclide inventory
- Temperature
- Pressure
- Tunnel geometry
- Mechanical stresses
- Material composition
- Groundwater composition.

The possible influences of these features on the processes considered to be significant for the long-term performance of the closure components are described in each FEP description.

Similarly, due to the interactions between the various parts of the disposal system, the evolution of the closure components can influence (or be influenced by) processes occurring in other parts of the repository system through interactions between various processes. For example, chemical degradation [9.2.8] interacts with groundwater flow and advective transport in the geosphere [10.3.5].
9.2 System evolution FEPs

The function of the closure backfill at repository level (mainly central tunnels) differs from that of the KBS-3V deposition tunnel backfill (discussed in Chapter 6 of Posiva 2012d) in that it is not required to restrain the swelling of the buffer installed in the deposition holes and is not required to have a substantial swelling capacity (swelling pressure). It does, however, have requirements that call for the use of uncompressible or swelling backfill (Sievänen et al. 2012, Section 3.2). There is, for example, a requirement to prevent the formation of preferential flow paths and to keep the KBS-3H drift materials in place should the drift plug be damaged.

Various chemical and mechanical processes, and their couplings, will affect the evolution of the closure components. Thermal processes are not explicitly considered because the heat source is not in the immediate surroundings of the closure backfill. The emphasis here is on the closure backfill at repository depth, as no materials have been yet selected for other parts of the closure. The behaviour of these components and the achievement of their safety functions will depend on the times and rates at which these processes occur. The following descriptions summarise each of these processes and the effects of the different variables on them. The couplings of these FEPs with other FEPs are thus indicated, but the consequences of the interaction or combinations of interactions will be discussed in Posiva (2016b).
9.2.1 Water uptake and swelling

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Alternative names:</th>
<th>Section in 2007-09:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water uptake; Swelling and mass distribution; Homogenisation (being the consequence)</td>
<td>Not applicable</td>
</tr>
</tbody>
</table>

**General description:**

Water uptake and swelling in the closure backfill is essentially the same process as water uptake in the buffer [5.2.2] although, at a detailed level, it is potentially a more complex mechanism affected by multiple variables due to:

- the greater potential for heterogeneity in the intersecting flowing fracture network in the rock that controls water flow; and
- the greater heterogeneity in subcomponents and material types, and layout (and void spaces) in the closure backfill than in the buffer.

The main factors affecting water uptake in the closure backfill (‘wetting’) are the prevailing groundwater pressure in the surrounding rock and the negative capillary pressure (total suction) drawing water into the backfill material. Water transport can take place either in the liquid or vapour phase, although vapour transport is less significant than for the buffer because of the lower temperatures that are expected.

The hydraulic conductivity of the closure backfill depends on the mineral composition, particularly the amount and type of expandable clay minerals, the density/porosity, degree of saturation (water retention curve) and salinity of the groundwater. The suction also depends on these factors, with suction reducing as the degree of saturation increases.

The closure backfill will have an initial water content depending on the composition of the Friedland or any other selected swelling clay and the nature of the backfill blocks. Groundwater will flow into the central tunnels from water-bearing fractures with varying inflow rate and pressure, and at different locations along the tunnel walls. The natural heterogeneity in the fracture network will mean that water uptake will be unequal along the mass of the backfill and, therefore, swelling will initially be heterogeneous.

As the closure backfill continues to absorb water and swell, further water uptake will depend on the evolving hydraulic conductivity and the pore water pressure gradient in
the backfill material. Once complete saturation is reached, the final swelling pressure and hydraulic conductivity will be such that diffusion will become the dominant transport process [9.3.1].

If free air is trapped in the tunnel, this will delay the saturation process while the air is compressed and becomes dissolved in the inflowing groundwater (Henry’s law). Only a limited amount of air can be dissolved into the water and, therefore, it may take some time for all of the free gas to be removed by dissolution and diffusion.

The time necessary for complete saturation of the closure backfill depends strongly on the local groundwater conditions and the fracture network. The water uptake and swelling process in the closure backfill is, however, expected to be faster than in the buffer because the tunnels will intersect more water-conducting fractures and the hydraulic conductivity of the closure backfill is higher than in the buffer (Sievänen et al. 2012). A high water pressure in the near-field rock may lead to mechanical erosion of the closure backfill during the early saturation stage [9.2.1] which may cause a slight increase in the overall saturation rate.

It is estimated that the time for complete saturation to be achieved could range from several months to a few thousand years for the case where there is low availability of water in the near field.

Continued water uptake and swelling will eventually lead to homogenisation of the backfill material and its density, and cause self-sealing of any voids and piping channels. The final swelling pressure will depend on the initial density and amount of swelling minerals within the Friedland or other selected swelling clay. Whether the swelling of backfill material is sufficient to fill the voids left after emplacement of the closure backfill depends importantly on the backfill geometry and extent of over-excavation of the tunnels (e.g. Åkesson et al. 2010).

Overall, water uptake and swelling of the closure backfill is influenced by the following features of the repository system.

− Temperature: the availability and behaviour of water in the closure backfill during saturation will depend on this variable.

− Pressure: Overall hydrostatic and swelling pressure will affect hydraulic conductivity in the closure backfill.

− Tunnel geometry: the size and distribution of void spaces between the backfill and the rock will influence the rate of water uptake and the final swelling pressure.

− Material composition: the proportion of swelling clays in the backfill material will affect the swelling pressure and hydraulic conductivity.

− Groundwater composition: the groundwater composition affects the backfill porewater composition, and the ionic concentration of the porewater may affect the hydraulic conductivity of the backfill.

**Uncertainties in the understanding of the FEP:**

Water uptake and swelling in the closure backfill is a process determined by many coupled sub-processes and influenced by features in the backfill and the near-field rock. Groundwater conditions (inflow, pressure, salinity) are Olkiluoto-specific and very localised (being strongly determined by the characteristics of fracture networks) and control the rate and heterogeneity of saturation. A key uncertainty is the density and
distribution of the fractures and their capacity to maintain a constant flow. The saturation
time and final swelling pressure is uncertain due to heterogeneities in the system.
Uncertainties are taken into account by conservatively assuming for the closure larger
hydraulic conductivity values than expected.

**Couplings to other FEPs:**
Water uptake and swelling of the closure backfill is directly affected by the following
FEPs:
- Mechanical erosion [9.2.2]
- Montmorillonite transformation [9.2.4]
- Alteration of accessory minerals [9.2.5]
- Freezing and thawing [9.2.7]
- Groundwater flow and advective transport (in the geosphere) [10.3.5]

Water uptake and swelling of the closure backfill directly affects the following FEPs:
- Mechanical erosion [9.2.2]
- Chemical erosion [9.2.3]
- Montmorillonite transformation [9.2.4]
- Alteration of accessory minerals [9.2.5]
- Microbial activity [9.2.6]
- Freezing and thawing [9.2.7]
- Physical degradation (closure plugs) [9.2.9]
- Transport through closure backfill and plugs [9.3.1]
- Stress redistribution (in the geosphere) [10.2.2]
- Rock mass damage (in the geosphere) [10.2.4]

**References:**
modeling of buffer, backfill and other system components. Critical processes and
scenarios, Stockholm, Sweden: Swedish Nuclear Fuel and Waste Management Co.

Production Line 2012 – Design, production and initial state of closure. Eurajoki,

9.2.2 Mechanical erosion

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:**
Piping and erosion

**Section in 2007-09:**
Not applicable

**General description:**
During the initial hydraulic saturation phase, significant volumes of groundwater may
flow into the central tunnels through intersecting, hydraulically active fractures. If
the rate of inflow exceeds the rate of water uptake [9.2.1] then active flow channels
or ‘pipes’ will develop in the closure backfill.
Mechanical erosion in the closure backfill is essentially the same process as in the buffer [5.2.3] although, at a detailed level, there may be differences due to:

− the greater potential for larger flowing fractures to intersect the central tunnels than the drifts; and
− the final swelling pressure is lower and the hydraulic conductivity is higher in the closure backfill than in the buffer.

The closure plugs (see below) will be important for minimising lateral movement of eroded backfill material along the length of the central tunnels. The risk of mechanical erosion is reduced as the closure backfill progressively absorbs groundwater because the consequent increase in swelling pressure limits further localized water inflow.

Mechanical erosion has been studied under laboratory conditions for both the buffer and the tunnel backfill materials (Sandén et al. 2008, Sandén & Börgesson 2010) for KBS-3V. Various laboratory experiments have also been performed on compacted blocks and pellets using MX-80 bentonite with different geometries of open flow channels, water flow rates and salinities. Erosion rates and accumulated eroded masses were observed to increase as a function of salinity, flow rate and the length of the erosion channel. Similar qualitative trends have been recorded in other experiments, and an empirical formulation for accumulated eroded mass as a function of total effluent volume has been developed (Sandén & Börgesson 2010).

Based on field-scale testing, the erosion of potential closure backfill materials having a content of swelling clay of the same order of magnitude as in Friedland clay or even higher, as in the case of pellets, depends on the inflow rate, the location of the piping channels, the density of the backfill materials and the salinity of the water (Dixon et al. 2008a, 2008b, 2011, Korkiala-Tanttu et al. 2011). In addition, the rate of erosion has the tendency to decrease over time. Nonetheless, given the total mass of backfill materials, the overall effect of erosion on the backfill materials is negligible (SKB 2010).

Overall, mechanical erosion is influenced by the following features of the repository system.

− Pressure: overall hydrostatic and swelling pressure will influence mechanical erosion.
− Backfill geometry: the size and distribution of void spaces between the backfill and the rock will influence the rate of water uptake and the potential for mechanical erosion.
− Material composition: affects pore geometry, swelling pressure and hydraulic conductivity.
− Groundwater composition: affects the rate and magnitude of free swelling.

**Uncertainties in the understanding of the FEP:**

Mechanical erosion and the subsequent sealing of the closure backfill are coupled processes that are highly dependent on the hydraulic behaviour of the rock. Uncertainties exist regarding both the influence of the rock hydrogeology and the ability of the closure backfill to respond to these processes.

Empirically, the understanding of when mechanical erosion may occur and the consequences are reasonably well understood. The specific dependence of the rate of erosion on features of the repository system (such as flow rate, salinity, initial water content and initial dry density) are less established.
**Couplings to other FEPs:**

Mechanical erosion in the closure backfill is directly affected by the following FEPs:
- Water uptake and swelling [9.2.1]
- Transport through closure backfill and plugs [9.3.1]
- Groundwater flow and advective transport (in the geosphere) [10.3.5]

Mechanical erosion in the closure backfill directly affects the following FEPs:
- Water uptake and swelling [9.2.1]
- Transport through closure backfill and plugs [9.3.1]
- Erosion and sedimentation in fractures (in the geosphere) [10.2.6]
- Colloid transport (in the geosphere) [10.3.6]

**References:**


### 9.2.3 Chemical erosion

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th>Process</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Class:</strong></td>
<td>System evolution</td>
</tr>
</tbody>
</table>

| **Alternative names:** | Chemical erosion |
| **Section in 2007-09:** | Not applicable |
General description:

Chemical erosion refers to the loss of swelling clay material from the closure backfill due to interactions with dilute groundwater. As the closure backfill saturates and swells, it will extrude into the hydraulically active rock fractures that intersect the tunnels. Upon contact with more dilute groundwater, the extruded backfill material may continue to expand and lose density until it begins to move in a gel state with the flowing groundwater. Clay particles are then removed from the extruded gel front due to shear forces and are dispersed as a colloidal sol, which is then transported away (Neretnieks et al. 2009, Moreno et al. 2010).

Chemical erosion in the closure backfill is essentially the same process as in the buffer [5.2.4] and KBS-3H filling components although, at a detailed level, there may be differences due to:

- the greater potential for larger flowing fractures to intersect the central tunnels than the drift;
- the larger perimeter of fracture intersection in the tunnel;
- the lower montmorillonite/smectite content of the closure backfill material relative to the buffer and filling component material;
- type of smectite; and
- the lower swelling pressure and higher hydraulic conductivity in the backfill than in the buffer and filling components.

The free-swelling behaviour of smectite is strongly dependent on the valency and ion concentration in the interlayer space of the mineral structure (Birgersson et al. 2009). The groundwater composition (primarily electrolyte content and pH), backfill composition, groundwater velocity and fracture aperture are the main parameters that control chemical erosion of the backfill in dilute groundwater. The groundwater composition defines the dilute conditions under which erosion may take place. The groundwater velocity controls the rate of mass loss for the flowing gel and dispersed particle erosion mechanisms as well as controlling the shear forces (Moreno et al. 2010). The fracture aperture will determine the surface area at the extruded clay/groundwater erosion interface. The smectite composition is important, because clays with a calcium fraction greater than 20 % are observed to be less susceptible to chemical erosion (Birgersson et al. 2009).

Numerous field and laboratory experiments have assessed montmorillonite colloid generation and stability (Wold 2010). The general consensus is that there is a critical groundwater salinity below which chemical erosion would occur and montmorillonite colloids would be stable.

Overall, chemical erosion is influenced by the following features of the repository system.

- Pressure: overall hydrostatic and swelling pressure will control chemical erosion.
- Tunnel geometry: influences the geometry of the backfill and thus its hydraulic conductivity as well as the total clay mass available for erosion.
- Material composition: defines the amount and nature of soluble accessory minerals which affect porewater composition and, thereby, the susceptibility of montmorillonite to erosion.
- Groundwater composition: primarily the cation content, affects the generation and stability of bentonite colloids.
Uncertainties in the understanding of the FEP:
Chemical erosion of the closure backfill in an intersecting, transmissive fracture environment by dilute groundwater is a highly complex, coupled transport process involving backfill material evolution, groundwater composition evolution, and bedrock hydrogeology. There is a possibility that, due to erosion, accessory mineral particles in the closure backfill will build-up and form a ‘filter cake’ limiting further loss of mass. Experimental results indicate that mass loss can slow down or possibly stop due to filtration effects (Birgersson et al. 2009, Schatz et al. 2011).

The potential presence of dilute groundwater in the geosphere is generally considered to result from the infiltration of glacial meltwaters. There is no palaeohydrogeochemical evidence, however, to indicate that dilute glacial meltwater has ever penetrated down to repository depths in the Olkiluoto area (Posiva 2013c) and, consequently, such meltwaters are not expected to do so in the future.

Couplings to other FEPs:
Chemical erosion in the closure backfill is directly affected by the following FEPs:
- Water uptake and swelling [9.2.1]
- Groundwater flow and advective transport (in the geosphere) [10.3.5]
Chemical erosion in the closure backfill directly affects the following FEPs:
- Water uptake and swelling [9.2.1]
- Transport through closure backfill and plugs [9.3.1]
- Erosion and sedimentation in fractures (in the geosphere) [10.2.6]
- Colloid transport (in the geosphere) [10.3.6]

References:


### 9.2.4 Montmorillonite transformation

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th><strong>Class:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

#### Alternative names:
Mineral (montmorillonite) transformation

#### Section in 2007-09:
Not applicable

#### General description:
The ability of the closure tunnel backfill to act as a diffusive, self-sealing barrier is due to the montmorillonite content in the backfill blocks and in the bentonite pellets placed in the void space between the backfill blocks and the rock.

Mineral transformations of the montmorillonite can potentially cause it to lose its swelling capability and increase its hydraulic conductivity so that, if transformation occurred throughout the bulk of the backfill, the swelling pressure could be reduced allowing advective flow (e.g. [5.3.5]) to occur.

Montmorillonite in the closure backfill can be altered in a number of different reactions and transformations. These can be divided into:
- cation-exchange reactions,
- protonation-deprotonation of mineral surfaces,
- alterations to the structural composition and layer charge,
- mineral transformations,
- cementation, and
- reactions with other repository materials.

These reactions and transformations are described for montmorillonite in the buffer [5.2.6] and the same processes will occur in the closure backfill although, at a detailed level, there may be differences due to:
- the maximum temperature reached in the closure backfill being less than that estimated for the deposition tunnel backfill in a KBS-3V repository (< 33–50 °C) and much less than in the buffer (95 °C), consequently dissolution/precipitation of minerals due to temperature effects is of no significance in the closure backfill;
- there are likely to be a larger number of flowing fractures that intersect the central tunnels than the KBS-3H supercontainer sections, and so the composition of groundwater may have a much higher impact on montmorillonite transformation than in the buffer; and
- the closure backfill is in direct contact with a range of other engineered materials, notably any cementitious closure plugs, which can promote local transformation of montmorillonite (Lehikoinen 2009), although at repository depth only low-pH cement will be used in the closure plugs.

Importantly, only a small fraction of the radionuclides that may be released from a failed canister are likely to reach the closure backfill (compared with the bentonite in the KBS-3H drift), and the consequences of montmorillonite transformation for radionuclide transport by advection in the central tunnels [9.3.1] are limited.
Overall, montmorillonite transformation processes in the closure backfill are influenced by the following features of the repository system.

- Temperature: controls the rate of the reactions that cause the mineral transformations, and the temperature gradients that can lead to silica migration.
- Material composition: significant for all chemical reactions in the closure backfill.
- Groundwater composition: significant for all chemical reactions in the backfill as it affects the porewater composition, especially its salinity and content of cations.

**Uncertainties in the understanding of the FEP:**

The composition of the closure backfill porewater and the near-field groundwater may vary during the evolution of the repository (especially salinity and the abundance of exchangeable cations such as Ca).

It has been acknowledged that the effects of cementitious material and external sources of silica (e.g. from low pH cement) on the long-term evolution of the backfill is not fully understood, but is thought to be negligible due to the large amount of backfill compared to the amount of cement or sources of silica.

**Couplings to other FEPs:**

Montmorillonite transformation in the closure backfill is directly affected by the following FEPs:

- Water uptake and swelling [9.2.1]
- Alteration of accessory minerals [9.2.5]
- Chemical degradation (of closure plugs) [9.2.8]
- Rock-water interaction (in the geosphere) [10.2.7]

Montmorillonite transformation in the closure backfill directly affects the following FEPs:

- Water uptake and swelling [9.2.1]
- Alteration of accessory minerals [9.2.5]
- Transport through closure backfill and plugs [9.3.1]

**References:**


### 9.2.5 Alteration of accessory minerals

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Alternative names:</th>
<th>Section in 2007-09:</th>
</tr>
</thead>
<tbody>
<tr>
<td>None</td>
<td>Not applicable</td>
</tr>
</tbody>
</table>

**General description:**

The hydraulic and physical properties of the closure backfill after water uptake are controlled by the swelling pressure generated by the montmorillonite. The chemical properties of the backfill are largely determined by accessory minerals, such as other
silicates (feldspars, quartz, cristobalite), sulphides (pyrite), sulphates (gypsum),
carbonates (calcite, dolomite, siderite), etc., some of which may generally be much
more reactive and soluble than montmorillonite under the geochemical conditions
expected in the near field.

Alteration of these accessory minerals is described for the buffer [5.2.7] and broadly
the same processes will occur in the closure backfill although, at a detailed level, there
may be differences due to:

− the maximum temperature reached in the closure backfill is less than that estimated
  for the backfill in a KBS-3V repository (< 33–50 °C) and much less than in the
  buffer (95 °C), consequently dissolution/precipitation of minerals due to
temperature effects are of no significance in the closure backfill;
− the backfill material contains a much greater proportion of accessory minerals
  compared with the bentonite planned to be used in the buffer, and the chemical
  composition of accessory minerals in the backfill may also be different from that
  of the buffer materials;
− there are likely to be many more large flowing fractures that intersect the tunnels
  than the KBS-3H drift, and so the turnover of water may be much higher than in
  the buffer, and
− the closure backfill is in direct contact with a range of other engineered materials,
  notably the cementitious closure plugs (of low-pH cement at repository depth),
  which may promote local transformation of accessory minerals within the backfill
  material.

It is assumed that the pH of the porewater in the closure backfill will be buffered by the
equilibrium with carbonates and also by proton buffering of clay (through reactions at
edge sites). Due to variations in the mineralogical composition of Friedland or other
swelling clay, the abundance of these pH buffering mineral phases is somewhat uncertain.

In contrast to the buffer, microbial activity is possible in the closure backfill [9.2.6].
The rate of redox reactions (e.g. sulphate reduction) can be increased by many orders
of magnitude in the presence of and due to the activity of such microbes.

Overall, the alteration of accessory minerals (and impurities) is influenced by the
following features of the repository system.

− Temperature: controls the rate of the reactions that cause mineral alteration and
temperature gradients can lead to silica migration.
− Material composition: significant for all chemical reactions in the closure backfill.
− Groundwater composition: significant for all chemical reactions in the closure
  backfill as it affects the porewater composition, especially its pH and silica
  content.

**Uncertainties in the understanding of the FEP:**

There is a natural variation in the initial mineralogical composition of batches of
Friedland clay (Kumpulainen & Kiviranta 2010). The main uncertainty regarding
transformation of accessory minerals is the definition of the range of mineralogical
compositions of the material allowed to be used in the repository system. Work is
ongoing to reduce this uncertainty.
No specific studies of chemical processes in the backfill have been done and the evaluation has to be based on the studies performed on bentonites and extrapolation from buffer studies. The differences in the composition, physical properties, temperature etc. have to be considered in the applicability of buffer data to the closure backfill. These differences are, however, considered to be adequately addressed when making bounding estimates of the potential effects of the accessory minerals assuming amounts and types of accessory minerals that are substantially different from those in the buffer.

**Couplings to other FEPs:**
Alteration of accessory minerals is directly affected by the following FEPs:
- Water uptake and swelling [9.2.1]
- Montmorillonite transformation [9.2.4]
- Microbial activity [9.2.6]
- Chemical degradation (of closure plugs) [9.2.8]
- Rock-water interaction (in the geosphere) [10.2.7]

Alteration of accessory minerals directly affects the following FEPs:
- Water uptake and swelling [9.2.1]
- Montmorillonite transformation [9.2.4]
- Transport through closure backfill and plugs [9.3.1]

**References:**

<table>
<thead>
<tr>
<th>9.2.6 Microbial activity</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Type:</strong> Process</td>
</tr>
<tr>
<td><strong>Alternative names:</strong> None</td>
</tr>
</tbody>
</table>

**General description:**
Microbes can exist naturally in deep rock and groundwater systems, and these may migrate into the closure backfill during saturation and water uptake [9.2.1]. Many other microbes will be introduced directly into the disposal facility from the surface with the backfill blocks and other engineering materials (e.g., Hallbeck 2010). These microbes may potentially affect the geochemical system in the backfill provided they maintain viable and active populations under repository conditions.

From a microbiological perspective, the backfill environment has several characteristics that significantly distinguish it from the geosphere. Those characteristics include the presence of organic impurities and stray materials (nutrients) in the backfill; the presence of oxygen (air) in the backfill pores and in infiltrating groundwater for a period of time until the oxygen has been consumed by microbial and/or redox reactions; and the presence of an air/water interface that will develop during the saturation process. All of these characteristics are conducive to the presence of active microbial populations.
Microbial activity in the closure backfill would, in general terms, consist of the same processes as in the buffer [5.2.8] and geosphere [10.2.10] although, importantly, microbial populations are considered much more viable and active in the closure backfill and at backfill-rock interfaces than in the buffer. This is due to the lower swelling pressure, higher water content, higher nutrient content and larger pore spaces in backfill materials and at backfill-rock interfaces (e.g., Stroes-Gascoyne et al. 2010, Stroes-Gascoyne et al. 2007). Consequently, their significance for the production of sulphide through sulphate reduction by sulphate-reducing bacteria (SRB) in the backfill and at interfaces may be greater than in the buffer though of less consequence as the closure backfill is far from the canister and buffer in the drift.

