DOPAS TRAINING WORKSHOP 2015

Integration of Experimental Work and Process Modelling in Safety Assessment

André Rübel (GRS)

D4 3.3
17 September 2015

The research leading to these results has received funding from the European Union's European Atomic Energy Community's (Euratom) Seventh Framework Programme FP7/2007-2013, under Grant Agreement No. 323273 for the DOPAS project.

Introduction of GRS

Who is GRS?

- The Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) is a non-profit organisation which deals with technical-scientific research and provides expertise
- GRS was established as a business in January 1977. The headquarters are in Cologne, other sites include: Berlin, Braunschweig and Garching
- GRS is only financed by contracts and the present annual volume of contracts is worth 57 million €
- Main customers are:
  - The Federal Ministry for the Environment, Nature Conservation, Building and Nuclear Safety (BMUB)
  - The Federal Ministry of Economic Affairs and Energy (BMWi)
  - The Federal Ministry of Education and Research (BMBF)
  - The Federal Foreign Office (AA)
  - The Federal Agency for Radiation Protection (BfS)
  - The European Commission

Major activities

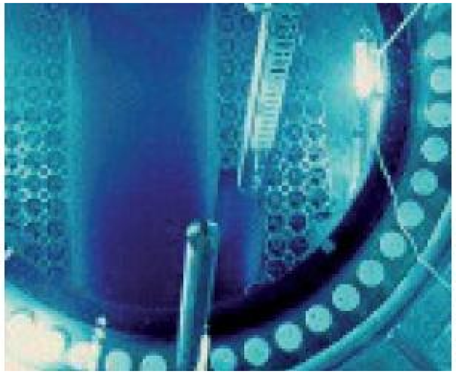
§ Research and development

- Reactor safety
- Radiation protection
- Waste disposal
- Environmental protection

Repository Safety Research Division
↳ Safety Analyses Department

§ Analyses, assessments and expert opinions

§ Scientific-technical services and support



What is safety?

Calvin and Hobbes are playing in the sandbox. Calvin builds a town out of sand. Hobbes is digging a hole.
Conversation:

Picture 1:	C: Here's a little town.
	H: Here's a steam shovel scooping out a giant hole.
Picture 2:	C: Here comes the bulldozer, pushing thousands of barrels of toxic nuclear waste into the giant hole.
Picture 3:	C: Over the years, these dangerous poisons seep into underground waterways.
Picture 4:	C: The cancer rate of the nearby little town triples.
	H: If you want me, I'll be under the bed.