After closure and backfilling of the tunnels, the saturation process by groundwater will proceed. Microbes will be present in the groundwater and these microbes will mix with the backfill, which also contains microbes. As the closure backfill candidate Friedland clay contains nutrients such as organic material (Kumpulainen & Kiviranta 2010), microbial activity will be initiated.

The initial oxygen, present in the air trapped in the backfill pores and in the groundwater infiltrating the backfill, will be consumed rapidly by microbial oxidation of organics (Lydmark & Pedersen 2011) including methane as the groundwater at Olkiluoto is rich in methane (Pedersen 2008). It is likely that all of the oxygen in the backfill pores and dissolved in the groundwater will be consumed within a short time after closure, although pockets of air may persist for longer.

Mass balance calculations can be used to evaluate how different kinds of residual materials remaining in the repository system could contribute to microbial oxygen reduction. Important nutrients are organic matter (including methane) and hydrogen gas. Microbes are expected to use all available organic matter first. The supply of hydrogen will be decisive for microbial activity in the long term. This implies that an enhanced effect of microbial activity must be expected until all organic matter has been consumed, and that subsequently an activity that is controlled by the supply of hydrogen will proceed. This means that oxygen, ferric iron, sulphate and carbon dioxide will be reduced to water, ferrous iron, sulphide and methane, respectively. The extent of these reactions is dependent on mass flows.

Overall, microbial activity in the closure backfill is influenced by the following features of the repository system.
- Temperature: temperature increase may enhance microbial activity.
- Material composition: the content of organic carbon is important as a nutrient.
- Groundwater composition: controls the availability of water and nutrients for microbial activity.
- Pressure: overall hydrostatic and swelling pressure may constrain activity by limiting pore size, although this is less significant in the backfill than in the buffer.
- Tunnel geometry: control the backfill geometry and thus the size and shape of the pores that may constrain microbial activity, thought material composition is the major influence.

Uncertainties in the understanding of the FEP:
There are a number of uncertainties related to the understanding of microbial activity in the closure backfill. The conceptual understanding of microbial processes in the backfill is not yet well supported by experimental data. Rather, the processes are inferred from research on microbial processes in the geosphere and in buffer materials.
**Couplings to other FEPs:**

Microbial activity in the closure backfill is directly affected by the following FEPs:

- Water uptake and swelling [9.2.1]
- Transport through closure backfill and plugs [9.3.1]
- Microbial activity (in the geosphere) [10.2.10]

Microbial activity in the closure backfill directly affects the following FEPs:

- Microbial activity (in the geosphere) [10.2.10]
- Alteration of accessory minerals [9.2.5]
- Transport through closure backfill and plugs [9.3.1]

**References:**


| 9.2.7  Freezing and thawing (in closure backfill) |
|---|---|
| **Type:** | Process |
| **Class:** | System evolution |
| **Alternative names:** | None |
| **Section in 2007-09:** | Not applicable |

**General description:**

Repeated glaciation and deglaciation events related to climate evolution [see 10.2.1 in Posiva 2012d] are expected to occur at Olkiluoto in the future.

The onset of glacial conditions [see 10.2.2 in Posiva 2012d] will be accompanied by permafrost [10.2.3 in Posiva 2012d]. Numerical simulations of ground temperature using pessimistic conservative boundary conditions indicate a maximum penetration depth of freezing temperatures to around 275–300 m (Hartikainen 2012).
In the very unlikely event of permafrost reaching repository depth, the backfill materials are expected to be fully water saturated when it might happen. The freezing point of porewater in the backfill is not precisely known but is likely to be lower than 0 °C. For example, considering saturated Friedland clay and Milos backfill materials with unfrozen swelling pressures close to 2 MPa, freezing points between −2 and −3 °C were experimentally observed (Schatz & Martikainen 2012, Birgersson et. al 2010). The primary consequence of confining water in porous material is a depression to lower temperature of the melting transition due to the Gibbs-Thomson effect (Dash et al. 2006). Additional factors, such as the specific surface area of the porous medium, its chemical and mineralogical composition, the nature of the exchangeable cations, and the content and composition of soluble compounds in the porewater affect the freezing point depression as well (Neresova & Tystovich 1966). Numerous experiments have demonstrated that the melting temperatures of materials are depressed in porous media (Dash et al. 2006).

If permafrost develops in the closure backfill, there will be a relative volume and stress increase resulting in increased pressure from the backfill on the bedrock. Two sets of independent experiments have investigated the effect of freezing and thawing on fully-saturated buffer and backfill materials (Birgersson et al. 2010, Schatz & Martikainen 2012). The main conclusions from these studies were that exposure to freezing temperatures results in a loss of swelling pressure until a critical temperature is reached followed by the development of significant internal pressures in compacted buffer and backfill samples, and that such pressures are attributed to the formation of ice in these samples.

It was shown that backfill swelling pressures will decrease when external water is frozen but the material itself remains unfrozen and that such decreases are expected on the basis of a theoretical description of the swelling pressure response at temperatures above the freezing point of the material (Birgersson et al. 2010). Increases in pressure, due to ice formation, were observed at temperatures below the freezing point (Schatz & Martikainen 2010). Furthermore, the effects of freezing were shown to be entirely reversible, because swelling pressure and hydraulic conductivity returned to the pre-freezing levels upon thawing, even after multiple freezing and thawing cycles.

When ice forms in freezing porous media, there is a corresponding increase in volume and/or pressure, depending on the particular confining stresses and the permeability of the material to water migration (Smith & Onysko 1990). For a situation involving equal pressure changes on the ice and water phases in the material, corresponding to a hydraulically closed frozen repository, the Clapeyron equation predicts a large increase in pressure for small changes in temperature below the freezing point, i.e. −13.49 MPa/°C. Alternatively, for a situation involving unequal pressure changes on the ice and water phases, corresponding to a hydraulically-open, partially frozen repository where the frozen material is connected to unfrozen groundwater, the generalised Clapeyron equation predicts a more modest increase in pressure for temperatures below the freezing point, i.e. −1.12 MPa/°C. The latter situation is thought to correspond to the phenomenon of frost heave, which is equivalent to the maximum pressure that can develop as a result of the flow of unfrozen liquid to the freezing front.

Additionally, the loss in swelling pressure between the freezing point of water in the host rock and the freezing point of water in the backfill, as well as the freezing point of water in the backfill, can be determined (Birgerssson et al. 2010). For example, in a
homogenised, fully-saturated backfill system with a swelling pressure of 3 MPa, a freezing point of –2.5 °C is estimated.

Overall, freezing and thawing in the closure backfill is influenced by the following features of the repository system.

- Temperature: the geothermal gradient and heat exchange across the atmosphere/ground interface controls the temperature in the rock.
- Pressure: the hydrostatic and swelling pressure will affect the temperature at which freezing of the porewater will occur.
- Tunnel geometry: the size and geometry of the tunnels potentially exposed to permafrost will affect the mass of backfill that can freeze.
- Material composition: the freezing point is affected by the specific surface area and soluble accessory mineral composition; the higher the material density the lower the freezing point.
- Groundwater composition: significant because the composition of the porewater affects the temperature at which it freezes, the higher the salinity the lower the freezing point.

**Uncertainties in the understanding of the FEP:**

The exact temperature evolution in the closure backfill is a source of uncertainty. It is also uncertain to what extent the Clapeyron and generalised Clapeyron equations can be considered to yield, possibly overly, conservative predictions with regard to pressure increases due to ice formation in backfill material.

**Couplings to other FEPs:**

Freezing and thawing in the closure backfill is directly affected by the following FEPs:

- Heat transfer [10.2.1]
- Water uptake and swelling [9.2.1]
- Permafrost formation [see 10.2.3 in Posiva 2012d]

Freezing and thawing in the closure backfill directly affects the following FEPs:

- Water uptake and swelling [9.2.1]
- Transport through closure backfill and plugs [9.3.1]

**References:**


9.2.8 Chemical degradation (of closure plugs)

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Alternative names:</th>
<th>Section in 2007-09:</th>
</tr>
</thead>
<tbody>
<tr>
<td>None</td>
<td>Not applicable</td>
</tr>
</tbody>
</table>

General description:

After closure of the disposal facility, groundwater will flow into the repository openings from the near-field rock [10.3.5] and the closure components will become water saturated. For some tunnel locations, unsaturated conditions may prevail longer than for others, depending on the local groundwater flow conditions. Concrete plugs in contact with groundwater may deteriorate due to leaching, alteration of their component minerals and gel phases, and by carbonation. Chemical degradation may also affect the clay-based closure components by mineralogical changes [9.2.4, 9.2.5].

The chemical degradation of the concrete plugs may have two significant effects. First, the increase potential for groundwater flow and advective transport. This will also increase their susceptibility to physical degradation [9.2.9]. Second, the alkaline plume generated by degradation of the plugs may interact with clay components causing a loss of swelling pressure and a reduction in the safety performance of the clay components in the KBS-3H deposition drifts and in the closure backfill. Depending on the composition of the groundwater, dissolved chloride, sulphate and magnesium can act as corroding agents for the concrete plugs. Chemical degradation of cement is mainly a coupled diffusion-reaction phenomenon, and the time needed for complete degradation of the concrete plugs will be highly dependent on the relative surface area of the concrete where diffusion exchange with water takes place as well as on the groundwater composition.

The plug(s) are to be constructed of low-pH cement intended to minimise the consequences of the alkaline plume causing a loss of swelling pressure in the buffer and closure backfill.

The chemical degradation of standard cementitious materials is well understood but there are fewer data on the mechanisms and rates of degradation of low-pH cement. Those studies that have been performed, however, found that they have broadly similar technical properties to more conventional cementitious materials (Martino 2005, Montori et al. 2008, Holt 2008).
The silica fume used in low-pH cements generally improves the durability of cement paste by increasing its strength, forming a less porous and less permeable matrix in concrete. This is due to the tendency for the silica to absorb moisture and swell slightly under wet conditions, which may help seal small fractures in the concrete if they form. Under drying conditions, however, low-pH concretes may shrink and crack as moisture is lost (Holt 2008), but drying is not likely to occur in the post-closure repository environment. The use of silica fume to enhance durability of injection grouts has also been recommended based on experimental studies (Orantie & Kuosa 2008).

In the water-saturated conditions expected in the repository, the low-pH cementitious materials will be more resistant to cracking than conventional cements and their rates of degradation will be slower. The development of pH conditions due to the degradation of low-pH cements has been studied in both stagnant (Vuorinen et al. 2005, Arenius et al. 2008) and flowing (Heikola 2008) conditions relevant to the repository environment. These studies show that the leachates will be less alkaline (pH ≤ 11) than the hyperalkaline leachates generated by degradation of traditional lime-rich cements (pH ~ 12.5). The pH in pore solutions has been observed to be dependent on the silica content of the cement (e.g. Calvo et al. 2010).

A conceptual model has been developed for the evolution of hyperalkaline leachates from conventional cements and their interaction with the host rock (Savage 1998). This model assumes that the leachates are released from the cement following mixing of groundwaters with the cement porewater. As the plume reacts with the host rock, the pH decreases, as Na, K, Ca, Al and Si in groundwater equilibrate with the cement leachates (Figure 9-1).

---

**Figure 9-1.** Conceptual model of hyperalkaline plume evolution in the aluminosilicate host rock from a cementitious repository. CSH = calcium silicate hydrates, CASH = calcium, aluminium silicate hydrates. From Savage (1998).

The extent of the cement/rock interaction depends greatly on the groundwater composition and the mineralogy of the rock. This model was developed, however, for ILW (intermediate level waste) repositories that will be backfilled with very large volumes of
a lime-based grout and it is not clear how relevant it is to the KBS-3 repository design that uses comparatively small and localised volumes of ordinary and low-pH cement.

The effects of grouting on rock-water interactions under Olkiluoto conditions have been modelled (Soler 2010). This work suggests that the formation of an alkaline plume will be extremely limited when a low-pH grout is used and, even when using grouts with lower silica fume contents, the extent and magnitude of the alkaline plume is likely to be limited. These results are in qualitative agreement with observations of cementitious materials in ONKALO (Soler 2010). Leaching tests with granitic groundwater have shown that low-pH concretes have good resistance to chemical degradation due to reaction with groundwater, although a thin altered front (in the order of a few to several hundred microns) has been observed showing incorporation of magnesium ions from groundwater into the CSH gels (Calvo et al. 2010). It should be noted that in a KBS-3H repository, deposition drifts will not be grouted even with a low-pH cement but with silica-based grouts, decreasing the possible alkaline plume as compared with a KBS-3V repository assumed in the above-mentioned studies. Local groundwater flow and transport conditions will have a major influence on the release and transport of cement leachate and on the development of the alkaline plume. Important controlling factors include the following (Metcalfe & Walker 2004):

- In a fractured rock, most of the leachate will be contained within a few active fractures and will not come into contact with the bulk of the rock. This source term dilution is enhanced by the fact that grouting is carried out at fracture zones and other locations where flow rates are highest.
- Further pH buffering and dilution may take place during transport through the fractures although, in open fractures with a limited buffering capacity and a small flow wetted surface area, the leachate may be transported over long distances with only limited buffering and dilution.

Any high pH leachate that is transported by groundwater will first interact with the host rock and fracture-filling minerals. This includes any porewaters held in the rock matrix, which can have a significant effect on mineral reactions, as was observed by the precipitation of calcite at the Maqarin natural analogue study site (Smellie 1998). Due to this interaction with the host rock, the pH of the leachate may be considerably lowered although no quantitative data on the pH buffering capacity of the Olkiluoto rocks are available.

Given these factors, it is possible that some high-pH leachate may interact with portions of the closure backfill or KBS-3H filling components. It is unlikely, however, that significant volumes of leachate will reach the buffer in the supercontainers because they will be located far away from the largest flowing fractures.

Groundwater chemistry is also affected by microbial activity [10.2.10]. Cementitious materials may act as energy sources for microbe populations (e.g. sulphur) but the long-term impact of microbial activity on cement degradation is not well understood. Chemical degradation may also affect the clay-based closure components by mineralogical changes, e.g. the alteration of montmorillonite in the closure backfill [9.2.4]. However, natural analogue studies on the long-term interaction of cement and rock and other EBS related materials (Pitty & Alexander 2011, Savage et al. 2011) have shown limited and local influence of cement leachate. In locations where clay and concrete materials are in contact, mineral transformations may occur locally within the plugs and this has to be taken into account in the design of composite structures.
Chemical degradation may also affect any metal reinforcements (e.g. rock bolts) left in the disposal facility after closure. In addition to a loss of isolation capacity, other consequences of chemical degradation will be an increase in susceptibility to physical degradation [9.2.9], an increase in the surface area that may be available for sorption, and an increase in the rate of colloid production [9.3.1].

Overall, chemical degradation of the closure plugs is influenced by the following features of the repository system.

- Temperature: the rate of degradation is affected by the temperature.
- Pressure: hydrostatic pressure differences cause groundwater flow and influence the availability of external water that may interact with grout and other cementitious materials. Groundwater flow controls the amount of dilution and, therefore, the spread and pH of the alkaline plume.
- Tunnel geometry: the location of the cementitious materials with respect to groundwater flow and distance from the buffer and other clay components are key factors controlling the impact of the alkaline plume.
- Material composition: the composition of the cement is a primary control on the pH of the alkaline leachates that will be generated.
- Groundwater composition: is a primary control on the degradation mechanisms and rates for both cementitious and clay-based closure components.

**Uncertainties in the understanding of the FEP:**

Although the mechanisms for concrete degradation are well known for conventional surface construction, there are significant uncertainties about the mechanisms and rates that may occur under deep repository conditions. The degradation of low-pH cementitious materials is less well studied than the degradation of ordinary cementitious materials, although it is clear that the leachates that are generated will have a lower pH than would be produced by degradation of conventional cements.

**Couplings to other FEPs:**

Chemical degradation of the closure components is directly affected by the following FEPs:

- Physical degradation (closure plugs) [9.2.9]
- Freezing and thawing (in closure plugs) [9.2.10]
- Rock-water interaction (in the geosphere) [10.2.7]
- Transport through closure backfill and plugs [9.3.1]

Chemical degradation of the closure components directly affects the following FEPs:

- Montmorillonite transformation [9.2.4]
- Alteration of accessory minerals [9.2.5]
- Physical degradation [9.2.9]
- Transport through closure backfill and plugs [9.3.1]
- Rock-water interaction (in the geosphere) [10.2.7]
- Aqueous solubility and speciation (in the geosphere) [10.3.1]
- Precipitation and co-precipitation (in the geosphere) [10.3.2]
- Colloid transport (in the geosphere) [10.3.6]
References:
9.2.9 Physical degradation (of closure plugs)

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Alternative names:</th>
<th>Section in 2007-09:</th>
</tr>
</thead>
<tbody>
<tr>
<td>None</td>
<td>Not applicable</td>
</tr>
</tbody>
</table>

**General description:**

Closure plugs in the deeper parts of the repository system will be subject to a range of mechanical loads and stresses that may cause physical degradation by a number of different mechanisms that are dependent, in part, on the composition of the closure plugs and their structural design.

Physical degradation of the closure plugs may cause the plugs to lose their strength, increasing the potential for groundwater flow and radionuclide transport. Physical degradation will also increase their susceptibility to chemical degradation [9.2.8].

The strength of a material is its ability to withstand applied stress without failure. Stress may be compressive, tensile or shearing in nature. Closure plugs will be subjected to the same stresses as the surrounding bedrock [10.2.2] and the stresses induced by the other engineered barriers, such as the swelling pressure from the closure backfill [9.2.1]. During water uptake and swelling of the closure backfill there may be significant differential pressures and loads on the closure plugs as the backfill swells unevenly on either side of the plugs. Over time, as full swelling and mass redistribution of the backfill is achieved, the hydrostatic and swelling pressures on either side of the plugs will equalise.

In broad terms, the clay-based components in the closure plug structures may respond to increased stress by plastic deformation, and may also be subject to mechanical erosion in essentially the same manner as the buffer [5.2.3] and the closure backfill [9.2.2]. In contrast, the cementitious closure components and construction materials will respond to increased stress by brittle deformation.

Physical degradation of cementitious materials generally leads to a loss of mechanical strength as well as a reduction of stiffness (Le Bellego et al. 2000, Carde et al. 1996). The mechanical strength of concrete is a function of its multiphase (aggregate and binder) nature, and concrete strength is affected by porosity, water/cement ratio, soundness of aggregate, aggregate-paste bond and other cement-related parameters such as chemical composition, cement surface area and particle-size distribution.

The final strength of concrete is achieved after a process of curing, which may take some months. Curing may be accompanied by shrinkage due to loss of water, and generation of internal tensile stress. Post-curing (autogenous) shrinkage can occur after the concrete has reached its final strength and is attributed to self-desiccation phenomena driven by internal mineral hydration reactions (Figure 9-2). Autogenous shrinkage is usually only a concern in high-performance concrete (with strengths > 40 MPa) where there is a low water/cement ratio of less than about 0.45. It can be more severe in concrete mixtures that have a very dense paste, without interconnected pores, such as mixtures containing silica fume (Holt 2005). Autogenous shrinkage may be significant at repository depth where high performance is needed, particularly for low pH material incorporating silica fume.
Continued chemical degradation [9.2.8] will cause a progressive reduction in the mechanical strength of the plugs. Prolonged chemical degradation may also lead to a reduction in the proportion of soluble compounds in the concrete, causing a loss of ability for concrete swelling and dilation. Over time, this mechanism will cause a change in the hydromechanical behaviour of the concrete-rock interface and a potential loss of isolation capability. The extent of this loss will be dependent on the initial binder/aggregate ratio, but prolonged leaching will eventually lead to a total loss of soluble compounds in the concrete, leaving only aggregates in place. This process has been studied for altered and unaltered concretes under a shearing load, and a loss of mechanical strength was observed for the degraded plug/rock interface (Buzzi et al. 2008). However, complete loss of isolation is not anticipated in the repository system due to the additional isolation capacity provided by the swelling clays in the closure backfill that will reduce the groundwater flow through the closure plugs.

Mechanical shearing is possible at the plug-rock interface due to differential pressures caused by uneven closure backfill swelling [9.2.1]. Shearing may cause additional physical degradation, but shrinkage of the concrete plug may reduce the shearing stresses on it (Haaramo & Lehtonen 2009). The report by Haaramo & Lehtonen (2009) discussed the deposition tunnel plug used in KBS-3V, but the processes are equally relevant for closure plugs.

Figure 9-2. Reactions causing autogenous and chemical shrinkage. C = unhydrated cement, W = unhydrated water, H_y = hydration products, and V = voids generated by hydration (Tazawa 1998).

In-situ rock stresses will be transferred to the plugs. The ambient stresses at Olkiluoto increase with depth and are well characterised (Aaltonen et al. 2010), but additional stresses will occur after closure of the disposal facility when the system moves towards a new mechanical, hydraulic and thermal equilibrium (Haaramo & Lehtonen 2009). The greatest differential loads and stresses are likely to be experienced by the closure components during hydraulic resaturation, but additional loads will develop during and after future glaciations [see 10.2.2 in Posiva 2012d], land uplift [see 10.2.4 in Posiva 2012b], and temperature changes [see 10.2.5 in Posiva 2012d].
Creep in the host rock may also affect the integrity of the closure plugs, but this process is anticipated to be of limited consequence because the additional loads induced by the rock are relatively small. Physical degradation may also affect the clay-based components in the plugs causing a loss in swelling pressure and isolation capacity. The main mechanisms are the same as those that will affect the closure backfill, notably mechanical [9.2.2] and chemical erosion [9.2.3], although flow rates may be higher in the upper part of the geosphere and, consequently, the rate of erosion may be higher.

Overall, physical degradation of the closure plugs is influenced by the following features of the repository system.

- Temperature: the rates of degradation processes are affected by temperature.
- Pressure: the water pressure and flow rate control the extent of any piping and erosion of the clay-based components in the closure plugs.
- Tunnel geometry: tunnel and repository geometry will affect the stresses acting on the system and, thus, the potential for mechanical damage to occur.
- Mechanical stress: the rock stress is a primary control on the physical degradation of the closure plugs.
- Material composition: the composition of the cement-based materials is a primary control on their strength.

**Uncertainties in the understanding of the FEP:**

Although the parameters that contribute to the strength of concrete and the mechanisms that can cause a loss of strength are generally well understood for conventional surface construction, there are uncertainties about the mechanisms and rates that may occur under deep repository conditions.

There is a lack of data on the long-term performance of concrete and cementitious structures in underground environments, particularly for the low-pH cements planned to be used in the deeper parts of the repository system. Those studies that have been performed on low-pH cement (Holt 2008), however, found that they have broadly similar technical properties to more conventional cementitious materials.

**Couplings to other FEPs:**

Physical degradation of the closure components is directly affected by the following FEPs:

- Water uptake and swelling (in the closure backfill) [9.2.1]
- Chemical degradation [9.2.8]
- Freezing and thawing [9.2.10]
- Stress redistribution (in the geosphere) [10.2.2]
- Reactivation-displacement along existing fractures (in the geosphere) [10.2.3]
- Creep (in the geosphere) [10.2.5]
- Glaciation [see 10.2.2 in Posiva 2012d]

Physical degradation of the closure components directly affects the following FEPs:

- Chemical degradation [9.2.8]
- Transport through closure backfill and plugs [9.3.1]
- Groundwater flow and advective transport (in the geosphere) [10.3.5]
9.2.10 Freezing and thawing (in closure plugs)

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Alternative names:</th>
<th>Section in 2007-09:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Freezing</td>
<td>Not applicable</td>
</tr>
</tbody>
</table>

**General description:**

The likelihood and consequence of freezing and thawing of the closure plugs depend on the depth. The annual (seasonal) development of frost and ice can be disregarded in this context because it affects the ground to a maximum depth of around 1 m. Development of much deeper permafrost will occur only in response to future climatic evolution [see 10.2.3 in Posiva 2012d] when the maximum depth of permafrost development at Olkiluoto is predicted to be between 200 and 300 m (Hartikainen 2012) using pessimistic and conservative boundary conditions. The unlikely formation of permafrost [see 12.2.3 in Posiva 2012d] at Olkiluoto at repository depth and then thawing during temperate periods would be a significant process that might affect the isolation capacity of these closure plugs. Freezing of concrete by permafrost can cause considerable mechanical damage because the water contained within its pore spaces will expand during freezing, producing an internal pressure. If the pressure exceeds the tensile strength of the concrete, the pore spaces will dilate and rupture.
The cumulative effect of successive annual (seasonal) freeze-thaw cycles can also cause progressive expansion and cracking, scaling and crumbling of the near-surface concrete structures. It is the weakly bound porewater that is almost exclusively responsible for the mechanical disruption, rather than water bound within the cement minerals. As a consequence, the greater the water-filled porosity, the more damage is likely to occur (Dahmani et al. 2006).

The deterioration of concrete associated with freezing has been very well studied and it has been concluded that it may take up to 30 freeze-thaw cycles to significantly diminish the strength of high performance concretes (Chatterji 2003). Frost damage in concrete has been shown to involve cement paste, aggregates, and the mineral and organic additives that comprise the structures (Pigeon & Pleau 1995). It should be noted that most of the reported studies on concrete damage due to freezing have been made on outdoor structures (e.g. Browne & Bamforth 1981) where the temperature variability in the atmosphere is much greater than will be experienced by the closure components below ground, suggesting that the damage to such components will not be as severe.

Laboratory studies of the concrete freezing mechanism have shown that the movement of the porewater within the concrete during freezing and thawing is enhanced in the aggregate-cement paste transition zone, which initiates and accelerates damage. Moderate additions of silica fume strengthen the microstructure of the cement paste-aggregate interfacial transition zone and reduce overall damage (Cwirzen & Penttala 2003).

For the repository system, the cementitious plugs will be manufactured from standard concrete in the upper parts of the repository system and from low-pH concrete at depth. Low-pH concrete is characterised by high silica fume content and a very low porosity and, thus, these closure plugs will be somewhat more resistant to freezing, but this is unlikely to be significant because permafrost is not expected to extend down to the lower parts of the repository system.

Other consequences of freezing will be an increase in the concrete surface area that may be available for chemical degradation [9.2.8] and radionuclide sorption [9.3.1] after thawing, although only very small amounts of the more strongly sorbing nuclides are expected to migrate to the upper geosphere.

In addition to the concrete plugs, preliminary closure plans for the repository system may include rock boulders in the topmost parts of the disposal facility to prevent inadvertent intrusion (Sievänen et al. 2012). Freeze-thaw cycles may also cause deterioration of these boulders and lead to a change in the grain size distribution, but this mechanism is not likely to be significant in terms of repository system performance.

Overall, freezing and thawing of the closure plugs is influenced by the following features of the repository system.

− Temperature: is the primary control on the process, and this is directly related to climate evolution.
− Pressure: affects the depth at which freezing and thawing may occur.
− Repository geometry: the location (depth) and size of the closure plugs will affect the amount of damage due to freezing and its impact on the hydraulic performance.
− Material composition: particularly the water content and particle size is significant for a material’s resistance to damage during freezing.
− Groundwater composition: in particular, salinity will affect the temperature at which freezing of water will occur.
**Uncertainties in the understanding of the FEP:**

The effect of multiple freezing and thawing cycles on the structural materials has not been studied under repository conditions. Most data relate to studies on outdoor freeze-thaw cycles. The available data mostly relate to conventional cementitious materials, and there is limited information on the impact of freezing on the high performance cementitious materials that will be used in the disposal facility.

There is some uncertainty regarding the actual maximum depth that permafrost can reach in the geosphere and the number of the freeze-thaw cycles that will occur, although there is confidence that permafrost will not penetrate to the depths of the KBS-3H deposition drifts at Olkiluoto.

**Couplings to other FEPs:**

Freezing and thawing of the closure components is directly affected by the following FEPs:

- Permafrost formation [see 10.2.3 in Posiva 2012d]

Freezing and thawing of the closure components directly affects the following FEPs:

- Chemical degradation [9.2.9]
- Physical degradation [9.2.10]
- Transport through closure backfill and plugs [9.3.1]

**References:**


9.3 Migration FEPs

With regard to migration, the safety functions provided by the closure are to prevent the formation of significant water conductive flow paths through the openings, and to limit and retard the inflow to and release of harmful substances from the repository. The ability of the closure backfill to provide these functions, as part of the engineered barrier system, strongly depends on its achieving a sufficiently high swelling pressure after complete hydraulic saturation, and maintaining that pressure over very long periods of time. In the case of canister failure, most radionuclides will diffuse through the buffer to the near-field rock. Because the processes that may control the transport of radionuclides and other substances through the closure backfill and plugs are mostly the same as for a tunnel backfill in a KBS-3V repository, only one overarching process has been considered that is [9.3.1] transport through closure backfill and plugs. Further discussion on the migration FEPs related to tunnel backfill can be found in Section 6.3 of the KBS-3V FEP report (Posiva 2012d).

9.3.1 Transport through closure backfill and plugs

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Alternative names:</th>
<th>Section in 2007-09:</th>
</tr>
</thead>
<tbody>
<tr>
<td>None</td>
<td>Not applicable</td>
</tr>
</tbody>
</table>

**General description:**

Transport/migration through closure backfill involves the same processes as migration in the buffer, although if data were needed to represent this process, these should be adapted for the closure backfill materials. For Friedland clay, data exist for the tunnel backfill in the KBS-3V concept that could be used (see Wersin et al. 2014, and also Posiva 2012d, Chapter 6).

In respect of the closure plugs, their primary purpose is to act as a barrier to groundwater flow along central and other tunnels and boreholes to prevent them from becoming significant pathways for groundwater flow or for rapid release of radionuclides to the surface. Progressive chemical [9.2.8] and physical [9.2.9] degradation of the closure plugs may affect their barrier function.

**Advection and diffusion**

In general, the closure plugs are designed to have low hydraulic conductivities, so that flow through them should be negligible unless they are degraded. Consequently, transport across the closure plugs will be predominantly by diffusion. Diffusion is an important process for cementitious closure components for two main reasons:

- it affects the transport of substances that may cause degradation of closure plugs, such as chloride and sulphate, and
- it affects the migration of radionuclides through the components, if there is a radionuclide release.
Diffusion is relevant for all periods. In the long term, degradation of the closure plugs causes changes in the hydraulic conditions that may lead to advection becoming the principal transport process.

In principle, diffusion through closure backfill and concrete plugs is the same as diffusion in other materials, such as in the buffer and filling components, and follows Fick’s law of diffusive transport in porous media.

In the context of concrete, diffusion has mostly been studied and modelled to estimate concrete durability (e.g. Bentz et al. 1997, Marchand et al. 2002). Concrete is a three-phase system consisting of aggregates, bulk cement paste and an interfacial transition zone between cement paste and aggregate. The cement paste surrounding each aggregate is characterised by a high porosity and, therefore, aggregate size directly affects the total porosity via the interfacial transition zone volume. Studies show that the concrete diffusivity depends on the water-cement ratio, the degree of hydration and the aggregate volume fraction (Bentz et al. 1998).

Most studies have examined Ordinary Portland Cement (OPC) and not the concretes that will be used in the disposal facility. The low-pH cementitious materials planned to be used at depth in the repository are characterised by high silica fume content and very low porosity and, therefore, have a different internal structure to OPC.

Studies that have been performed on high silica fume concretes have shown that the silica has a significant effect on diffusivity. The addition of 10 % of silica fume to achieve a water-cement ratio of 0.3 reduces diffusivity of chloride by a factor of 15 or more, increasing the durability of the concrete (Bentz et al. 2000). Due to the extremely fine pore structure, the relative effects of the different parameters on diffusion depend on the specific diffusing species.

Some diffusivity data for radionuclides in cementitious materials (mostly concrete) are available, for example $10^{-11}$ to $10^{-15}$ m$^2$/s for iodine and $10^{-12}$–$10^{-14}$ m$^2$/s for rhenium in concrete containing 4 % fly ash (Wellman et al. 2006). Other studies have investigated the diffusion of Cs, Am and Pu in concrete and found that the diffusivity for Cs was in the range of $10^{-12}$ to $10^{-13}$ m$^2$/s but no movement could be measured for Am and Pu (Albinsson et al. 1996).

Most radionuclide diffusivity data have been derived for LLW and ILW repositories that will be backfilled with very large volumes of a lime-based grout (e.g. Johnston & Wilmot 1992). It is not clear that these data are directly applicable to the KBS-3H repository design, which uses very small and localised volumes of low-pH cement-based materials.

The porosity and diffusivity of the concrete will affect the surface area accessible for radionuclide sorption, although only very small amounts of more highly sorbing nuclides are expected to migrate to the upper geosphere.

Advective conditions may form in the cementitious structures in the long term due to their progressive chemical and physical degradation. Diffusion through the closure backfill will be effectively the same as diffusion through the buffer and filling components and may be enhanced due to mechanical erosion. One distinct process that may have a significant effect on groundwater flow is settlement of the materials used to backfill the vertical shafts, which has to be taken into account in the overall design.
Sorption

Sorption on cementitious closure components may be a significant process for repository performance because it may retard radionuclide transport or enhance transport if radionuclides sorb onto mobile colloids. Calcium aluminates and calcium silicate hydrates in cement provide efficient sorption sites. Other components in the cement may also sorb radionuclides, but the extent and mechanisms are not well established (Cocke & Mollah 1993).

The sorption of radionuclides on cementitious materials is quantified by the distribution ratio (K_d) between the quantity of a radionuclide sorbed per unit mass of cement and the equilibrium concentration of the radionuclide in the porewater. There is a considerable body of sorption data that has been derived for LLW and ILW repositories that will be backfilled with very large volumes of a lime-based grout. The most recent data for safety relevant radionuclides have been derived for the planned Swiss ILW repository in Opalinus Clay, and take account of the different phases in the degradation of cement-based concrete or grout and the resulting degradation products (Wieland & van Loon 2002). The sorption behaviour of anions in cementitious systems has been less studied because these radionuclides are more mobile than cations. Organic ligands may compete with anionic radionuclide uptake in cement (Pointeau et al. 2008).

There are relatively few radionuclide sorption data that are directly relevant to the low-pH cement-based materials that will be used at depth in the KBS-3 repository, but some analogue data are available from studies on colloidal silica which is used as an injection grout in geotechnical engineering projects (Hölttä & Hakanen 2008). These studies show that Eu sorption onto silica colloids is strongly dependent on pH (Hölttä et al. 2009, p. 25). The significance of sorption onto cementitious closure components is, however, limited by the very small volume of cement in the KBS-3 repository design and the fact that only poorly-sorbing radionuclides are anticipated to migrate beyond the buffer (e.g. I-129, Tc-99).

Sorption onto the closure backfill is effectively the same as sorption in the buffer [5.3.3], although any differences in material composition will need to be taken into account.

Colloid transport

Colloids may form during chemical or physical degradation of the closure plugs and this may be a significant process because radionuclide transport in the geosphere could be either enhanced or retarded by association with colloids [10.3.8]. Hydrogeochemical conditions in the disposal facility will constrain the significance of colloid-mediated radionuclide transport through their influence on colloid populations and stability, radionuclide sorption and mobility.

A compilation of data on near-field cementitious colloids from laboratory and in-situ experiments and natural analogues shows that the colloidal populations varied over several orders of magnitude (Alexander & Moeri 2003). The highest populations (10^7 colloids/mL) were observed at the site of the Maqarin natural analogue study and the lowest in laboratory batch studies using crushed OPC (10^3 colloids/mL).
Overall, transport through closure backfill and plugs is influenced by the following features of the repository system.

- Radionuclide inventory: controls the radionuclides that are available for transport through the closure plugs.
- Temperature: is a control on diffusion rates but at the temperatures expected, this may not be a significant effect at depth.
- Tunnel geometry and overall repository geometry control the volume of closure backfill, and the size, shape and location of the closure plugs and affect the transport across them.
- Groundwater composition: the composition of the natural groundwater affects the solubility and speciation of radionuclides, and their transport processes as well as the solubility of the plug components and their chemical equilibration processes.

**Uncertainties in the understanding of the FEP:**

The radionuclide transport characteristics of the materials used for the closure plugs, especially low-pH cementitious materials, are less well understood than for conventional materials. In the case of degraded concrete, the data are very limited, but the significance of this should be low because of the very small volume and limited distribution of cementitious materials in the KBS-3H repository system and due to their location mainly far away from the deposition drifts. There are uncertainties regarding the mechanisms and rates of colloid formation due to the degradation of cementitious closure components. The interactions between natural colloids and those formed from the bentonite and degradation of cementitious components are unclear (Hölttä et al. 2009).

**Couplings to other FEPs:**

Transport through closure backfill and plugs is directly affected by the following FEPs:

- Water uptake and swelling (in the closure backfill) [9.2.1]
- Chemical degradation [9.2.8]
- Physical degradation [9.2.9]
- Freezing and thawing (in closure plugs) [9.2.10]
- Groundwater flow and advective transport (in the geosphere) [10.3.5]

Transport through closure backfill and plugs directly affects the following FEPs:

- Groundwater flow and advective transport (in the geosphere) [10.3.5]

**References:**


10 GEOSPHERE

10.1 Description

The geosphere is defined here as the volume of rock that hosts the disposal facility and, in simple terms, comprises:

- the solid rock matrix and its constituent minerals,
- the various fractures and deformation zones, and other discontinuities that divide the rock mass into discrete blocks or zones, and
- the groundwater contained in the matrix pores and the fractures.

The boundary between the geosphere and the surface environment is the geosphere-biosphere interface: although commonly referred to as an ‘interface’, this boundary is, in reality, a zone characterised by changing physico-chemical characteristics with depth. Many processes in the upper geosphere are coupled with processes in the biosphere across the interface, such as groundwater flow and advective transport [10.3.5], which is coupled with groundwater recharge and discharge [see 9.2.7 in Posiva 2012d].

The geosphere at Olkiluoto has been characterised to confirm its suitability as a host for the proposed spent nuclear fuel repository, and to provide information for the safety case and technical design. The understanding of the present state and past evolution of the Olkiluoto site is described in a series of Olkiluoto site description reports. The most recent Site Description report (Posiva 2013c) presents the site’s geology, rock mechanics, surface hydrology, hydrogeology, and solute transport properties. The likely future evolution of the site has been previously reported for KBS-3H by Smith et al. (2007), and will be updated in Posiva (2016b).

The crystalline bedrock of Finland is a part of the Precambrian Fennoscandian Shield, which, in south-western Finland, consists mainly of Early Palaeoproterozoic metamorphic and igneous rocks, belonging to the Svecofennian Domain. This domain developed between 1930 Ma and 1800 Ma ago, either during one long Svecofennian orogeny, or during several, separate orogenies. The rocks of Olkiluoto can be divided into two major classes (Aaltonen et al. 2010). The first are supracrustal high-grade metamorphic rocks including various migmatitic gneisses, tonalitic-granodioritic-granitic gneisses, mica gneisses, quartz gneisses, and mafic gneisses. The second are igneous rocks including pegmatitic granites and diabase dykes. The metamorphic supracrustal rocks have been subjected to polyphase ductile deformation producing thrust-related folding, strong migmatisation and pervasive foliation. The most important rock forming minerals in the Olkiluoto rocks are quartz, potassium feldspar, plagioclase, biotite (± other micas) and hornblende (± other amphiboles).

The bedrock at Olkiluoto has been subject to extensive hydrothermal alteration processes, which are estimated to have taken place at temperatures from slightly over 300 °C down to 50 °C (Gehör et al. 2002). Based on the grade of alteration, two different types of hydrothermal alteration can be distinguished: a fracture-controlled type and a pervasive (or disseminated) type. The fracture-controlled alteration indicates that hydrothermal
fluids have passed through the rock along planar features, with the alteration being restricted to incipient fractures or narrow zones adjacent to them. The pervasive alteration indicates the strongest type of alteration that occurs as spots or is finely disseminated throughout the rock and in the fracture fillings. Three main hydrothermal alteration types have been identified at Olkiluoto: (i) clay mineral formation, which has two main subtypes; illitisation and kaolinisation, (ii) sulphidisation, and (iii) carbonatisation.

The fault zones at Olkiluoto are mainly SE-dipping thrust faults formed during contraction in the latest stages of the Fennian orogeny, approximately 1800 Ma ago, and were reactivated in several deformation phases. In addition, NE-SW striking strike-slip faults are also common. Fracturing varies between different rock domains, but the following three fracture sets are typical for the site (i) east-west striking fractures with generally subvertical dips to both the north and south, (ii) north-south striking fractures with generally subvertical dips to both the east and the west and (iii) moderately-dipping to gently-dipping fractures with strikes that are generally subparallel to the aggregate foliation directions in a particular fracture domain.

The strength and deformation properties of the intact rock, as well as its thermal properties, depend essentially on the intact rock’s mineral composition and structure. The heterogeneity of the rock properties at Olkiluoto is, therefore, reflected in the variation of the thermal and rock mechanics properties and seen e.g. in the anisotropic thermal properties due to foliation and gneissic banding. In Fennoscandia, the orientation of the major principal stress is attributed to an E-W compression from the mid-Atlantic ridge push and a N-S compression from the Alpine margin, resulting in a roughly NW-SE orientation of the major principal stress (Heidbach et al. 2008). This is also supported by the regional in situ data from Olkiluoto and other Finnish sites studied during the site selection programme. Changes in isostatic load due to glaciations and related isostatic adjustment and the existence of the brittle deformation zones change the stress regime at the site. Currently, a thrust faulting stress regime is present, i.e. the horizontal stresses are larger than the vertical stress, $\sigma_H > \sigma_h > \sigma_v$ and the principal stresses are approximately oriented horizontally and vertically, respectively. The orientation of $\sigma_H$ at the site is found to vary slightly with depth and at the repository depth be in the range NW-SE and E-W. The vertical stress is generally close to that expected due to the weight of the overlying rock. The rock stresses increase with increasing depth and, at repository depth, the stress magnitudes based on in situ stress data are approximately $\sigma_H = 25$ MPa, $\sigma_h = 13$ MPa and $\sigma_v = 11$ MPa (Posiva 2013c, Table 5-2).

In the crystalline bedrock at Olkiluoto, groundwater flow takes place in hydraulically active deformation zones (hydrogeological zones) and fractures. The larger-scale hydrogeological zones, which are related to brittle deformation zones, carry most of the volumetric water flow rate in the deep bedrock. There is a general decrease of transmissivity of both fractures and the hydrogeological zones with depth. Under natural conditions, groundwater flow at Olkiluoto occurs mainly as a response to freshwater infiltration dependent on the topography, although salinity (density) variation driven flow also takes place to a lesser extent. The porewater within the rock matrix is stagnant but exchanges solutes by diffusion with the flowing groundwater in the fractures.
Figure 10-1. Illustrative hydrogeochemical site model of baseline groundwater conditions with the main water-rock interactions at Olkiluoto. Changes in colour indicate alterations in water type. The hydrogeologically most significant zones are represented. Blue arrows represent flow directions. Rounded rectangles contain the main sources and sinks affecting pH and redox conditions. Enhanced chemical reactions dominate the infiltration zone at shallow depths, and at the interface between Na-Cl-SO4 and Na-Cl groundwater types. The illustration depicts hydrogeochemical conditions in the water-conductive fracture system, not in the diffusion-dominated rock matrix (Posiva 2013c, Chapter 7).

The distribution of the groundwater types is the result of progressive mixing of groundwaters and the slow interaction between the groundwater, porewater and the minerals of the rocks (see Figure 10-1 and Posiva 2013c). The groundwater composition is also affected by microbial activity. Water-rock interactions, such as carbon and sulphur cycling and silicate reactions, buffer the pH and redox conditions and stabilise the groundwater chemistry.

Weathering processes during infiltration play a major role in determining the shallow groundwater composition. Pyrite and other iron sulphides are common in water conducting fractures throughout the investigated depth zone indicating a strong lithological buffer against oxic waters over geological time scales. Groundwaters, in the range down to 300 m depth, show indications of having been affected by infiltrating waters of glacial, marine and meteoric origin during the alternating periods of glaciations and interglacials during the Quaternary. On the other hand, these indications are absent in fracture groundwaters below 300 m, implying that these groundwaters are older.
The current fracture groundwater is characterised by a significant, depth-dependent variation of salinity (see Figure 10-1). Fresh waters (salinity <1 g/L) rich in dissolved carbonate are found at shallow depths, in the uppermost tens of metres. Brackish groundwater, with salinity up to 10 g/L dominates at depths between 30 m and about 400 m. Sulphate-rich waters are common in the depth layer 100−300 m, whereas brackish chloride water, poor in sulphate dominates at depths of 300−400 m. Saline groundwaters (salinity >10 g/L) dominate at still greater depths. The matrix porewaters seem to be in equilibrium with the fracture groundwaters in the upper part of the bedrock (0−150 m), suggesting a similar origin and strong interaction between groundwater in fractures and matrix at these depths. At deeper levels (150−500 m), the matrix porewater is less saline and increasingly enriched in $\delta^{18}$O; this has been interpreted to represent fresh water conditions during a warm climate, probably during the preglacial Tertiary period (Posiva 2009).

A Rock Suitability Classification (RSC) system has been developed for KBS-3V (McEwen et al. 2012) and is being updated for KBS-3H. The classification system will assist in defining suitable rock volumes for repository panels, assessing whether deposition drifts or sections of them are suitable for the supercontainers. The classification system will aim to locate the deposition drifts in such a way that the surrounding host rock favours the long-term performance of the engineered barriers and contributes to the retardation of any radionuclides released in the event of canister failure.

In defining the repository panels, those deformation zones that are classified as layout determining features (LDFs) are avoided together with the surrounding rock volumes affected by those zones, referred to as the ‘respect volumes’. LDFs are large deformation zones that form the main groundwater flow routes or are large enough to be the location of significant (post-glacial) earthquakes that could lead to canister failure either by rock shear in the zone or its respect volume, or by secondary rock shear movements on large fractures intersecting the deposition drifts.

10.1.1 Long-term safety and performance

The long-term safety requirements for the geosphere are that the characteristics of the host rock, and the depth of the repository, are selected in such a way as to make it possible for the engineered barriers to fulfil their containment function.

The safety functions assigned to the host rock are to (Posiva 2016c):

- Isolate the spent nuclear fuel repository from the surface environment and normal habitats for humans, plants and animals and limit the possibility of human intrusion, and isolate the repository from changing conditions at the ground surface.
- Provide favourable and predictable mechanical, geochemical and hydrogeological conditions for the engineered barriers.
- Limit the transport and retard the migration of harmful substances that could be released from the repository.
It is intended that the host rock shall retain its favourable properties over hundreds of thousands of years (Posiva 2016c). As described above, Rock Suitability Classification (RSC) criteria are defined for the KBS-3H deposition drifts so that favourable conditions prevail in the vicinity of the canisters at the time of supercontainer emplacement and also in the long term. These favourable conditions are achieved at the selected repository depth by avoiding LDFs and their associated respect volumes when locating the repository panels and by avoiding other deformation zones, flowing features and fractures with large extent when selecting locations for the deposition drifts and the supercontainers. As a consequence, the potential impact of processes and events related to external climate evolution, such as intrusion of dilute (glacial) meltwaters or shear displacement caused by post-glacial faulting, is minimised.

The mechanical and thermal properties of the host rock will also be taken into account when defining the orientation and separation distance between the underground openings, to minimise any damage to the host rock and to control the near-field temperature. Due to natural variations in rock properties, it is not possible completely to exclude unfavourable conditions near a few canisters at the time of emplacement or the possibility that unfavourable conditions will develop in the future. Nonetheless, the use of the RSC system is intended to minimise the occurrence of unfavourable conditions.

The impact of the repository on the geosphere will be most pronounced during operations and in the first few hundred to a few thousand years after closure, when the hydraulic and thermal gradients are at their greatest. Due to the smaller excavation volumes, the disturbances caused by a KBS-3H repository are likely smaller than those of a KBS-3V repository. The most significant impacts on the geosphere due to external processes will be related to climate evolution and land uplift. Although the timing and duration of the different phases of climate evolution is uncertain, several repeated phases of temperate, permafrost and glacial periods are expected over the next 120,000 years. The current interglacial period is expected to last at least up to 50,000 years AP (Pimenoff et al. 2011).

10.1.2 Overview of the potentially significant FEPs

There are a number of processes that are considered to be significant for the long-term safety performance of the geosphere that relate to system evolution and to the migration of radionuclides and other substances.

Processes related to system evolution are:

10.2.1 Heat transfer
10.2.2 Stress redistribution
10.2.3 Reactivation-displacement along existing fractures
10.2.4 Rock mass damage
10.2.5 Creep
10.2.6 Erosion and sedimentation in fractures
10.2.7 Rock-water interaction
10.2.8 Methane hydrate formation
10.2.9 Salt exclusion
10.2.10 Microbial activity
Processes related to the migration of radionuclides and other substances are:

10.3.1 Aqueous solubility and speciation
10.3.2 Precipitation and co-precipitation
10.3.3 Sorption
10.3.4 Diffusion and matrix diffusion
10.3.5 Groundwater flow and advective transport
10.3.6 Colloid transport
10.3.7 Gas transport

These processes are each potentially affected by a number of features of the repository system that can influence the occurrence, rate, activity and potential couplings between the processes. These features relate either to aspects of the design of the repository or to characteristics of the geosphere that might be time-dependent during the repository lifetime. The most significant features are:

- Radionuclide inventory
- Temperature
- Groundwater pressure
- Groundwater flux
- Rock stress
- Repository geometry
- Fracture geometry
- Rock matrix properties
- Fracture properties
- Groundwater composition
- Gas composition.

The possible influences of these features on the processes considered to be significant for long-term performance of the geosphere are described in each FEP description, and are summarised in Table 10-1.

Many of the processes occurring within the geosphere are interdependent and directly coupled to each other. For example, the reactivation of an existing fracture [10.2.3] will directly affect groundwater flow and advective transport through the geosphere [10.3.5]. The direct couplings are listed in each FEP description, and are summarised in the matrix shown in Table 10-2.

Similarly, due to the complex interactions between the various parts of the disposal system, the evolution of the geosphere can influence (or be influenced by) processes occurring in other parts of the repository system through interactions between various processes. For example, groundwater flow and advective transport in the geosphere [10.3.5] interacts with groundwater discharge and recharge in the surface environment [see 9.2.7 in Posiva 2012d]. The interactions between the geosphere and other components of the disposal system are summarised in Table 10-3.
References


Posiva 2016b. Safety evaluation for a KBS-3H spent nuclear fuel repository at Olkiluoto – Performance Assessment. Eurajoki, Finland: Posiva Oy. POSIVA 2016-02 (in prep.).


Table 10-1. The possible influences of features of the disposal system on the processes considered to be significant for the long-term performance of the geosphere (marked with Y). These influences and couplings are discussed in more detail in each FEP description.

<table>
<thead>
<tr>
<th>Processes</th>
<th>Features</th>
<th>Radionuclide inventory</th>
<th>Temperature</th>
<th>Groundwater pressure</th>
<th>Groundwater flux</th>
<th>Rock stress</th>
<th>Repository geometry</th>
<th>Fracture geometry</th>
<th>Rock matrix properties</th>
<th>Fracture properties</th>
<th>Groundwater composition</th>
<th>Gas composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Processes related to system evolution:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.2.1 Heat transfer</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.2.2 Stress redistribution</td>
<td></td>
<td>Y</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.2.3 Reactivation-displacement of existing fractures</td>
<td></td>
<td></td>
<td></td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.2.4 Rock mass damage</td>
<td></td>
<td>Y</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.2.5 Creep</td>
<td></td>
<td>Y</td>
<td></td>
<td>Y</td>
<td></td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.2.6 Erosion and sedimentation in fractures</td>
<td></td>
<td>Y</td>
<td></td>
<td></td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.2.7 Rock-water interaction</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.2.8 Methane hydrate formation</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.2.9 Salt exclusion</td>
<td></td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.2.10 Microbial activity</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Processes related to the migration of radionuclides and other substances:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.3.1 Aqueous solubility and speciation</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.3.2 Precipitation and co-precipitation</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.3.3 Sorption</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.3.4 Diffusion and matrix diffusion</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.3.5 Groundwater flow and advective transport</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.3.6 Colloid transport</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.3.7 Gas transport</td>
<td></td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 10-2. Possible couplings between FEPs within the geosphere considered significant for the long-term performance of the disposal system. The numbers on the leading diagonal refer to the FEPs listed in Section 10.1.2. As an example of how to read this table, the blue coloured square means that “Reactivation-displacements along existing fractures” [10.2.3] directly affects “Groundwater flow and advective transport” [10.3.5].

|     | 10.2.1 | 10.2.2 | 10.2.3 | 10.2.4 | 10.2.5 | 10.2.6 | 10.2.7 | 10.2.8 | 10.2.9 | 10.2.10 | 10.3.1 | 10.3.2 | 10.3.3 | 10.3.4 | 10.3.5 | 10.3.6 | 10.3.7 |
|-----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 10.2.1 | X      | X      | X      | X      | X      |        |        |        |        |        |        |        |        |        |        |        |        |
| 10.2.2 | X      | X      | X      | X      |        |        |        |        |        |        |        |        |        |        |        |        |        |
| 10.2.3 |        | X      |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| 10.2.4 | X      |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| 10.2.5 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| 10.2.6 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| 10.2.7 | X      |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| 10.2.8 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| 10.2.9 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| 10.3.1 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| 10.3.2 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| 10.3.3 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| 10.3.4 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| 10.3.5 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| 10.3.6 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| 10.3.7 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
Table 10-3. Interaction matrix for the geosphere. FEPs in italics are addressed in other chapters. A short name for some of the FEPs is used in the table: Diffusion (Diffusion and matrix diffusion), Precipitation (Precipitation and co-precipitation), Erosion & sedim. (Erosion and sedimentation in fractures), GW flow (Groundwater flow and advective transport).

<table>
<thead>
<tr>
<th>Buffer</th>
<th>Heat transfer</th>
<th>Heat transfer</th>
<th>GW flow; Colloid transport; Diffusion; Gas transport; Heat transfer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Filling components</td>
<td>Heat transfer</td>
<td>Heat transfer</td>
<td>GW flow; Colloid transport; Diffusion; Gas transport; Heat transfer</td>
</tr>
<tr>
<td>Compartment and drift plugs</td>
<td></td>
<td></td>
<td>Gw flow</td>
</tr>
<tr>
<td>Closure</td>
<td>Heat transfer</td>
<td>Heat transfer</td>
<td>Heat transfer</td>
</tr>
<tr>
<td>Rock matrix</td>
<td>Diffusion; Precipitation; Rock-water interaction; Sorption</td>
<td>Diffusion; Erosion &amp; sedim.; Gas transport; Gw flow; Precipitation; Rock-water interaction; Sorption</td>
<td></td>
</tr>
<tr>
<td>Fractures and deformation zones</td>
<td>Diffusion; Precipitation; Rock-water interaction; Sorption</td>
<td>Diffusion; Erosion &amp; sedim.; Gw flow; Precipitation; Rock-water interaction; Sorption</td>
<td></td>
</tr>
<tr>
<td>Groundwater (Gw)</td>
<td>Agri- &amp; aquaculture; Gas transport; Gw discharge&amp;recharge; Gw flow; Ingestion of drinking water</td>
<td>Heat transfer</td>
<td></td>
</tr>
<tr>
<td>Surface environment</td>
<td>Construction of a well; Gw discharge and recharge</td>
<td>Glaciation; Inadvertent human intrusion; Land uplift &amp; depression; Permafrost formation</td>
<td></td>
</tr>
<tr>
<td>External</td>
<td></td>
<td></td>
<td>Glaciation; Land uplift &amp; depression; Climate evolution; Glaciation; Inadvertent human intrusion; Land uplift &amp; depression; Permafrost formation</td>
</tr>
</tbody>
</table>
10.2 System evolution FEPs

Various thermal, chemical, hydraulic and mechanical processes (and their couplings) will affect the evolution of the geosphere. The nature and significance of some of these processes will vary with depth and with time. In turn, these processes can affect the performance of the engineered barriers and the migration behaviour of radionuclides and other substances in the geosphere (Section 10.3). The following descriptions summarise each of these processes and the effects of the different variables on them. The couplings of these FEPs with other FEPs are thus indicated, but the consequences of the interaction or combinations of these interactions will be discussed in detail in Posiva (2016b).

References

Posiva 2016b. Safety evaluation for a KBS-3H spent nuclear fuel repository at Olkiluoto – Performance Assessment. Eurajoki, Finland: Posiva Oy. POSIVA 2016-02 (in prep.).

<table>
<thead>
<tr>
<th>10.2.1 Heat transfer</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Type:</strong> Process</td>
</tr>
<tr>
<td><strong>Alternative names:</strong> Heat transport</td>
</tr>
</tbody>
</table>

**General description:**

Thermal energy will be generated by the spent nuclear fuel (radiogenic heat) [3.2.2] and this will be transferred through the canister [4.2.2] and the buffer [5.2.1], and to a lesser extent through filling components, to the geosphere. This radiogenic heat will then be transferred outwards from the near field, through the geosphere, by a combination of conduction in the solid rock and advection in groundwater flowing through fractures [10.3.5].

The rates of heat conduction and convection in the geosphere are dependent on the thermal properties of the rock/groundwater system. These thermal properties depend mainly on the mineral composition of the rock and also on the temperature. In transient heat transfer by conduction, diffusivity is the most important thermal parameter, and is a function of thermal conductivity, specific heat capacity and the bulk density of the rock mass.

The temperature at any given time and place in the geosphere will be controlled by the heat balance, which in turn will be affected by the natural geothermal gradient, the ambient surface temperature and radiogenic heat generation. The natural geothermal gradient at Olkiluoto is currently nearly constant at 1.5 °C/100 m (Posiva 2013c, Section 2.5.6), whereas the surface temperature is largely controlled by the prevailing climatic conditions, which will evolve with time [see 10.2.1 in Posiva 2012d]. Changing surface temperature conditions will affect, though with delay, the geothermal gradient.

The maximum temperature in the geosphere will occur in the near-field rock adjacent to the buffer, approximately 20–60 years after the emplacement of the nearby canisters (Ikonen & Raiko 2015, Figure 39). The maximum temperature is dependent on the heat generation in the spent nuclear fuel [3.2.2], and the spacing between the canisters and
KBS-3H deposition drifts. For the KBS-3H repository design, the maximum temperature at the buffer/rock interface will be approximately 60 °C, which is about 50 °C above the ambient temperature of the rock. The temperature in the near-field rock will remain above the ambient temperature at the repository level for thousands of years. After about 20,000 years, the temperature in the near-field rock will be less than 5 °C above the natural rock temperature, and the geothermal gradient will again mainly control the temperature in the geosphere (Ikonen & Raiko 2015, Figure 39). Overall, the temperatures are slightly lower in KBS-3H than in KBS-3V if the same canister spacings are assumed (Ikonen & Raiko 2015).

Heat generation in the spent nuclear fuel will decrease over time and will effectively cease after about 50,000 years (Raiko 2013). Transfer of radiogenic heat in the geosphere is, thus, of most significance during the early thermal phase of repository evolution. The early thermal peak will cause the near-field rock to expand and may result in rock mass damage [10.2.4]. Temperatures in the geosphere will be lower than in the engineered barriers, largely because of the larger distance from spent fuel canister(s) and larger volume of rock into which thermal energy is dissipated and the low thermal conductivity of the buffer with respect to the rock.

The lowest temperatures in the geosphere will occur close to the surface, in response to the surface temperatures, particularly during future glacial cycles [see 12.2.2 in Posiva 2012d], when permafrost forms [see 10.2.3 in Posiva 2012d]. Overall, heat transfer in the geosphere is influenced by the following features of the repository system.

- Radionuclide inventory: controls the radiogenic heat output from the spent nuclear fuel.
- Temperature: conductive heat flow is proportional to the thermal gradient at any point in time caused by natural thermal boundary conditions and heat generation in the spent nuclear fuel.
- Groundwater flux: controls the generally minor proportion of heat transfer that occurs by advection through the fracture network.
- Repository geometry: in particular the depth that controls the natural, ambient temperature and the heat source distribution according to the repository layout.
- Rock matrix properties: the mineralogy and foliation control the thermal properties of the bulk rock.

Uncertainties in the understanding of the FEP:

Heat transfer and the factors affecting it are well understood. There is generally high confidence in the thermal data (Posiva 2013c). Thermal properties are mainly measured in the laboratory on small-scale samples (Kukkonen et al. 2011) but additional data are obtained from in-situ measurements (Kukkonen et al. 2005), which provide data on the relevant metre scale. Current results suggest reasonable agreement between these larger-scale data and the upscaled laboratory data, thereby enhancing confidence in the upscaling. Minor uncertainties in the temperature estimates are due to spatial variation of the thermal properties of the host rock, uncertainties in climatic evolution and on how the sequence of canister deposition in time and space will influence the near-field rock temperatures in the first decades after deposition.

The estimates of rock mass damage due to the rising temperatures in the early phase are affected by these uncertainties, though rock mass damage depends also on the rock mechanic properties.
**Couplings to other FEPs:**

Heat transfer in the geosphere is directly affected by the following FEPs:
- Heat transfer (in the buffer/drift) [5.2.1]
- Groundwater flow and advective transport [10.3.5]

Heat transfer in the geosphere directly affects the following FEPs:
- Heat transfer (in the buffer/drift) [5.2.1]
- Stress redistribution [10.2.2]
- Reactivation-displacement along existing fractures [10.2.3]
- Rock mass damage [10.2.4]
- Creep [10.2.5]
- Rock-water interaction [10.2.7]
- Microbial activity [10.2.10]
- Groundwater flow and advective transport [10.3.5]
- Permafrost formation [see 10.2.3 in Posiva 2012d]

**References:**


**10.2.2 Stress redistribution**

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th>Process</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Class:</strong></td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:**
- 

**Section in 2007-09:**
- 7.6

**General description:**

Prior to excavation of the underground openings, the geosphere is initially in a pre-stressed state due to the regional tectonic and gravitational stresses, and residual stress from the last period of ice loading (Posiva 2013c). When an excavation is made in the
rock (e.g. access tunnel, central tunnel, deposition drift), the stresses will be locally realigned to become parallel and perpendicular to the excavation surfaces, causing corresponding changes in the magnitude of the stresses (Andersson et al. 2007, p. 96). Stress concentrations occurring in KBS-3V tunnels around the deposition holes will be lacking from KBS-3H drifts, which have a much simpler (cylindrical) geometry. Stress redistribution will occur almost immediately after excavation but could subsequently be affected by other tunnel excavations nearby. Small changes in the stress distributions are possible during the entire programme of excavation of underground openings and operations (over decades).

Stress redistribution is also possible in the post-closure period due to thermal expansion of the rock caused by the thermal gradient [10.2.1] and due to the swelling pressure of bentonite in the buffer [5.2.2] and the KBS-3H filling components. Land uplift [see 10.2.4 in Posiva 2012d] and glaciation [see 10.2.2 in Posiva 2012d] will also cause changes in the stress state and, hence, the stress distribution, and may also affect the fracture network (Hökmark et al. 2010, Valli et al. 2011, p. 38).

As a result of the stress redistribution, high stresses may develop and different types of rock damage may take place. The possibility and extent of the damage depends on the rock strength, which in turn is dependent on the rock type and rock structure (e.g. foliation). In the immediate vicinity of the excavation (due to blasting, if used, and stress concentration), an excavation damaged zone (EDZ) will be created that is characterised by irreversible structural changes to the rock, such as the formation of microcracks. It should be mentioned that the KBS-3H deposition drifts will be bored, not blasted, and will thus probably have a much more limited EDZ than the 3V deposition tunnels (cf. Smith et al. 2007, Section 4.1.2). The extent and properties of the EDZ depend on bedrock properties and boring technique, especially cutter head design (Gribi et al. 2007, Section 7.6.3). Stress redistribution can result in rock mass damage [10.2.4] and the formation of new fractures or, more likely, reactivation and displacement along existing fractures, which may change the properties of the fractures [10.2.3]. Further away from the excavation, an excavation disturbed zone (EdZ) will be formed where less intensive changes may occur that are potentially reversible, such as elastic displacements.

The extent of rock mass damage, stress redistribution and the nature of the EDZ and EdZ will be influenced by the design of the repository and the geometry of the excavations. The orientation of the KBS-3H deposition drifts with respect to the orientation of the major principal stress will affect the resulting stress magnitudes. The excavation method will also influence the extent of the EDZ (Pastina & Hellä 2006, Mustonen et al. 2010). The access and central tunnels will be constructed using the drill and blast method, whereas the shafts and deposition drifts will be bored. Although, in general, drill and blast method produces a more pronounced EDZ than boring, by using controlled excavation in connection with the drill and blast method, the extent of the EDZ and the formation of continuous pathways can be reduced.

Stress redistribution may cause dilation of fractures and affect the groundwater flow paths in the near-field rock due to changes in the extent and geometry of, and connections between, the hydraulically active fractures. This will, in turn, influence the rate of water uptake by the buffer [5.2.2]. After failure of the canister, the disturbances of the rock caused by stress redistribution (formation of EDZ or rock mass damage) will influence the mass transfer between the near field and geosphere, and the migration
of radionuclides in the near-field rock by groundwater flow and advective transport [10.3.5] and matrix diffusion [10.3.4]. Overall, stress redistribution in the geosphere is influenced by the following features of the repository system.

- Temperature: higher temperatures cause thermal expansion potentially resulting in rock mass damage, whilst cooling may cause cracks and fractures.
- Rock stress: the initial stress field in the rock is a primary control for the magnitude of near-field stress redistribution, subsequent events such as glaciation and deglaciation loading cycles will change the stress distribution.
- Repository geometry: the design and geometry of the repository (including orientation, shape of the tunnels and tunnel spacing) is a primary control on stress redistribution in the near-field rock.
- Fracture geometry: the geometry of the fractures influences the stress pattern in the rock; in particular, the large-scale deformation zones may have effects on stress redistribution.

**Uncertainties in the understanding of the FEP:**
The stress redistribution process is well understood from modelling studies. There are data uncertainties regarding the elastic and strength parameters of the rock at Olkiluoto and especially concerning the in-situ stress state related to the large scatter of the available data. However, the general directions of in-situ stress components are well known from recent measurement data.
The hydraulic properties of the EDZ and the impact of the EDZ on the groundwater flow are not yet fully understood. Based on the EDZ characterisation studies at ONKALO (Mustonen et al. 2010), it has been shown that blast-induced fracturing is likely to occur, whatever form of drill and blast system is employed, and that some of these fractures may be water-conducting. However, the studies also indicated that this blast-induced fracturing does not form a continuous, connected network over larger distances along the tunnel.

**Couplings to other FEPs:**
Stress redistribution in the geosphere is directly affected by the following FEPs:
- Water uptake and swelling (in the buffer) [5.2.2]
- Water uptake and swelling (in the filling components) [7.2.2]
- Heat transfer [10.2.1]
- Rock mass damage [10.2.4]
- Glaciation [see 10.2.2 in Posiva 2012d]
- Land uplift and depression [see 10.2.4 in Posiva 2012d]

Stress redistribution in the geosphere directly affects the following FEPs:
- Physical degradation (of closure plugs) [9.2.8]
- Deformation (of compartment and drift plugs) [8.2.2]
- Reactivation-displacement along existing fractures [10.2.3]
- Rock mass damage [10.2.4]
- Creep [10.2.5]
- Groundwater flow and advective transport [10.3.5]
References:

10.2.3 Reactivation-displacement along existing fractures

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Alternative names:</th>
<th>Section in 2007-09:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reactivation – displacements along existing discontinuities</td>
<td>7.6.2</td>
</tr>
</tbody>
</table>

General description:
All deep rock, including the bedrock at Olkiluoto, contains physical discontinuities in the form of various kinds of fractures (e.g. joints and faults). These may have different geometries and spatial dimensions. Some of these discontinuities may be ‘open’,
particularly in the near-surface zone, and serve as routes for groundwater flow and advective transport [10.3.5], whereas others may be ‘closed’ due to compressive stresses or ‘sealed’ by the precipitation of secondary, fracture-filling minerals.

When there is a change in the stress pattern in the rock mass, causing stress redistribution [10.2.2], it is more likely that any displacement will occur along these pre-existing discontinuities than that new fractures will form in intact rock. This conclusion is supported by recent studies at Olkiluoto (Mattila & Viola 2014). There are five, quite different types of processes that may occur in the near-field rock causing displacement (shear, closure and opening) and dilation in the pre-existing fractures in the rock.

- Tectonically induced: these result from stresses accumulated from plate tectonic (Atlantic ridge push and Alpine collision) processes (Heidbach et al. 2008, Posiva 2013c). Due to the large distance of Finland from active plate margins, however, this type of activity is of little relevance over the timescales of most importance to long-term safety (i.e. hundreds of thousands of years).

- Excavation induced: the design and layout of the repository will be based on Rock Suitability Classification criteria that are intended to avoid major geological features (see Section 10.1). There could, however, potentially be displacement along other more minor features due to the stress redistribution caused by the excavation of the repository and other underground openings [10.2.2].

- Thermally induced: heat generated from the waste canisters will change the stress distribution around the repository. This may cause shear displacements in the fractures and fracture zones and, hence, possible changes in fracture transmissivity. Such changes are, however, evaluated as being quite insignificant (Hökmark et al. 2010, p. 92).

- Seismically induced: seismic activity can cause changes in the pre-existing fractures and fracture zones. Seismic activity is, however, low in the Finnish bedrock (Posiva 2013c) and consequently reactivation during the current temperate climate is expected to remain very limited. More pronounced seismic activity may, however, be related to post-glacial faulting.

- Glaciation induced: glacial cycles will substantially change the stress state in and around the repository due to changes in loading caused by the advance and retreat of an ice sheet [see 10.2.2 in Posiva 2012d], and this may cause reactivation of pre-existing features. The changes in stress state depend on the time-dependent ice load magnitude as well as on the elastic properties of the lithosphere and the viscoelastic properties of the mantle. Ice loading will increase the vertical loads in the rock mass and, thereby, induce differential horizontal loads. Deglaciation and the resulting differential stresses may cause dynamic effects in the geosphere and is the most likely cause of fault reactivation (Ojala et al. 2004). Non-dynamic stress changes may also need to be considered (Hökmark et al. 2010, Chapter 7). In addition, permafrost development [10.2.3] may cause dilation of fractures due to the expansion of water during freezing.

Glacial loading and unloading is, therefore, judged to be the most likely cause of reactivation or displacement along existing fractures during the period of hundreds of thousands of years in which the long-term safety of the repository must be demonstrated [see 10.2.2 in Posiva 2012d].
Because of reactivation-displacement, the hydraulic properties of fractures may change and cause localised changes in the groundwater flow paths and their transport properties. Reactivation would also cause the groundwater in the fracture to be displaced. Such changes are, however, considered to be of limited importance because analyses have shown that the impact of stress changes and shear displacements on hydraulic properties of fractures is either negligible or very limited (Hökmark et al. 2010). Larger reactivation-displacements are possible in connection with earthquakes, but the likelihood of large magnitude earthquakes is low at Olkiluoto (Saari 2012).

The buffer in the KBS-3H deposition drifts mitigates the effects of the displacements on the canister. In the worst case, displacement could cause disruption to a deposition drift at the location of a canister, leading to mechanical failure of the canister. It has been shown that with the current design of the canister and buffer, the canister will not fail if the shear displacement is $< 5 \text{ cm}$ and the shear velocity is $< 1 \text{ m/s}$ (see Posiva 2016c, Appendix B). Furthermore, the probability of this process occurring is minimised by locating the deposition drifts and canisters away from deformation zones and large fractures.

Although the process for shear movement is the same for KBS-3H and 3V, different sets of fractures are of relevance as the canister orientation and the orientation of rock stresses are different. The main concern for KBS-3H are movements on subvertical fractures (Gribi et al. 2007, Section 7.6.2).

Major deformation zones capable of accommodating significant slip should be readily identified and KBS-3H drifts will not be constructed within, or in the immediate vicinity of such zones. An earthquake occurring on a major deformation zone may, however, give rise to stress changes in the rock that trigger the reactivation of smaller-scale fractures that cannot be avoided when constructing the drifts (Gribi et al. 2007, Section 7.6.1).

Laboratory scale experiments indicate that fracture transmissivities increase considerably after shear displacements of more than a couple of millimetres, although this increase is very sensitive to normal load variations (Hökmark et al. 2010, Section 3.5.2). Shear displacements taking place under effective normal stresses higher than around 6–7 MPa are considered to cause negligible transmissivity increases (Hökmark et al. 2010). The effective normal stress is defined as the normal stress less the hydraulic pressure. Low normal stresses could exist only in the tunnel vicinity, e.g. at a distance of a few metres from the underground openings, although effective normal stresses will even then be larger than 6–7 MPa, typically 10 MPa or more. Shear displacements of the magnitudes produced in the laboratory, i.e. typically 5 mm and more, are only possible for very large fractures and only away from the fracture edges. Close to the edges, shear displacements are close to zero regardless of the fracture size (Hökmark et al. 2010, Section 3.5.2).

Even if the displacements along fractures that intersect the KBS-3H deposition drifts do not cause failure of the canister, they may cause deformation of the canister [4.2.3] or mass redistribution of the buffer [5.2.2] within the deposition drift.

Overall, reactivation-displacements along existing fractures in the geosphere are influenced by the following features of the repository system.

- Rock stress: the initial stress state of the rock is a key control.
- Repository geometry: the design and geometry of the repository is a primary control on the potential for fracture reactivation-displacement in the near-field rock.
− Fracture geometry: the geometry of the fractures influences how and where the excavations intersect the existing discontinuities.
− Fracture properties: the fracture properties (e.g. fracture coating materials, roughness and mechanical properties) affect the response of fractures to loads.

**Uncertainties in the understanding of the FEP:**

The reactivation-displacement process is fairly well understood from modelling studies, but uncertainties exist concerning the mechanical loads and stresses that will result from future glaciations and how these will affect existing discontinuities. There is also uncertainty concerning the mechanical properties of fracture zones.

In addition, there is considerable uncertainty regarding the effect on flow properties of fractures or fracture zones due to reactivation-displacements and on resulting groundwater flow. The timing of future glacial cycles is also subject to considerable uncertainty.

Although these uncertainties affect the assessment of the reactivation displacements, the impact of the uncertainties can be scoped by modelling using conservative assumptions and also reduced by repository design. The reactivation displacements, except for the seismically induced displacements in connection with large earthquakes, are limited and are not expected to affect long-term safety. The likelihood of large earthquakes is low at Olkiluoto and the potential magnitudes of shear displacements of fractures around the repository are further reduced by locating the repository so that major deformation zones are avoided.

**Couplings to other FEPs:**

Reactivation-displacement along existing fractures in the geosphere is directly affected by the following FEPs:
− Stress redistribution [10.2.2]

Reactivation-displacement along existing fractures in the geosphere directly affect the following FEPs:
− Deformation (of the canister) [4.2.3]
− Deformation (of the supercontainer shell) [6.2.2]
− Deformation (of compartment and drift plugs) [8.2.2]
− Physical degradation (of closure plugs) [9.2.9]
− Erosion and sedimentation in fractures [10.2.6]
− Diffusion and matrix diffusion [10.3.4]
− Groundwater flow and advective transport [10.3.5]

**References:**


Hökmark, H., Lönnqvist, M. & Fälth, B. 2010. THM issues in repository rock. Thermal, mechanical, thermo-mechanical and hydro-mechanical evolution of the rock at the
10.2.4 Rock mass damage

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th>Process</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Class:</strong></td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:**
Spalling; Fracturing; Fracturing and spalling; Fracture initiation and propagation; Structurally controlled failure

**General description:**
Rock mass damage (in underground openings at Olkiluoto) is a process of structurally controlled failure, concentrated on naturally existing flaws or planes of weaknesses occurring within the rock mass. Rock mass damage occurs at the surface of a rock excavation when there are large shear stresses prevailing just beyond the tunnel/drift perimeter.

In the repository near-field environment, rock mass damage is most likely to occur on the surfaces of the excavations when their geometry causes the stresses to be concentrated at localised areas of the exposed rock wall, and those stresses exceed the local rock strength. The different rock types at Olkiluoto have slightly different strength properties, and so may respond to stress in different ways (Posiva 2013c). These stresses occurring around different parts of the repository can result from thermal expansion due to heat transfer from the spent nuclear fuel [10.2.1] or due to mechanical readjustment of the prevailing in-situ stress field [10.2.2].

The potential for rock mass damage in the rock around the disposal facility will be greatest during the operational period, when the rock mass responds to the substantial changes in near-field stress caused by the excavation and the thermal impact from the spent nuclear fuel. Heat transfer [10.2.1] from the emplaced canisters will cause
additional thermal stresses and will induce damage in the rock mass around the excavation perimeter. Additional loads arising from glaciation/deglaciation can also contribute to the extension of the rock damage zone around the perimeter of the drift/tunnels. The extent of rock mass damage is reduced once the buffer and the KBS-3H filling components have reached their full swelling pressures [5.2.2], because this will reduce the stress gradients across the near field.

There is a range of possible mechanical impacts of rock mass damage at Olkiluoto, from slight cracking through to complete failure of the excavation. The mechanical impacts on the rock adjacent to the excavation due to rock mass damage contribute to the evolution of the near-field rock characteristics. In-situ experiments at Olkiluoto have provided estimates of the likely changes of the rock properties in the near field due to rock mass damage. Figure 10-2 illustrates microscopic spalling and structurally controlled failure on the wall of a test deposition hole at ONKALO. Changes in the hydraulic characteristics and the possible formation of transport paths with enhanced transmissivity are of importance for the long-term safety.

The likelihood of rock mass damage taking place is controlled by the geometry of the pre-existing features in the rock (fractures, joints, foliation planes, etc.), which can affect the local rock strength. Furthermore, the swelling pressure of the buffer will control rock mass damage because of the supporting pressure on the rock walls.

Figure 10-2. Example of rock mass damage as structurally controlled crack growth and microscopic spalling around a 1.8 m diameter borehole during Posiva’s Spalling Experiment (POSE). From Siren et al. (2015).
For KBS-3H, thermomechanical and fracture mechanics based model calculations using the 3DEC and Fracod3D codes have been performed (Suikkanen et al. 2016). Due to the alignment of the deposition drifts with the major in-situ stress component $s_H$, and thanks to the smaller diameter and simpler geometry of the deposition drift, KBS-3H is less prone to thermally induced rock mass damage compared with KBS-3V. The simpler geometry particularly refers to the absence of vertical deposition holes and deposition tunnel. Because artificial watering is used, rock mass damage may be mitigated by the increased buffer saturation in drift sections where the groundwater inflow is very low.

Boundary element modelling results of two KBS-3H drifts, niches and a central tunnel show that stress values in the drifts are moderate being up to 65 MPa during the construction period (Hakala et al. 2008).

The likelihood of rock mass damage will be higher in weaker rock volumes, e.g. in mica-rich layers and in highly fractured sections. During construction and operation of the disposal facility, some parts of the excavations will need to be supported to minimise the likelihood of rock mass damage and to ensure operational safety. This is particularly the case for the central and access tunnels, which may remain open for a long period (up to about 100 years) to allow for phased excavation and operation of the disposal facility. Consequently, these tunnels will be open during the initial stages of the thermal phase.

Overall, rock mass damage is influenced by the following features of the repository system.

− Temperature: heat flow and thermal gradients can cause expansion and thermal stresses and, as a consequence, rock mass damage.
− Rock stress: the initial and evolving stress state of the near-field rock is a primary control on rock mass damage.
− Repository geometry: the orientation of the KBS-3H deposition drifts has a significant effect on the stress magnitudes around the excavations and hence on the extent of possible rock mass damage.
− Rock matrix properties: the mineral composition varies between the different rock types at Olkiluoto and this further affects their respective strengths.

**Uncertainties in the understanding of the FEP:**

Due to the heterogeneity of the rock at Olkiluoto, the exact location of rock mass damage events within the excavations cannot be predicted, but the broad extent of rock mass damage that will occur across the entire repository system is understood. Ongoing characterisation of the geosphere at Olkiluoto has provided better understanding of the in-situ stresses but further work is ongoing.

The probability and extent of rock mass damage in a KBS-3H deposition drift will depend on the local rock conditions and on the rate of bentonite swelling, which itself depends on local rock permeability, which is both heterogeneous and uncertain. The artificial wetting used in the DAVE design reduces this uncertainty to some extent, by increasing the early buffer saturation in the dry drift sections.
**Couplings to other FEPs:**
Rock mass damage is directly affected by the following FEPs:
- Water uptake and swelling (in the buffer) [5.2.2]
- Water uptake and swelling (in the filling components) [7.2.2]
- Heat transfer [10.2.1]
- Stress redistribution [10.2.2]
- Creep [10.2.5]

Rock mass damage directly affects the following FEPs:
- Stress redistribution [10.2.2]

**References:**

### 10.2.5 Creep

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th><strong>Class:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Alternative names:</strong></th>
<th><strong>Section in 2007-09:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>None</td>
<td>7.6.4</td>
</tr>
</tbody>
</table>

**General description:**
Creep of the rock mass is a slow, quasi-continuous (time-dependent) physical deformation process that occurs mainly along pre-existing discontinuities in the rock. Very slow creep can, however, also take place in the rock matrix due to differential stress fields.

In the repository environment, creep may occur due to the imposition of stresses resulting from tectonic, isostatic land uplift [see 10.2.4 in Posiva 2012d], climatic (e.g. ice loading and unloading) [see 10.2.1 in Posiva 2012d] and excavation processes. Heat transfer from the spent nuclear fuel may also cause an increase in the rate of creep, but the effect will be minor and limited to the thermal phase of repository evolution. Rock creep will occur continuously at a slow rate throughout the lifetime of the repository, although it is unlikely to be as significant for repository evolution as the more rapid stress redistribution [10.2.2] and pre-existing fault reactivation/displacement [10.2.3] processes.
There is no relevant difference in processes related to creep between KBS-3H and 3V (Gribi et al. 2007, Section 7.6.4). The main consequence of creep in the far-field rock is likely to be a change to the hydraulic and transport properties of fractures (Eloranta et al. 1992). In particular, the fracture connectivity and channelling properties could change, such that the preferential flow paths through the rock mass could alter over time. Creep of the near-field rock around the repository excavations may deform the deposition drifts, and thus impact on the swelling pressure in the buffer [5.2.2] and filling components [7.2.2]. Rock creep is not expected to cause damage to the canister because rock movements, if any, due to creep are limited, and the buffer will mitigate their impact. Reviews of the long-term physical properties of crystalline rocks indicate that there is a ‘stress threshold’ that can be sustained indefinitely, i.e. below which creep processes can be disregarded. This value is of the order of 40–60% of the unconfined compressive strength for laboratory specimens under unconfined compressive loading and increases rapidly under increasing confining pressures (Damjanac & Fairhurst 2010; Hagros et al. 2008).

Overall, creep in the geosphere is influenced by the following features of the repository system.  
- Temperature: heat flow and thermal gradients can affect creep but, given the temperatures likely to occur in the geosphere in the very long term, this will be a minor control given the very slow pace at which creep takes place.  
- Rock stress: the initial and evolving stress state of the rock is a primary control on creep.  
- Fracture geometry: the orientation of the fractures is relevant because creep occurs predominantly along pre-existing discontinuities.  
- Rock matrix properties: the mineral composition varies between the different rock types at Olkiluoto and this affects their respective strengths.

**Uncertainties in the understanding of the FEP:**

The very long-term creep processes are not well understood or predictable, but this uncertainty is not considered to be significant for evaluating repository safety. This is because it is very unlikely that loads in the rock will change so much over time that the long-term stress thresholds for the occurrence of creep are reached.

**Couplings to other FEPs:**

Creep in the geosphere is directly affected by the following FEPs:  
- Heat transfer [10.2.1]  
- Stress redistribution [10.2.2]  
- Glaciation [see 10.2.2 in Posiva 2012d]  
- Land uplift and depression [see 10.2.4 in Posiva 2012d]

Creep in the geosphere directly affects the following FEPs:  
- Deformation (of the supercontainer shell) [6.2.2]  
- Deformation (of compartment and drift plugs) [8.2.2]  
- Physical degradation (of closure plugs) [9.2.9]  
- Reactivation-displacement along existing fractures [10.2.3]  
- Rock mass damage [10.2.4]  
- Groundwater flow and advective transport [10.3.5]
**References:**


---

**10.2.6 Erosion and sedimentation in fractures**

<table>
<thead>
<tr>
<th>Type</th>
<th>Class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:**

Erosion/sedimentation in fractures

**Section in 2007-09:**

7.6.6

**General description:**

Groundwater flow in the geosphere predominantly takes place in hydraulically active deformation zones (hydrogeological zones) and fractures [10.3.5]. During and after the operational phase, the groundwater flow around the KBS-3H deposition drifts may increase significantly. This may lead to erosion, transport and sedimentation of fault gouge material and to buffer erosion, possibly changing the hydraulic properties of fractures intersecting the deposition drifts (Gribi et al. 2007, Section 7.6.6). In the far future, the increase in flow associated with the passage of an ice margin over the site and the injection of acidic, oxygenated glacial water, the groundwater chemistry may become more acidic and oxidising. The consequence would be an increased potential for fracture-filling materials, such as carbonates and sulphides, to be dissolved and eroded and for the transmissivity of the fractures to increase (Pitkänen et al. 2004). This phenomenon affects especially the groundwaters close to the ground surface, but calcite and sulphides observed in overburden (Breitner 2011) will limit the significance of reactive water infiltration in fractures. Any loose material present, due to repository construction, may also be eroded and redistributed during saturation. After complete saturation of the buffer and the tunnel backfill, however, the groundwater flow rates and chemistry in the geosphere will return to natural conditions.
Erosion and sedimentation in fractures is most likely to occur during the early period of hydraulic saturation, although glacial meltwaters, if they reach repository depths, might also lead to some erosion in fractures later. There is also the possibility for bentonite particles eroded from the buffer [5.2.3] or KBS-3H filling components [7.2.3] to be carried into water-bearing fractures where they can accumulate and cause sedimentation. This sedimentation process can potentially restrict the flow of groundwater through the fractures [10.3.5], alter their channelling properties and reduce their transmissivity. This may be beneficial for reducing the flow in fractures that intersect the deposition drifts. Furthermore, the released bentonite particles may act as colloids and influence the transport of radionuclides through the geosphere [10.3.6]. Nonetheless, erosion and sedimentation in fractures is not expected to lead to any significant changes to the bulk hydraulic or transport properties of the geosphere. This is because bentonite erosion is expected to remain limited, as the KBS-3H deposition drifts are located in rock volumes with limited flow. During construction, when the flow rates are expected to be at highest due to the gradients caused by the open excavation, the groundwater flow can be reduced by grouting. Post-grouting with silica-based grouts is planned to be used in the deposition drifts (Posiva 2012b, Section 9.7.1).

Overall, erosion and sedimentation in fractures in the geosphere is influenced by the following features of the repository system.

- Groundwater flux: the flux and flow rate can affect the transport capacity for bentonite particles eroded from the buffer and KBS-3H filling components, as well as the rate of erosion.
- Fracture geometry: in particular, the interconnected fracture network geometry and the channel aperture within the plane of the fracture through which groundwater flows.
- Fracture properties: the mineralogy affects the susceptibility of the fracture coating or infill minerals to dissolution and erosion.
- Groundwater composition: affects the chemical reactions and consequently the rate of dissolution of the fracture-filling materials and also the stability (agglomeration and subsequent filtration) of bentonite colloids released from the buffer and KBS-3H filling components, as well as the rate of release of these colloids.

**Uncertainties in the understanding of the FEP:**

Erosion and sedimentation processes are considered to be of limited importance based on expert judgement concerning the current understanding of the processes controlling fracture minerals.

The extensive studies of the fracture properties at Olkiluoto and the understanding of the geological history of the area show that the fracture fillings are controlled mainly by geologically old processes occurring over the past hundreds of millions of years. The infiltration experiment at Olkiluoto studied the influence of increased infiltration on fracture calcites and sulphides. The results do not indicate any significant loss of fracture minerals (Posiva 2013c). There is no indication of any significant erosion or sedimentation processes in the fractures in geologically recent times, including in the deeper parts of the rock at repository depth.
### Couplings to other FEPs:

Erosion and sedimentation in fractures is directly affected by the following FEPs:
- Mechanical erosion (in the buffer) [5.2.3]
- Chemical erosion (in the buffer) [5.2.4]
- Mechanical erosion (in the filling components) [7.2.3]
- Chemical erosion (in the filling components) [7.2.4]
- Reactivation-displacement along existing fractures [10.2.3]
- Rock-water interaction [10.2.7]
- Groundwater flow and advective transport [10.3.5]

Erosion and sedimentation in fractures directly affects the following FEPs:
- Rock-water interaction [10.2.7]
- Diffusion and matrix diffusion [10.3.4]
- Groundwater flow and advective transport [10.3.5]
- Colloid transport [10.3.6]

### References:


### 10.2.7 Rock-water interaction

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th><strong>Class:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Alternative names:</strong></th>
<th><strong>Section in 2007-09:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Reactions groundwater/rock matrix</td>
<td>7.7</td>
</tr>
</tbody>
</table>

**General description:**

Groundwater in the geosphere will interact with the mineral surfaces it is in contact with. These rock-water interactions will occur at all times, although different reactions
may dominate at different times in response to the forcing and dynamic nature of the climatic and groundwater systems. The importance of these interactions is due both to their potential to affect the hydrogeochemical evolution of the geosphere and to their influence on radionuclide migration through the geosphere by a number of mechanisms:

− they control the overall hydrogeochemical system in the geosphere, notably the redox state, and thus are a major influence on the solubility and speciation of radionuclides released from the near field [10.3.1];
− precipitation and dissolution of fracture-coating minerals [10.2.6, 10.3.2] can alter the groundwater flow system, and flow rate, thus affecting the radionuclide transport time through the geosphere; and
− radionuclides may be sorbed [10.3.3] or incorporated into secondary alteration products formed by rock-water interaction, thus retarding transport.

The porewater composition occurring within the buffer and KBS-3H filling components depends on the composition of the saturating groundwater, the results of rock-water interactions in the geosphere and further reactions with the buffer and filling materials. The porewater composition in the buffer and filling components affects the swelling of the buffer [5.2.2] as well as the sorption capacity [5.3.3].

The fractures in the geosphere are the most important pathway for groundwater flow within the geosphere and, thus, interactions between the groundwater and the fracture coating minerals and mixing between the groundwater types will dominate changes in the hydrogeochemical system relevant for long-term safety. Fracture-coating minerals may not be representative of the bulk mineralogy of the rock because they are, themselves, likely to be the solid products of previous rock-water interactions.

The fracture-coating minerals at Olkiluoto are dominated by carbonates and clays, and these are accompanied by minor sulphides and oxides. Notably, the fractures at Olkiluoto lack ferric oxyhydroxide precipitates. In comparison, the bulk rock matrix is composed predominantly of silicate minerals (Pitkänen et al. 1999).

Compared with most other common mineral-water interactions, calcite is quickly equilibrated and, in most cases, the reaction is described adequately with equilibrium thermodynamics. Calcite is a significant pH buffer, especially against low pH. Calcite equilibrium is strongly coupled to the consumption and production of CO₂ by biological processes. The most common sulphide mineral in the Olkiluoto fractures is pyrite, though pyrrhotite, sphalerite and chalcopyrite are also found but less frequently. All sulphides as well as dissolved SO₄ are redox sensitive because sulphur is both a potential electron donor and acceptor in redox processes. Among the sulphide phases, pyrite and pyrrhotite are, however, most effectively dissolved in oxic conditions, because both ferrous iron and sulphur can be oxidised in redox processes. The reaction rates for oxidation of these sulphide phases are several orders of magnitude higher than for silicates. Various rock-water interaction processes may be mediated by microbial action [10.2.10].

The bedrock at Olkiluoto consists of high-grade metamorphic schists and gneisses and, therefore, many of the minerals were originally stabilised at high temperatures and pressures (e.g. cordierite, garnet and sillimanite). On the other hand smectite, sericite, pinite at Olkiluoto, in the rock matrix and in the fracture zones result from retrograde metamorphism and though susceptible of low temperature rock-water interactions, no detailes on the potential alteration products are known.
Most silicate minerals in the fractures and the rock matrix are prone to mineral alterations under typical geosphere conditions. Partial or incongruent decomposition of silicates is often energetically more favourable than direct breakdown by complete dissolution, for example, K-feldspar typically alters to form illite and kaolinite. At ambient temperatures, all usual silicate reactions are surface area, rate and mineral saturation controlled (Lasaga 1984). An additional factor that affects silicate dissolution reactions is the presence of redox-sensitive elements, such as Fe. Often, silicate reactions take place in conditions far from thermodynamic equilibrium, but the specific reaction rates of silicates are usually several orders of magnitude slower than for the carbonates and sulphide minerals (Luukkonen 2006).

Typically, the most active part of the geosphere for water-rock interactions is the upper oxidising, low pH (~6) zone. Geochemical studies at Olkiluoto indicate that dissolution of calcite, plagioclase and mafic minerals, and the precipitation of quartz and kaolinite occur in the overburden and upper bedrock (Pitkänen et al. 1999). The driving force for dissolution reactions lies in the low ionic strength and acidity of meteoric water. Future climate evolution [see 10.2.1 in Posiva 2012d] and the development of permafrost [see 10.2.3 in Posiva 2012d] will affect the duration of rock-water interactions, and the flux and composition of recharge water [see 9.2.7 in Posiva 2012d]. In post-glacial melt conditions, low ionic strength glacial meltwater may intrude down into the geosphere. This can have a long-term, significant impact on rock-water interactions, especially if the melt waters contain dissolved oxygen. There is, however, no palaeohydrogeological evidence to suggest that there has been any significant influence of oxidising glacial waters from any past glaciations on the deep groundwater conditions at Olkiluoto (Posiva 2013c). In the near-field rock, alkaline groundwaters may be created due to chemical degradation of concrete components of the repository system, such as closure plugs [9.2.8]. The alkaline groundwater may cause degradation of silicates around the repository and precipitation further along fractures, where more neutral pH conditions prevail (Baker et al. 2002). Interactions between the cement leachate and the rock are a potentially important factor for altering flow in the near-field rock, e.g. clogging of fractures and/or formation of secondary minerals has been suggested. Similarly, during the period of radiogenic heating, calcite may be precipitated in the near-field rock because it has lower solubility at higher temperatures [10.3.2].

During disposal, the KBS-3H deposition drifts will be filled with drift components and closed relatively soon. Parts of the central tunnels will, however, be left open for tens of years and the access tunnel and shafts will be left open for the whole operational period of approximately 100 years. In the case of extended periods of open tunnels, rock-water interactions will be enhanced. Under these open conditions, the most important reaction is likely to be the oxidation of pyrite. This process is known to occur very rapidly and can locally lead to very low pH groundwaters (pH < 3) and is the cause of ‘acid mine drainage’ that is often observed in deep mines and excavations. The significance of the reaction depends entirely on the amount of pyrite present. The total excavated volume in KBS-3H is smaller and in KBS-3V, resulting in a smaller interface area and smaller amount of engineering materials. Taking also into account the smaller and tighter EDZ (due to the use of boring instead of blasting), it can be concluded that generally the impacts of chemical interactions between engineered barriers and the rock are expected to be less significant in KBS-3H compared with KBS-3V (Gribi et al. 2007, Section 7.7).
Geochemical conditions and rock-water interactions may also be influenced by microbial activity, which can affect redox conditions [10.2.10].

Overall, rock-water interaction in the geosphere is affected by the following features of the repository system.

- **Temperature:** is an important control and, as a simple rule, typically a 10 °C increase in temperature will cause a 2–3 fold increase in reaction rates.
- **Groundwater flux:** has an indirect effect, in that movement of groundwater can introduce new chemical species to depth and transport dissolved substances throughout the geosphere.
- **Rock matrix properties:** the mineralogy is important when fracture-coating minerals are scarce, because the rock matrix will then be the solid phase in direct contact with the groundwater.
- **Fracture properties:** fracture mineralogy is important when fracture-coating minerals are present, because they will be the solid phases in direct contact with the groundwater.
- **Groundwater composition:** is fundamental for controlling reactions, particularly pH, redox and ionic strength.

**Uncertainties in the understanding of the FEP:**

Conceptually, rock-water interactions are well understood, but there are a number of parameter uncertainties that affect the modelling of future rock-water systems. These include both rate constants and thermodynamic data for the fracture-coating minerals. The significance of the silicate minerals in rock-water interactions is also not well understood.

With regard to the future evolution of the Olkiluoto groundwater system, there is some uncertainty about future climate evolution and the impact this may have on groundwater flow and chemistry. These uncertainties mostly relate, however, to rock-water interactions at shallow depths. Current understanding of the Olkiluoto groundwater chemistry and its past evolution suggests that the deep groundwater system is stable over the long term. Infiltrating waters of glacial, marine and meteoric origin have penetrated only to a maximum depth of approximately 300 m.

**Couplings to other FEPs:**

Rock-water interaction in the geosphere is directly affected by the following FEPs:

- Chemical degradation (of closure plugs) [9.2.8]
- Heat transfer [10.2.1]
- Erosion and sedimentation in fractures [10.2.6]
- Microbial activity [10.2.10]
- Groundwater flow and advective transport [10.3.5]
- Glaciation [see 10.2.2 in Posiva 2012d]
- Permafrost formation [see 10.2.3 in Posiva 2012d]
Rock-water interaction in the geosphere directly affects the following FEPs:
- Montmorillonite transformation (in the buffer) [5.2.6]
- Alteration of accessory minerals (in the buffer) [5.2.7]
- Montmorillonite transformation (in the filling components) [7.2.5]
- Alteration of accessory minerals (in the filling components) [7.2.6]
- Chemical degradation (of closure plugs) [9.2.8]
- Erosion and sedimentation in fractures [10.2.6]
- Methane hydrate formation [10.2.8]
- aqueous solubility and speciation [10.3.1]
- Precipitation and co-precipitation [10.3.2]
- Sorption [10.3.3]
- Diffusion and matrix diffusion [10.3.4]
- Groundwater flow and advective transport [10.3.5]
- Colloid transport [10.3.6]
- Gas transport [10.3.7]

References:
### 10.2.8 Methane hydrate formation

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th><strong>Class:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:**
None

**Section in 2007-09:**
7.7

**General description:**

Methane hydrates (also called methane ice or clathrates) are solid crystalline compounds of methane and water having an approximate formula of CH₄•nH₂O, where n ≈ 5–7. They are found abundantly on the sea floor and in the Arctic permafrost areas associated with oil and gas (methane) in sedimentary rocks (Ahonen 2001). There is very limited (if any) evidence to suggest significant methane hydrate accumulations occur in crystalline rocks.

An important precondition of their formation is that a CH₄ gas phase separates from groundwater under supersaturated conditions or that methane hydrate separates directly from the liquid phase when temperatures decrease, such as during the onset of permafrost conditions (Buffet 2000).

Within the mineral structure, methane is trapped within hydrogen-bonded water molecules, contributing to solid stability by its small molecular size. Methane hydrates are stable under specific pressure and temperature conditions (Sloan 2004) and may be stable at temperatures above 0 °C if the hydrostatic pressure is in excess of 20 bars, which is equivalent to around 200 m depth (Figure 10-3).

![Figure 10-3. Phase diagram for a methane-water mixture as a function of depth (equivalent to a hydrostatic pressure of 10 bar = 100 m) and temperature. Grey area defines the limits of methane hydrate stability in the temperature-pressure field. T_m represents the melting temperature of ice. T_c corresponds to the current temperature profile at Olkiluoto and T_p represents the temperature profile under long-term permafrost conditions with a permafrost thickness of about 100 m. After Buffet (2000).](image-url)
Currently, the geosphere temperatures are too high and the \( \text{CH}_4 \) contents in the groundwater too low to allow the formation of methane hydrates at any depths at Olkiluoto (Gascoyne 2005, Paloneva 2009, Keto 2010, Tohidi et al. 2010). Nonetheless, methane hydrates could theoretically form under possible future glacial conditions. The rate of accumulation of \( \text{CH}_4 \) in the Finnish bedrock is not well known; however, it is estimated to be slow at Olkiluoto (Delos et al. 2010).

It is unlikely that methane hydrates could ever form in the near field because permafrost is not predicted to reach to repository depths [10.2.3] and because of the groundwater composition and slow migration rate of \( \text{CH}_4 \) at Olkiluoto (Tohidi et al. 2010).

An important potential consequence of the formation of methane hydrates relates to their melting when the temperature increases (or pressure drops). Melting releases significant amounts of \( \text{CH}_4 \) in a gas phase in a very short time period, which may cause a rapid gas overpressure and mechanical disruption to the rock or other materials around it. Melting would also enhance two-phase flow and any radionuclides dissolved in the far-field groundwater could be expelled upwards with the methane gas.

Overall, methane hydrate formation (and melting) is influenced by the following features of the repository system.

− Temperature: the onset of permafrost conditions in a future glacial cycle is a requirement for the process to occur.
− Groundwater pressure: is important because methane hydrates form only at hydrostatic pressures in excess of that equivalent to 200 m depth.
− Groundwater composition: is a dominant control because methane hydrates can form only when the methane content is close to its solubility limit.

**Uncertainties in the understanding of the FEP:**

The processes leading to methane accumulation and hydrate formation are relatively well understood, but there is very limited evidence to suggest they ever occur within crystalline rock environments. In the most recent reviews on the worldwide occurrence of clathrates, no references are found for their existence in crystalline rock formations, but only in sediments along the Arctic coast of Alaska and Canada, and in sedimentary basins such as the Atlantic regions near the Caribbean (e.g. Carroll 2009, Demirbas 2010).

At Olkiluoto, methane clathrates have been observed within a few microscopic fluid inclusions within quartz grains (Eichinger et al. 2010). These inclusions were formed at very high temperatures and pressures (up to 400 °C), in conditions when \( \text{CH}_4 \) dissolves in water. As these fluid inclusions cooled, the gas and water phases separated, leading to very high gas pressures within the quartz grains.

This formation mechanism differs significantly from the processes that lead to large-scale methane accumulation in sedimentary systems, and applies in conditions that are grossly different from those in the repository system. As a consequence, the formation of methane clathrates in the crystalline rocks at Olkiluoto is considered to be very unlikely.

**Couplings to other FEPs:**

Methane hydrate formation in the geosphere is directly affected by the following FEPs:

− Rock-water interaction [10.2.7]
− Groundwater flow and advective transport [10.3.5]
− Permafrost formation [see 10.2.3 in Posiva 2012d]
Methane hydrate formation in the geosphere directly affects the following FEPs:
- Aqueous solubility and speciation [10.3.1]
- Precipitation and co-precipitation [10.3.2]
- Groundwater flow and advective transport [10.3.5]
- Gas transport [10.3.7]

References:

10.2.9 Salt exclusion

<table>
<thead>
<tr>
<th>Type: Process</th>
<th>Class: System evolution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alternative names: None</td>
<td></td>
</tr>
<tr>
<td>Section in 2007-09: 7.7</td>
<td></td>
</tr>
</tbody>
</table>

**General description:**
During permafrost conditions [see 10.2.3 in Posiva 2012d], the ground temperature remains perennially below zero and, as a consequence, groundwater freezes, although the actual temperature at which it freezes is dependent on the groundwater composition and pressure, and may be below zero.
Any dissolved species (salts) in freezing groundwater tend not to be incorporated into the ice lattice structure and, instead, are preferentially segregated into a separate phase. This salt exclusion process may lead to the formation of a saline water body moving ahead of an advancing freezing front, isolation of liquid brine pockets within the solid ice phase, accumulation of salts on the grain-boundaries or in the rock matrix, or crystallisation of cryogenic minerals. Cold, saline waters and brines associated with permafrost are called cryopegs.

If this process were to occur in the geosphere, the high density of the excluded saline water might potentially cause it to sink downwards to repository level, where it could interact with the clay in the buffer and KBS-3H filling components, causing it to lose some of its swelling capacity [5.2.2].

The freezing point of saline groundwaters may be significantly below 0 °C, depending on the salt content (Figure 10-4). With decreasing temperature, a brine phase with increasing salinity forms and is segregated as a saline front moving ahead of the propagating permafrost if the rate of movement of the brine is faster than the rate of progression of the freezing front. Scoping calculations indicate that the rate of permafrost advance in low-porosity crystalline rock may be of the order of 5 cm/a (Ahonen 2001). Under these conditions, the rate of advance of the permafrost is faster than the rate of migration of salinity, since the properties of the rock mean that this migration is diffusion dominated. Thus, the salinity is trapped and the formation of segregated intra-permafrost cryopegs, cryogenic mineralisation or sorbed grain-boundary salts occur within the frozen domain.

At the Palmottu natural analogue study site in Finland, a brackish Na-SO₄ type groundwater with very low stable isotopic signature was observed at depths of a few hundred metres. Permafrost development accompanied by salt exclusion was considered to be one potential explanation for its hydrogeochemical evolution (Blomqvist et al. 2000). Similarly, at Olkiluoto, SO₄-rich Littorina-derived groundwater dominates in the upper part of the geosphere and overlies a brackish Na-Cl type groundwater with high Na/Ca ratio at depths of 200–300 m. It has previously been suggested that these brackish waters (and similar saline waters found at depth in the Canadian Shield) developed as a result of salt exclusion during the last permafrost period. This explanation has, however, now been ruled out on the basis of their isotopic compositions (Posiva 2013c).

Due to the salinity of the groundwaters at Olkiluoto, the salt exclusion process may potentially occur during future permafrost periods, with the earliest predicted onset of permafrost being 50,000 years in the future [see 10.2.3 in Posiva 2012d].
Overall, salt exclusion is influenced by the following features of the repository system.

- Temperature: the onset of freezing conditions is a requirement for the process to occur.
- Groundwater composition: specifically, salinity is important because this controls the potential for the process and the nature of salts that can be excluded by the process.

**Uncertainties in the understanding of the FEP:**

The salt exclusion process is well understood and proven in the laboratory. Large-scale occurrence of salt exclusion in nature has been suggested as one possible explanation of relatively shallow saline waters in palaeohydrogeological interpretations of groundwater chemistry from field and natural analogue studies (e.g. Ruskeeniemi et al. 2004). The recent chemical and isotopic results from Olkiluoto and similar sites in Scandinavia and Canada, however, indicate that salt exclusion did not occur during the last permafrost cycle (Posiva 2013c, Stotler et al. 2012). In addition, there is no hydrogeochemical indication in fracture or matrix pore groundwater that permafrost would have approached repository depth. This process is, therefore, considered very unlikely to occur in the future at Olkiluoto.

**Couplings to other FEPs:**

Salt exclusion in the geosphere is directly affected by the following FEPs:

- Groundwater flow and advective transport [10.3.5]
- Permafrost formation [see 10.2.3 in Posiva 2012d]

Salt exclusion in the geosphere directly affects the following FEPs:

- Aqueous solubility and speciation [10.3.1]
- Precipitation and co-precipitation [10.3.2]
References:

10.2.10 Microbial activity

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>System evolution</td>
</tr>
</tbody>
</table>

**Alternative names:** Microbial processes

**Section in 2007-09:** 7.7

**General description:**
Microbes are ubiquitous forms of life and different species of microbes are adapted to different physicochemical conditions. It is also known that active microbial populations and processes extend deep into the bedrock to repository depths, and that deep subsurface microbes may differ substantially from those in the near-surface environment (Pedersen 2008).

In the geosphere, microbes are most likely to be located on the surfaces of fracture coating minerals and may, therefore, influence rock-water interactions [10.2.7], or are suspended in the groundwater in fractures. Microbes are considered important for influencing or even controlling (at least localized) geochemical conditions such as redox potential, and microbial reduction of sulphate to sulphide may influence the corrosion of the copper overpack. In general, however, microbial populations and
processes in the geosphere are likely to be less significant than in the near field, where microbes have a greater potential to become involved in corrosion of the copper overpack on the canister [4.2.5].

Microbiological processes in the geosphere will remain potentially active for the complete lifetime of the repository. Microbial populations will tend to respond to all nutrients available or intruding with time into the geosphere from the ground surface, from deeper depths or from the engineered barrier system.

In near-surface oxidising conditions, oxygen is consumed by microbes through aerobic respiration, aerobic methane oxidation, and oxidation of iron and sulphur compounds. Carbon dioxide is generated by microbes during aerobic oxidation of organic carbon. In deeper reducing conditions, microbes take advantage of a broad range of reactions, such as denitrification, fermentation and reduction of manganese, iron and sulphate, using methane, hydrogen and carbon dioxide of crustal origin (e.g. Itävaara et al. 2011).

The microbial populations present in the Olkiluoto groundwater have been studied and the data show that aerobic bacterial activity is restricted to the upper few metres, with anaerobic microbes dominant at all greater depths (Haveman et al. 1998, 2000, Pedersen 2008, Pedersen et al. 2010, Itävaara et al. 2011). Increased activities of several species are recorded at a depth of around 300 metres, which is considered to be significant because, at Olkiluoto, it denotes the greatest depth to which sulphate-containing ancient seawater has infiltrated. It is suggested that anaerobic methane oxidation (ANME) with sulphate reduction (SRB) may occur at this depth (Nyyssönen et al. 2012).

However, the results of stable isotope analyses of groundwater and fracture calcites indicate that microbial sulphate reduction by anaerobic methane oxidation has been very limited (not pervasive) at the site. Sulphur ($\delta^{34}$S (SO$_4$)) isotopic results from pyrites in the fractures indicate that microbial SO$_4$ reduction has occurred at relatively low temperatures. $\delta^{13}$C(DIC) results from monitored groundwater samples with elevated sulphide contents or $\delta^{13}$C from fracture calcites do not indicate significant anaerobic CH$_4$ oxidation (ANME) during the long term, although it is possible in minor amounts (Posiva 2013c). The results suggest the oxidation of hydrocarbons other than methane to be the energy source in microbial sulphate reduction. The potential role of other short-chain hydrocarbons as an energy source in sulphate reduction has been emphasised by Kniemeyer et al. (2007). The first results from the SURE experiment (first lab tests) also suggest that methane alone is not a “proper” energy source in sulphate reduction, rather microbes will use preferably hydrogen when present (Pedersen et al. 2013, Pedersen 2013).

Microbial activity in the geosphere is important for controlling certain aspects of the geochemical system, for example by maintaining reducing conditions. Microbial activity may, therefore, be important for controlling the solubility and speciation of radionuclides released from the near field [10.3.1].

In addition to affecting the geochemical conditions, microbes may also exert a direct control on radionuclide transport, if nuclides become attached to sessile (attached) or planktonic (mobile) microbes, which may then affect their migration behaviour. Microbial populations and processes in the geosphere are affected by a number of features of the repository system.
− Groundwater flux: the movement of water can introduce new microbial species to depth, transport populations throughout the geosphere and cause mixing of groundwaters, which may enhance microbial activity.
− Fracture properties: the fracture coating minerals may act as the main substrate onto which microbial populations form, and from which they derive some nutrients.
− Groundwater composition: provides nutrients to microbes in the form of dissolved or colloidal species derived from rock-water interactions.
− Gas composition: may also provide nutrients to microbes in the form of dissolved gas.
− Temperature: the activity of microbial species is temperature dependent.

Uncertainties in the understanding of the FEP:

It is evident that viable microbial populations will occur in the geosphere and that they are important for controlling the redox system in the rock. It is uncertain, however, how important this influence may be for the performance of the repository system. The impact of microbes on radionuclide transport in the geosphere is, however, expected to be limited (Pedersen et al. 2014).

There is considerable uncertainty about the nature and populations of microbes that would be viable in the long term in the geosphere. The current sampling and culturing methods indicates several microbial groups to be present across a broad range of depths within the bedrock at Olkiluoto but when some culturing process is being strongly activated several of the less abundant populations cannot be observed. It is not clear, therefore, what processes are actively influenced by the presence of microbes, or will be during repository construction and operation, and after closure of the facility.

The quantification of microbial activity, particularly the rate of sulphate reduction, is uncertain. Some minor microbial SO₄ reduction with anaerobic CH₄ oxidation may be active at the interface of SO₄ and CH₄ rich groundwaters, particularly if the system is disturbed by excavation and groundwater mixing occurs. But likely other short-chain hydrocarbons or hydrogen are the main energy sources (Posiva 2013c).

Couplings to other FEPs:

Microbial activity in the geosphere is directly affected by the following FEPs:
− Heat transfer [10.2.1]
− Groundwater flow and advective transport [10.3.5]

Microbial activity in the geosphere directly affects the following FEPs:
− Microbial activity (in the buffer) [5.2.8]
− Corrosion (of the supercontainer shell) [6.2.1]
− Microbial activity (in the filling components) [7.2.7]
− Corrosion (of compartment and drift plugs) [8.2.1]
− Rock-water interaction [10.2.7]
− Aqueous solubility and speciation [10.3.1]
− Precipitation and co-precipitation [10.3.2]
− Sorption [10.3.3]
− Colloid transport [10.3.6]
References:


10.3 Migration FEPs

Once a canister has failed, water has entered the canister and radionuclides have been released from the spent nuclear fuel and have migrated through the engineered barriers, they will be subject to migration (transport) and retardation processes operating in the geosphere. Other substances naturally present in the groundwater (such as organic and inorganic ligands) will be affected by the same transport processes and their presence may also potentially influence the migration and mobility of radionuclides. A summary of the main transport processes is shown in Figure 10-5 and the following descriptions summarise each of these processes, and the effects of the different variables on them.
Figure 10-5. The main transport processes in the geosphere. In flow and transport models, diffusion-accessible pore space may be assumed to exist throughout the rock matrix, or to be confined to spatially limited zones adjacent to transmissive fractures.

<table>
<thead>
<tr>
<th>10.3.1 Aqueous solubility and speciation</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Type:</strong> Process</td>
</tr>
<tr>
<td><strong>Alternative names:</strong> Speciation and sorption</td>
</tr>
</tbody>
</table>

**General description:**

Some radionuclides released from a failed canister will diffuse through the buffer [5.3.4] and be available for transport in the geosphere. According to the current understanding of the evolution of the disposal system, radionuclides will remain contained within most of the canisters for several hundred thousand years.

Groundwater flow and advective transport in the geosphere predominantly takes place in hydraulically active deformation zones (hydrogeological zones) and fractures. The radionuclides present in the geosphere will be present either in the aqueous phase or sorbed to the fracture-coating minerals [10.3.3] or will diffuse into the rock matrix [10.3.4], where they may be sorbed onto mineral surfaces. Smaller fractions of the inventory in the geosphere may also be associated with colloids [10.3.6] or the gas phase [10.3.7].

In this context, solubility refers to the maximum possible aqueous concentration of an element in all dissolved chemical forms (species) in the groundwater, which are in equilibrium with each other and the minerals in contact with the groundwater. Due to
past rock-water interactions [10.2.7], it is probable that the rock matrix will be altered along fractures and, therefore, the relevant mineral surfaces for controlling solubility and speciation will be the secondary alteration minerals that coat the fracture walls, rather than the minerals in the rock matrix.

The speciation of dissolved radionuclides is very important for radionuclide transport in the geosphere because it is the major control on their solubility and reactivity (sorption).

Generally, speciation of the radionuclides and solubility in the geosphere are controlled by the groundwater composition. Important for radionuclide solubility and speciation are pH, the redox conditions and the concentrations of dissolved gases, inorganic anions such as carbonate and chloride, and organic complexants. Solubility may be additionally controlled by co-precipitation and the formation of solid solutions [10.3.2].

The groundwater composition itself is controlled by the rock-water interactions [10.2.7] that take place as groundwater flows through the fractures and mixes with other groundwater types. The groundwater composition, as well as radionuclide solubility and speciation, may also be affected by microbial activity [10.2.10].

A significant issue for understanding solubility in the geosphere is that radionuclides will be dissolved in the groundwater in much lower concentrations than in the near field, because of the substantial dilution of the radionuclide concentrations entering and migrating through the geosphere. Under the most likely line of evolution, only a very small proportion of the total radionuclide inventory is estimated to migrate from the near field to the geosphere, and typically it is only the long-lived, poorly sorbing and highly soluble radionuclides that will do so (e.g. Cl-36, I-129, C-14). As a result, it is much less likely that radionuclide concentrations in groundwater in the geosphere will be solubility limited, compared with the engineered barrier system (e.g. within the canister or buffer). This means that precipitation is unlikely to be a significant immobilisation process in the geosphere, although co-precipitation with major elements may occur [10.3.2].

As noted above, the speciation of radionuclides in the geosphere will be controlled by the natural groundwater composition and, in particular, the presence of strong complexing ligands, such as carbonate and Cl– ions. In the presence of strong complexants, the formation of stable aqueous species may decrease the degree to which radionuclides are sorbed. The low-sorbing radionuclide complexes are mostly anionic. This is exemplified by the behaviour of uranium in fresh groundwaters, where the presence of a high concentration of carbonate leads to the formation of calcium-uranium(VI)-carbonate complexes and reduces the degree of sorption (Prat et al. 2009).

The redox state of the system also significantly affects the aqueous speciation of radionuclides for the redox-sensitive elements, such as Se, Tc, U, Np and Pu.

A thorough study of the radionuclide speciation in the Olkiluoto reference groundwaters has been conducted, taking account of the likely effects of climate evolution on future groundwater compositions (Grivé et al. 2007, Hakanen et al. 2014). The present-day Olkiluoto groundwater composition at the depth of the planned repository is characterised by a fairly high ionic strength (TDS 10–12 g/L), low redox potential and slightly basic pH. The fractures in the rock are typically coated with carbonates, clays and sulphides, which may provide sites for sorption or new mineral co-precipitation (Posiva 2013c, Hakanen et al. 2014).
There is a significant variation in the natural groundwater composition with depth at Olkiluoto and, consequently, radionuclide solubility and speciation may vary substantially during transport through the geosphere. The groundwater composition will also change in response to climate evolution [see 10.2.1 in Posiva 2012d]. Over time, the upper geosphere may be recharged with meteoric water, seawater and glacial meltwater, each with different redox potential, pH and ionic strength. Changes in the groundwater composition mean that the fracture-filling minerals with which radionuclides are associated via co-precipitation or sorption may be dissolved or new sorbing phases may be formed. The speciation of radionuclides in the groundwater at repository depth is of most interest because it is the rock immediately around the repository that contributes most to the overall transport resistance of the geosphere (Poteri 2009, Hodgkinson et al. 2009, Poteri et al. 2014).

Overall, aqueous solubility and speciation are influenced by the following features of the repository system.

− Radionuclide inventory: controls the types and amounts of radionuclides that may be available for transport and, in the geosphere, their expected low concentrations mean that solubility limits are unlikely to be reached.

− Temperature: the solubility of radionuclides is temperature dependent, although this is likely to be a second-order control in the geosphere.

− Groundwater pressure: the groundwater pressure will influence solubility and speciation, but is also a second-order control in the geosphere.

− Groundwater flux: is important because the movement of groundwater reduces the concentration of radionuclides due to dilution and dispersion.

− Rock matrix properties: the rock mineralogy is important when fracture-coating minerals are scarce because the rock matrix will then be the solid phase controlling groundwater chemistry.

− Fracture properties: the fracture mineralogy is important when fracture-coating minerals are present, because they act as the main solid phase for controlling groundwater chemistry.

− Groundwater composition: is a first-order control on the solubility and speciation of radionuclides, particularly the pH, Eh plus the type and concentration of dissolved species in the groundwater.

− Gas composition: will affect the groundwater composition (redox) if a two-phase system develops.

**Uncertainties in the understanding of the FEP:**

Radionuclide solubility and speciation are well understood from a conceptual model perspective. Similarly, the radionuclide solubilities are generally well characterised in thermodynamic databases, although there are numerical uncertainties for some of the safety relevant radionuclides and the matching solubility limiting phases. This may not be as significant for the geosphere as it is for the canister interior or buffer, because it is unlikely that the concentrations of the radionuclides that most contribute to the releases from the geosphere will be solubility limited.

The speciation of radionuclides is uncertain because of the uncertain spatial and temporal variation in groundwater composition. This is accounted for to a large extent by defining reference and bounding groundwaters as a function of time for different climatic periods. For many elements, the geochemical uncertainty is larger than the thermodynamic uncertainty.
**Couplings to other FEPs:**

Aqueous solubility and speciation is directly affected by the following FEPs:
- Chemical degradation (of closure plugs) [9.2.8]
- Rock-water interaction [10.2.7]
- Methane hydrate formation [10.2.8]
- Salt exclusion [10.2.9]
- Microbial activity [10.2.10]
- Precipitation and co-precipitation [10.3.2]
- Groundwater flow and advective transport [10.3.5]
- Colloid transport [10.3.6]

Aqueous solubility and speciation directly affects the following FEPs:
- Precipitation and co-precipitation [10.3.2]
- Sorption [10.3.3]
- Groundwater flow and advective transport [10.3.5]
- Colloid transport [10.3.6]
- Gas transport [10.3.7]

**References:**


10.3.2 Precipitation and co-precipitation

<table>
<thead>
<tr>
<th>Type: Process</th>
<th>Class: Migration</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Alternative names:</em></td>
<td></td>
</tr>
<tr>
<td><em>Section in 2007-09:</em></td>
<td></td>
</tr>
</tbody>
</table>

**General description:**

Precipitation and co-precipitation processes are very strongly dependent on radionuclide solubilities [10.3.1]. Due to the anticipated very small release rates of radionuclides from the near field and subsequent dilution in the geosphere, radionuclide concentrations in the geosphere are expected to be at trace levels and are unlikely ever to reach solubility limits under the expected hydrogeochemical conditions. Precipitation of single radioelement solid phases is, therefore, not expected to be a significant immobilisation process in the geosphere but co-precipitation may occur.

Co-precipitation is the precipitation of a radionuclide with a naturally occurring major element species (e.g. Ca) to form a solid solution. This might occur in the geosphere at the interface between groundwaters with different compositions where minerals are precipitated (e.g. oxic/anoxic water boundaries).

Co-precipitation of naturally occurring radionuclides is commonly observed in geological systems, and has been studied as part of several natural analogue studies such as that at Palmottu (Blomqvist et al. 2000).

Co-precipitation of radionuclides has been considered within the engineered barriers, for example co-precipitation of Ra-226 with Ba (Bosbach et al. 2010), but there is limited information on the potential for co-precipitation of repository derived radionuclides to occur in the geosphere, and co-precipitation is usually not accounted for in performance assessments (Bruno et al. 2007).

Precipitation and co-precipitation, occurring on solid surfaces such as the fracture walls, would retard radionuclide transport. The mechanism is considered to be irreversible unless a change in geochemical conditions causes the precipitated mineral phases to redissolve. It is possible that precipitation could cause the formation of suspended colloids directly from solution and, if this were to occur, it might enhance radionuclide transport, depending on the mobility of the colloid phase [10.3.6].

Overall, precipitation and co-precipitation are influenced by the following features of the repository system.

- Radionuclide inventory: controls the radionuclides that are available for inclusion in precipitates.
- Temperature: the solubility of radionuclides is temperature dependent, although this is likely to be a second-order control over precipitation in the geosphere.
- Groundwater pressure: can influence solubility limits and, thus, precipitation, but is a second-order control in the geosphere.
- Groundwater flux: the movement of groundwater through the rock controls the distribution of radionuclides in the geosphere and, therefore, their concentrations and the overall groundwater composition.
− Rock matrix properties: the rock mineralogy is important when fracture-coating minerals are scarce because the rock matrix will then be the solid phase controlling groundwater chemistry.
− Fracture properties: the fracture mineralogy is important when fracture-coating minerals are present because they act as the main solid phase for controlling groundwater chemistry.
− Groundwater composition: particularly pH, carbonate concentration, redox conditions, and dissolved gases are the primary controls on the potential for precipitation and co-precipitation.
− Gas composition: will affect the groundwater composition (including the redox potential) if a two-phase system develops.

**Uncertainties in the understanding of the FEP:**

There is a good conceptual understanding of radionuclide precipitation and co-precipitation mechanisms, and the factors that control radionuclide and major element solubilities. It is unlikely that precipitation will be a significant process in the geosphere, but co-precipitation is possible. There is, however, considerable uncertainty regarding the nature of the co-precipitate phases that may form in the geosphere.

Broadly, the uncertainties that apply to solubility and speciation [10.3.1] also apply to precipitation and co-precipitation. The added complexity relates to the formation of co-precipitated solid solutions, for which there are currently very few data relevant to the conditions expected in the geosphere.

**Couplings to other FEPs:**

Precipitation and co-precipitation are directly affected by the following FEPs:
− Chemical degradation (of closure plugs) [9.2.8]
− Rock-water interaction [10.2.7]
− Methane hydrate formation [10.2.8]
− Salt exclusion [10.2.9]
− Microbial activity [10.2.10]
− Aqueous solubility and speciation [10.3.1]
− Sorption [10.3.3]
− Groundwater flow and advective transport [10.3.5]

Precipitation and co-precipitation directly affect the following FEPs:
− Aqueous solubility and speciation [10.3.1]
− Sorption [10.3.3]
− Diffusion and matrix diffusion [10.3.4]
− Groundwater flow and advective transport [10.3.5]
− Colloid transport [10.3.6]

**References:**

10.3.3 Sorption

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Alternative names:</th>
<th>Section in 2007-09:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Speciation and sorption</td>
<td>7.7</td>
</tr>
</tbody>
</table>

**General description:**

The migration of radionuclides dissolved in the groundwater within geosphere fractures [10.3.1] may be retarded by sorption on the surfaces of the minerals that coat the fracture surfaces (e.g. clays, carbonates, sulphides and oxides) and on the pore surfaces of the host rock surrounding the fractures. The fracture-coating minerals at Olkiluoto typically have a very limited thickness of only a few millimetres at most. In addition, there is often an altered layer of the host rock that ranges in thickness from millimetre to centimetre scale present adjacent to the fracture surfaces (Posiva 2013c, Chapter 8).

Sorption is element specific and depends on the speciation of the element (valency state, hydrolysis and complexation), the groundwater ionic strength and the solid phase surface characteristics. Radionuclides may be sorbed by either surface complexation or ion exchange.

Surface complexation is a mechanism involving a covalent or electrostatic bond between the hydrated surface of the solid and a radionuclide. This mechanism is most efficient for cations that are strongly hydrolysed, and is very important for radionuclides with a high positive charge and high electronegativity (Bradbury & Baeyens 2009a, 2009b). Surface complexation is also the main sorption mechanism for oxyanions.

Ion exchange is a mechanism involving substitution of a radionuclide for an ion in the mineral structure. It occurs strongly on clay and mica minerals due to the exchangeable cations that compensate for the negative charge in the mineral structure. This mechanism is effective even for non-hydrolysed cationic radionuclide species.

Sorption is typically characterised by the distribution coefficient, which is the ratio between the concentration of the radionuclide in the solid phase and in solution. For most of the radionuclides, trace concentrations and linear sorption are assumed in the far field. For radionuclides with elevated concentrations in groundwater, the distribution coefficient is based on a non-linear sorption isotherm. Many of the radionuclides transported to the geosphere are not strongly sorbing (Altmann et al. 2001) and, in the...
absence of co-precipitation [10.3.2], their retardation in the geosphere will occur mainly as a result of matrix diffusion [10.3.4] under expected evolution conditions. The fracture-coating minerals that have formed due to rock-water interaction [10.2.7] will provide effective sorption sites in the geosphere, but, because the coatings are very thin, the most abundant surfaces for sorption will be the altered and unaltered rock behind the fracture coatings.

There is a significant change in the nature of the fracture-coating mineral assemblage with depth at Olkiluoto and, consequently, the potential for sorption may vary substantially during radionuclide transport through the geosphere. The fracture-mineral assemblage and groundwater composition, particularly in the upper geosphere, may also evolve in response to climate evolution and the changing nature of the recharging water. Sorption is a reversible reaction and there may be a net release (desorption) of radionuclides if, for example, there are changes to the groundwater chemistry. It is possible that radionuclides could sorb onto suspended colloids directly from solution, and this might enhance radionuclide transport, depending on the mobility of the colloid phase [10.3.6].

Overall, sorption is influenced by the following features of the repository system.
- Radionuclide inventory: controls the radionuclides that are available for sorption.
- Temperature: is a control over the efficiency of radionuclide sorption, although this is likely to be a second-order effect in the geosphere.
- Groundwater flux: is important because groundwater movement controls the distribution of radionuclides in the geosphere.
- Rock matrix properties: the rock mineralogy is important when fracture-coating minerals are scarce, because the rock matrix will then be the solid phase on which sorption may occur.
- Fracture properties: the fracture mineralogy is important when fracture-coating minerals are present, because they can act as the solid phase for sorption.
- Groundwater composition: particularly the pH, Eh and speciation may affect the rate and degree of sorption.

**Uncertainties in the understanding of the FEP:**

There is a good conceptual understanding of the mechanisms that control sorption. Sorption in the geosphere is significant only for a limited set of radionuclides under expected evolution conditions, because most of the radionuclides that can readily migrate through the buffer demonstrate conservative, non-reactive transport behaviour. The quantitative evaluation of sorption is limited by the very large uncertainties in the future changes to the hydrogeochemical system in the geosphere in response to climate evolution.

The primary uncertainties relate to the sorption capacity of the various fracture-coating minerals and rock types that are available for sorption, and the spatial and temporal variation in that sorption capacity.
**Couplings to other FEPs:**

Sorption is directly affected by the following FEPs:
- Rock-water interaction [10.2.7]
- Microbial activity [10.2.10]
- Aqueous solubility and speciation [10.3.1]
- Precipitation and co-precipitation [10.3.2]
- Diffusion and matrix diffusion [10.3.4]
- Groundwater flow and advective transport [10.3.5]

Sorption directly affects the following FEPs:
- Precipitation and co-precipitation [10.3.2]
- Groundwater flow and advective transport [10.3.5]
- Colloid transport [10.3.6]

**References:**


---

**10.3.4 Diffusion and matrix diffusion**

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
</tr>
</tbody>
</table>

**Alternative names:**

None

**Section in 2007-09:**

7.7

**General description:**

In fractured crystalline rocks, bulk solute transport and groundwater movement at the macroscopic scale usually takes place by flow (advection) through the fracture network [10.3.5].

At the microscopic scale, however, radionuclides may also move within the fractures by diffusion and this may be an important transport mechanism in low flow or stagnant conditions when advection is not occurring. This may, for example, occur beneath a permafrost layer [see 10.2.3 in Posiva 2012d] when groundwater flow stops after recharge and discharge zones are shut off by the frozen layer.
In a flowing fracture, radionuclides may also move laterally out of the fracture and into an intricate network of interconnected microfractures and micropores within the rock by molecular diffusion. This process is called matrix diffusion (Neretnieks 1980). The water in the interconnected microporosity will be very slow moving or even immobile and, therefore, the transport of radionuclides subject to matrix diffusion will be retarded relative to the flowing water in a fracture. The retardation effect may be increased for sorbing nuclides because the surface area of the microporosity can typically be 3 to 6 orders of magnitude larger than that of the flowing fractures, providing abundant sorption sites (EC 2005, p. 25).

Matrix diffusion may prove to be effective for retarding even non-sorbing species depending on how long they remain isolated within the microporosity before diffusing back out into the flowing fracture. This is particularly relevant, because typically it is mainly the long-lived, poorly sorbing and highly soluble radionuclides (e.g. Cl-36, I-129 and C-14) that will be able to diffuse through the buffer and reach the geosphere before they decay to insignificant levels.

There may be differences in the matrix diffusion behaviour of anions, cations and neutral species. Anions may be excluded to some extent from the smallest micropores due to their repulsion from negatively charged mineral surfaces, and diffusion tests have indicated in practice that anionic exclusion may take place in the rocks at Olkiluoto (Kaukonen et al. 1997). For cations the effect is the opposite because of their attraction towards the mineral surfaces. Cations enter the matrix more frequently than neutral species, whereas anions have a smaller probability to enter the matrix.

It has also been speculated that radionuclides associated with colloids or microbes could be retarded by matrix diffusion. The diffusion of such relatively large particles into the rock would, however, be much less than that of dissolved radionuclides. In performance assessments, it is generally conservatively assumed that such particles are excluded from rock matrix pores due to their size or charge.

Evidence for matrix diffusion comes from laboratory measurements, in-situ tracer experiments and natural analogues (EC 2005, p. 26). In some cases, there is an observed increase in the matrix porosity (and thus an increase in the effective diffusivity) within the first few centimetres of rock adjacent to water-bearing fractures due to mineral alteration. Any fracture coating present may be porous and allow matrix diffusion to take place but, in some cases, the coatings could ‘seal’ the underlying rock porosity and limit the effect of matrix diffusion.

The significance of matrix diffusion for radionuclide transport in the geosphere depends, in part, on the volume of rock available for the process. In turn, this volume may be restricted by the accessible depth of the interconnected microporosity within the rock mass. Many observations show, however, that the interconnected porosity extends throughout large volumes of the rock types abundant at Olkiluoto. The flow rate in the fracture also affects the coupling between transport along the fracture and the diffusion into the rock matrix, and, therefore, the overall retardation effect due to matrix diffusion.

At Olkiluoto, the nature of fracture-coating minerals and the depth of the interconnected porosity and alteration halos adjacent to fractures are being investigated (Posiva 2013c, Chapter 8) and an in-situ investigation programme has also been started in the ONKALO underground laboratory that aims to quantify the diffusivity and
The porosity of the rock matrix (Aalto et al. 2009). The results of those investigations that are already available have been used to establish site-specific models of the rock matrix structure and retention processes (Hakanen et al. 2014). Future results will be used to evaluate and enhance these models.

Matrix diffusion will be relevant for all time frames after radionuclides have been released from the failed canister and have migrated through the buffer or other KBS-3H drift components. Variations in the flow field [10.3.5] due to geological and climatic processes [see 10.2.1 in Posiva 2012d], and processes such as stress redistribution [10.2.2], erosion and sedimentation in fractures [10.2.6] and precipitation [10.3.2] may change the geometry of the flowing fracture network and, therefore, potentially affect the flow rates and flow paths.

Overall, diffusion and matrix diffusion in the geosphere are influenced by the following features of the repository system.

- Radionuclide inventory: controls the radionuclides that are available for matrix diffusion.
- Temperature: controls the rate of diffusion, although this is of secondary importance.
- Groundwater flux: is important because advection, together with the fracture geometry, controls retardation due to matrix diffusion.
- Fracture geometry: in particular, the width of flow channels and fractures, together with the groundwater flow, and the depth of the interconnected porosity in the rock adjacent to flowing fractures, are important.
- Rock matrix properties: these are important for defining the extent of microporosity.
- Fracture properties: fracture-coating minerals can have different diffusion properties from those of the host rock. Often the diffusion coefficients are higher due to the enhanced microporosity of the fracture-coating minerals. On the other hand, fracture coatings can potentially seal the surfaces of the rock and limit the potential for matrix diffusion.

**Uncertainties in the understanding of the FEP:**

Although matrix diffusion is a well understood and documented process, there are significant uncertainties regarding its quantification, in particular, with respect to the different matrix diffusion behaviour of anions, cations and neutral species.

A key uncertainty is the description of matrix heterogeneity, which is strongly site-specific, and is likely to vary with depth in the geosphere and with distance from the major hydraulically-active fractures and alteration zones.

Another significant uncertainty relates to the evolution of the fracture network and hydraulic conditions over time due to natural geological and climate processes, and due to repository related processes. These processes may affect the flow-rate distributions in the bedrock.
**Couplings to other FEPs:**

Diffusion and matrix diffusion in the geosphere are directly affected by the following FEPs:
- Reactivation-displacement along existing fractures [10.2.3]
- Erosion and sedimentation in fractures [10.2.6]
- Rock-water interaction [10.2.7]
- Precipitation and co-precipitation [10.3.2]
- Groundwater flow and advective transport [10.3.5]

Diffusion and matrix diffusion in the geosphere directly affects the following FEPs:
- Corrosion (of supercontainer shell) [6.2.1]
- Corrosion (of compartment and drift plugs) [8.2.1]
- Sorption [10.3.3]
- Groundwater flow and advective transport [10.3.5]
- Colloid transport [10.3.6]

**References:**


**10.3.5 Groundwater flow and advective transport**

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
</tr>
</tbody>
</table>

**Alternative names:**
Advection/mixing; Transport of radionuclides in water phase

**Section in 2007-09:**
7.7 and 7.8

**General description:**
In crystalline rocks, such as those at Olkiluoto, groundwater flow (advection) takes place predominantly in a fracture network and is, therefore, strongly heterogeneous on all scales. On a scale of metres or larger, flow is concentrated in a small number of flowing features, typically formed by fracture zones or along intersecting fractures. On a smaller scale (centimetre scale), flow within a single fracture is often channelled through interconnected void spaces in between any constrictions in the fracture aperture and filling minerals. The hydraulic properties of the rock and, hence, the velocity and direction of flow can vary widely throughout the rock mass. Stress redistribution [10.2.2] may cause fractures in the network to open or close and, therefore, may affect the groundwater flow system over time. Flow through the fracture network may also be affected by erosion of fracture-filling minerals and sedimentation [10.2.6].

A KBS-3H repository will probably cause a smaller hydraulic disturbance than a KBS-3V repository, because of the smaller excavated volume (Gribi et al. 2007, Section 7.7). In the period immediately after waste emplacement, groundwater flow in the near-field rock is important because it controls the availability of water for uptake by the buffer [5.2.2] and filling components [7.2.2], and controls the time until full swelling pressure is achieved. During this initial period, groundwater flow in the near-field rock may also be affected by the temperature gradient driven by radiogenic heat output [10.2.1].

Over much longer periods of time, groundwater flow is important because it will be the primary process responsible for transporting any radionuclides that are released from the near field through the geosphere and towards the surface environment (advective transport). This is not expected to occur until long after the thermal period has ended and, consequently, thermally driven convection in the geosphere is not considered to be a significant process for radionuclide transport.

Groundwater flow will control the rate at which corrosive agents affecting the canister, especially sulphide, will be conveyed from the geosphere to the near field. After the canister has failed, groundwater flow will transport dissolved radionuclides [10.3.1] and potentially those in colloidal form [10.3.6], and in the gas phase by entraining bubbles in the flowing groundwater [10.3.7]. Radionuclide transport in flowing groundwater may, however, be retarded by a number of physical and chemical processes, including sorption [10.3.3] and matrix diffusion [10.3.4]. Precipitation is unlikely to be a significant retardation process in the geosphere due to the expected low radionuclide concentrations but co-precipitation may occur [10.3.2].

Groundwater flow in the geosphere is mainly driven by the hydraulic gradient, which is the change in groundwater pressure head per unit distance. The hydraulic gradient is created by differences in the elevation of the groundwater table, which are controlled mainly by the topography and sea level. Groundwater flow at depth is also affected by
density differences between fresh and saline water bodies. Saline waters are denser than fresh water, and so tend to sink. Saline waters occur at depth in many crystalline rocks and can originate from seawater or from long-term rock-water interactions. The saline/fresh water interface at a coastal margin together with the groundwater table also affects groundwater flow patterns. Temperature also affects the density of the water, and can contribute to density driven flow.

The majority of the rain and surface waters that infiltrate into the geosphere will circulate in the shallow, local groundwater system contained within the overburden and topmost part of the bedrock. Only a very small proportion of the recharge will reach the deep groundwater flow system [see 9.2.7 in Posiva 2012d] and can be involved in radionuclide transport processes within the geosphere (Pitkänen et al. 2009).

The natural variability of groundwater flow systems in fractured crystalline rock, such as at Olkiluoto, will result in a significant variation in the water flow velocities and the transport routes through the fracture network followed by the radionuclides, leading to dispersion of migrating solutes (Figure 10-6). The geometry and degree of connectivity of the fracture network has a dominant control on the extent of dispersion. Dispersion can occur in the direction of flow (longitudinal dispersion) and perpendicular to the direction of flow (transverse dispersion). Mixing of groundwaters of different composition may also affect the chemical and physical retardation of radionuclides.

The effect of mixing and dispersion (and matrix diffusion [10.3.4]) is that radionuclide concentrations in the groundwater tend to be progressively reduced as they become diluted over a larger volume of rock, and releases to the surface environment take place over a longer period of time with the maximum (peak) release delayed and more diluted than would be the case if mixing and dispersion did not occur.

In response to evolving hydrogeological and climatic conditions at the surface, the groundwater pattern at the Olkiluoto will change over the lifetime of the repository. Simulations have indicated that, regardless of transient effects, the range of possible groundwater flow patterns at Olkiluoto will be well constrained by the site-scale topography and local hydraulic zones (Nykyri et al. 2008).

Initially, continued isostatic uplift of the land will cause progressive retreat of the Baltic Sea and alter the groundwater flow system until about 10,000 years AP. The later onset of glacial conditions [see 10.2.2 in Posiva 2012d] and permafrost [see 10.2.3 in Posiva 2012d] will have an even more significant effect. Permafrost is estimated to develop at Olkiluoto to a maximum depth of around 200–300 m (Hartikainen 2012). An extensive permafrost layer will effectively prevent infiltration and remove the hydraulic gradient, causing groundwater flow to cease. Even in case of discontinuous permafrost (i.e. where taliks are present), the infiltration will be very limited compared with unfrozen ground conditions.
Groundwater flow could also be significantly affected due to methane hydrates if they were to form during permafrost conditions and subsequently melt rapidly, releasing large amounts of CH₄ that could drive groundwater flow upwards [10.2.8].

Overall, groundwater flow in the geosphere, and advective transport, is influenced by a number of features of the repository system.

- Radionuclide inventory: controls the radionuclides that are available for transport by groundwater flow.
- Temperature: the geothermal gradient will have a minor influence on groundwater flow after the thermal period has ended.
- Groundwater pressure: the variation in groundwater pressure (head) is the primary driver for groundwater flow.
- Groundwater flux: the flux of groundwater is the primary measure of the volume of groundwater and amount of dissolved radionuclides that are transported through the rock.
- Rock stress: may have a local effect causing the fractures to open or close and thus indirectly affecting the flow.
- Fracture geometry: the fracture geometry is a dominant control on flow in the geosphere because flow is restricted to the active fracture network.
- Fracture properties: in particular, properties such as the aperture of the fracture that control transmissivity are important for controlling groundwater flow.
- Groundwater composition: any differences in salinity (TDS) can cause density driven flow.
- Gas composition: is important for controlling the potential for two-phase flow, which may influence advection.

**Uncertainties in the understanding of the FEP:**

The main driving forces for groundwater flow and advective transport through the fractures and deformation zones that comprise the main flow paths are well understood. There are, however, uncertainties associated with the different conceptualisations of
the heterogeneous fractured crystalline rock mass in the numerical models used in performance assessments. Updating the site descriptive models in the ongoing site characterisation work at Olkiluoto is reducing the uncertainty about the location and characteristics of the hydraulically active deformation zones and characteristics of the fracture network.

There is also uncertainty about the connectivity and transmissivity within the fracture networks. The Posiva Flow Log (PFL, Öhberg & Rouhiainen 2000) primarily measures the connected transmissive features and there are many detailed hydraulic data that make it possible to set bounds on the uncertainties. There is a high level of confidence regarding the flow system in the central part of the island at Olkiluoto, but less confidence outside this area because the locations and properties of the hydro-zones and fracture networks that underpin the hydrological DFN model are not as comprehensively sampled and measured as in the central area.

The biggest uncertainties may, however, relate to the evolution of the groundwater flow conditions over time in response to both geological and climatic changes that will affect the hydraulic head (pressure) distribution, the rate of flow and the locations of recharge and discharge zones.

As well as large-scale uncertainties, there are also uncertainties associated with understanding of flow on a small scale, within individual fractures, such as the coupling between advection in a fracture and matrix diffusion in the rock.

**Couplings to other FEPs:**

Groundwater flow in the geosphere and the advective transport of radionuclides are directly affected by the following FEPs:

- Physical degradation (of closure plugs) [9.2.8]
- Transport through closure backfill and plugs [9.3.1]
- Heat transfer [10.2.1]
- Stress redistribution [10.2.2]
- Reactivation-displacement along existing fractures [10.2.3]
- Creep [10.2.5]
- Erosion and sedimentation in fractures [10.2.6]
- Rock-water interaction [10.2.7]
- Methane hydrate formation [10.2.8]
- Aqueous solubility and speciation [10.3.1]
- Precipitation and co-precipitation [10.3.2]
- Sorption [10.3.3]
- Diffusion and matrix diffusion [10.3.4]
- Gas transport [10.3.7]
- Construction of a well [see 9.2.30 in Posiva 2012d]
- Glaciation [see 10.2.2 in Posiva 2012d]
- Permafrost formation [see 10.2.3 in Posiva 2012d]
- Land uplift and depression [see 10.2.4 in Posiva 2012d]
- Inadvertent human intrusion [see 10.2.5 in Posiva 2012d]
Groundwater flow in the geosphere and the advective transport of radionuclides directly affects the following FEPs:

- Water uptake and swelling (in the buffer) [5.2.2]
- Mechanical erosion (in the buffer) [5.2.3]
- Chemical erosion (in the buffer) [5.2.4]
- Water uptake and swelling (in the filling components) [7.2.2]
- Mechanical erosion (in the filling components) [7.2.3]
- Chemical erosion (in the filling components) [7.2.4]
- Advection (in the filling components) [7.3.5]
- Transport through closure backfill and plugs [9.3.1]
- Heat transfer [10.2.1]
- Erosion and sedimentation in fractures [10.2.6]
- Rock-water interaction [10.2.7]
- Methane hydrate formation [10.2.8]
- Salt exclusion [10.2.9]
- Microbial activity [10.2.10]
- Aqueous solubility and speciation [10.3.1]
- Precipitation and co-precipitation [10.3.2]
- Sorption [10.3.3]
- Diffusion and matrix diffusion [10.3.4]
- Colloidal transport [10.3.6]
- Gas transport [10.3.7]
- Groundwater discharge and recharge [see 9.2.7 in Posiva 2012d]
- Construction of a well [see 9.2.30 in Posiva 2012d]

References:


10.3.6 Colloid transport

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
</tr>
</tbody>
</table>

**Alternative names:**
Colloid formation and transport

**Section in 2007-09:**
7.7

**General description:**
Colloids are small particles suspended in the groundwater that typically range in size from about 1 nm to 1 µm. They are naturally occurring and ubiquitous in deep groundwaters, but may also be generated by physical and chemical processes resulting from the presence of the repository. In particular, colloidal particles may be released to the geosphere by chemical erosion of the buffer [5.2.4] and the KBS-3H filling components [7.2.4], or by chemical degradation of cementitious materials [9.2.8]. Colloids may affect the flow in fractures if they are transported away from the deposition drift materials and later deposited within the fracture network [10.2.6].

Radionuclide-bearing colloids may, in principle, also be formed by direct precipitation or co-precipitation within the geosphere, but because radionuclide concentrations in the geosphere are expected to be at trace levels, precipitation is not expected to be a significant mechanism for radiocolloid formation [10.3.2].

Colloidal transport of radionuclides in the geosphere cannot occur until after the canister has failed and radionuclides have migrated through the buffer to the geosphere. Radionuclide-bearing colloids would only be formed after radionuclides have diffused through the buffer. Colloids formed by precipitation or co-precipitation within the canister are expected to be filtered by the buffer [5.3.6] unless the buffer becomes substantially eroded.

The radionuclides that reach the geosphere most readily under normal conditions will generally be poorly sorbing and highly soluble and, therefore, are less likely to be associated with colloids than other radionuclides. The association mechanisms between radionuclides and colloids may be weak ion-exchange, stronger complexation or direct incorporation (EC 2005, p. 35).

The transport and retention processes of radionuclides that become associated with colloids in the geosphere will be different from those of dissolved radionuclides. Depending on the abundance and nature of the colloids, and the characteristics of the fracture network, radionuclide transport may be enhanced or retarded by different mechanisms involving the colloids.

Radionuclide transport may be enhanced, particularly for the sorbing nuclides, if they are attached to mobile colloids. In general, colloids will not be retarded by sorption or matrix diffusion to the same extent as dissolved radionuclides. Furthermore, electrostatic repulsion between the colloids and fracture-coating minerals may keep colloids to the central parts of the flowing fractures, where flow velocities are higher than the average. Colloids may also be attached to buoyant and mobile gas bubbles [10.3.7]. Radionuclide transport may be retarded, however, if nuclides are strongly sorbed onto immobile colloids that are subject to agglomeration and filtration processes in the fractures.
In general, colloid-facilitated transport may increase radionuclide transport only if the following conditions are met (Gardiner et al. 2001).

− There is a large population of colloids occurring naturally in groundwater or arising from the presence of the repository.

− Fracture apertures and other pore spaces that conduct flowing groundwater are sufficiently large to allow colloids to pass without significant physical or chemical filtration.

− The groundwater chemistry is conducive to colloid stability.

− Radionuclide sorption on colloids is favoured by electrostatic attraction and groundwater chemistry, and desorption processes are irreversible, or at least slow relative to transport times through the geosphere.

Colloids are not expected to be stable under the high ionic strength groundwaters found at depth at Olkiluoto, and present-day colloid concentrations are low. In the event of infiltration of low ionic strength glacial water to repository depth, however, colloidal stability will be enhanced. These are also the conditions under which mechanical erosion of the buffer and KBS-3H filling components by flowing groundwater is likely to be most significant [5.2.3 and 7.2.3], and this would provide a source of colloids in the geosphere.

Overall, colloid transport in the geosphere is influenced by the following features of the repository system.

− Radionuclide inventory: controls the radionuclides that may be available for association with colloids.

− Temperature: the stability of colloids may be temperature dependent, although this is only a second-order control.

− Groundwater flux: the movement of groundwater is important for controlling the rate of colloid migration.

− Fracture geometry: controls the overall flowpath for groundwater that may contain colloids.

− Fracture properties: in particular, the aperture of the fractures will control the potential for colloids to be filtered from the flowing groundwater.

− Groundwater composition: controls the potential for colloid formation and the stability of colloids, as well as the sorption and solubility properties of radionuclides.

**Uncertainties in the understanding of the FEP:**

Radionuclide uptake on colloids must be considered in terms of a ternary system, where radionuclides are distributed between the aqueous phase, the colloids and the fixed (rock mineral) sorption sites. There is significant uncertainty associated with the understanding of such complex systems.

The significance of colloid-facilitated radionuclide transport is increased if radionuclide uptake on colloids is irreversible or only slowly reversible. The understanding and quantification of radionuclide sorption/desorption kinetics over time frames relevant to performance assessment, are not well advanced.
Filtration theory, which describes colloid immobilisation processes, works well for certain well-defined systems. It is, however, inadequate for many natural, heterogeneous geological systems.

Finally, the evolution of the population of colloids in the geosphere (especially those associated with degradation of the engineered barrier system and foreign materials), and their mobility and stability, under different groundwater conditions are not well defined.

**Couplings to other FEPs:**

Colloid transport in the geosphere is directly affected by the following FEPs:

- Mechanical erosion (of the buffer) [5.2.3]
- Chemical erosion (of the buffer) [5.2.4]
- Colloid transport (in the buffer) [5.3.6]
- Mechanical erosion (of the filling components) [7.2.3]
- Chemical erosion (of the filling components) [7.2.4]
- Colloid transport (in the filling components) [7.3.6]
- Chemical degradation (of closure plugs) [9.2.8]
- Erosion and sedimentation in fractures [10.2.6]
- Rock-water interaction [10.2.7]
- Microbial activity [10.2.10]
- Aqueous solubility and speciation [10.3.1]
- Precipitation and co-precipitation [10.3.2]
- Sorption [10.3.3]
- Diffusion and matrix diffusion [10.3.4]
- Groundwater flow and advective transport [10.3.5]
- Gas transport [10.3.7]

Colloid transport in the geosphere directly affects the following FEPs:

- Aqueous solubility and speciation [10.3.1]

**References:**


### 10.3.7 Gas transport

<table>
<thead>
<tr>
<th>Type:</th>
<th>Class:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Migration</td>
</tr>
</tbody>
</table>

**Alternative names:**
- Formation/dissolution/reaction of gaseous species;
- Transport of radionuclides in gas phase

**Section in 2007-09:**
- 7.7 and 7.8

**General description:**
Dissolved gases occur in most deep groundwater systems and are commonly derived from:
- air dissolved in groundwater during recharge (predominantly N₂, O₂, Ar),
- dissolved gases produced in the bedrock by radioactive decay (He, Ar, Rn),
- crustal degassing and diffusion (He, N₂, CH₄, H₂), and
- thermogenic and microbial processes (CH₄ and heavier hydrocarbons, H₂S, CO₂, N₂).

In the repository near field, additional gas may also be formed by radiolysis of the canister water [3.2.6], anaerobic corrosion of the iron insert of the canister [4.2.6] and microbial activity in the buffer [5.2.8] and KBS-3H filling components [7.2.7]. Of these, anaerobic corrosion of iron will produce the greatest volume of gas (hydrogen) under the expected near-field conditions. Due to the change of the plug and supercontainer shell material to titanium (previously steel), the additional contribution of KBS-3H-specific materials is not significant for gas formation. Rapid evolution of gas in the geosphere is also possible only in the very unlikely presence of methane hydrates if these were to melt, causing the release of significant amounts of CH₄ [10.2.8].

The solubility of gases in groundwater depends mostly on the hydrostatic pressure and temperature. Their solubility tends to increase with depth, due to the increase in hydrostatic pressure, but is reduced by an increase in groundwater temperature and salinity.

A free gas phase (bubbles) will form if the aggregate partial pressure of the dissolved gases exceeds the hydrostatic pressure. This typically occurs when groundwater flows from depth towards the surface and the hydrostatic pressure becomes progressively lower. Once a free gas phase has formed in the groundwater, a two-phase (water and gas) system is created. In a fractured crystalline rock, the free gas will migrate upwards through the fracture network towards the surface.

While the gas pressure in the repository is below the hydrostatic pressure of 4 MPa, slow inflow of water from the host rock occurs and water saturation in the KBS-3H deposition drifts increases. Any residual air in the void space between the supercontainer and rock as well as between the distance block and rock will be trapped. This concerns also the DAWE design – despite the fact that a significant part of the air is evacuated during watering – because the large quantity of air trapped within the fine pore structure of the bentonite cannot be removed by this technique. Full saturation is, therefore, not likely to be reached before the start of gas generation and a residual free gas phase will remain (Gribi et al. 2007, Section 7.5.2).

Two-phase flow may occur in the period shortly after closure of the disposal facility, when air trapped in the excavations and in fractures in the rock is displaced or is dissolved in groundwater saturating the near field. This will be a transient process and is unlikely to affect the remainder of the geosphere.
Two-phase flow involving radionuclides cannot occur until after the canister has failed and radionuclides have migrated through the KBS-3H drift components to the geosphere. Depending on the characteristics of the fracture network and the groundwater flow system [10.3.5], the transport of radionuclides in a two-phase system may be enhanced or retarded by different mechanisms. The significance of a gas phase is very largely dependent on the volume of free gas present.

Enhanced radionuclide transport may occur if the radionuclides are directly incorporated into gases (e.g. C-14 in methane) and the gas bubbles move freely through the fractures due to their buoyancy, allowing them to travel faster than the mean groundwater flow rate. In addition, other radionuclides in colloidal form may also be carried with the mobile bubbles, because colloids are often preferentially attached to the gas-water interface (i.e. the bubble surface). Radionuclides dissolved in the groundwater may also be pushed ahead of the gas bubbles as they travel through the fractures, causing a localised groundwater flow rate faster than otherwise.

Radionuclide transport may be retarded, however, if radionuclides are associated with gas bubbles that become trapped and accumulate within kinks and bends in fractures, forming an airlock. These trapped bubbles will also restrict further groundwater flow through the fractures, because the groundwater cannot pass through the accumulation of trapped gas.

At Olkiluoto, the most abundant naturally occurring dissolved gases are CO$_2$, H$_2$, N$_2$, O$_2$ and He. In addition, the deep, saline groundwaters also contain methane close to its saturation point (Gascoyne 2005, Pitkänen et al. 2004, Pitkänen & Partamies 2007). The impact of these gases on the current groundwater flow system is low, however, because they remain in solution.

Regarding gas transport, the most important consideration for the repository, after waste disposal, is the high CH$_4$ concentration in the deep, saline groundwater. Continuous accumulation of CH$_4$ over time could lead to the formation of a free gas phase in the geosphere if the gas solubility decreased due to heat output from the spent nuclear fuel [10.2.1] or due to upconing of deeper groundwater. The first of these mechanisms is not likely to be significant for radionuclide transport under normal conditions, however, because most of the canisters are expected to remain intact long after the thermal phase has ended. The significance of the second mechanism in the very long term is uncertain because it depends on future geological and climate variability.

Both CH$_4$ and H$_2$ are also important gases that can be used by microbes in sulphate reduction processes in the geosphere.

Overall, gas transport in the geosphere is influenced by the following features of the repository system.

- Radionuclide inventory: controls the radionuclides that may be available for gas transport.
- Temperature: is a first-order control on gas solubility.
- Groundwater pressure: the hydrostatic pressure is also a first-order control on gas solubility.
- Groundwater flux: the movement of water is important for controlling the transport of entrained gas bubbles.
- Fracture geometry: the geometry of the fracture network controls the transport of any free gas once it forms and, in particular, determines whether it can move upwards due to buoyancy or instead form an airlock.
- Groundwater composition: is fundamental because the concentration of dissolved gases in the groundwater is a primary control over the formation of a free gas phase.
- Gas composition: different gases and compositions will present different solubilities under the expected geosphere conditions.

**Uncertainties in the understanding of the FEP:**

There is a good fundamental understanding of the gas formation and two-phase flow processes. It is uncertain, however, whether the rate of gas generation will be sufficient to enable two-phase flow to occur in the geosphere and, if it does, whether it will be significant in controlling radionuclide transport processes.

The potential for gas generation at Olkiluoto due to the methane content of the deep, saline groundwaters remains an open question.

**Couplings to other FEPs:**

Gas transport in the geosphere is directly affected by the following FEPs:
- Gas transport (through the buffer) [5.3.7]
- Gas transport (through the filling components) [7.3.7]
- Rock-water interaction [10.2.7]
- Methane hydrate formation [10.2.8]
- Aqueous solubility and speciation [10.3.1]
- Groundwater flow and advective transport [10.3.5]

Gas transport in the geosphere directly affects the following FEPs:
- Groundwater flow and advective transport [10.3.5]
- Colloid transport [10.3.6]
- Gas origin and implications (in the surface environment) [see 9.2.22 in Posiva 2012d]

**References:**


<table>
<thead>
<tr>
<th>Report Number</th>
<th>Title</th>
<th>Authors</th>
<th>ISBN</th>
</tr>
</thead>
<tbody>
<tr>
<td>POSIVA 2016-01</td>
<td>Simplified transport modelling of a disposal system and doses using probabilistic methods</td>
<td>Pekka Kupiainen &amp; Olli Nummi (Fortum Power and Heat Oy)</td>
<td>978-951-652-246-6</td>
</tr>
<tr>
<td>POSIVA 2016-02</td>
<td>Safety Evaluation for a KBS-3H spent nuclear fuel repository at Olkiluoto – Performance Assessment</td>
<td>Posiva Oy</td>
<td>978-951-652-249-7</td>
</tr>
<tr>
<td>POSIVA 2016-03</td>
<td>Safety Evaluation for a KBS-3H spent nuclear fuel repository at Olkiluoto – Features, events and processes</td>
<td>Posiva Oy</td>
<td>978-951-652-250-3</td>
</tr>
</tbody>
</table>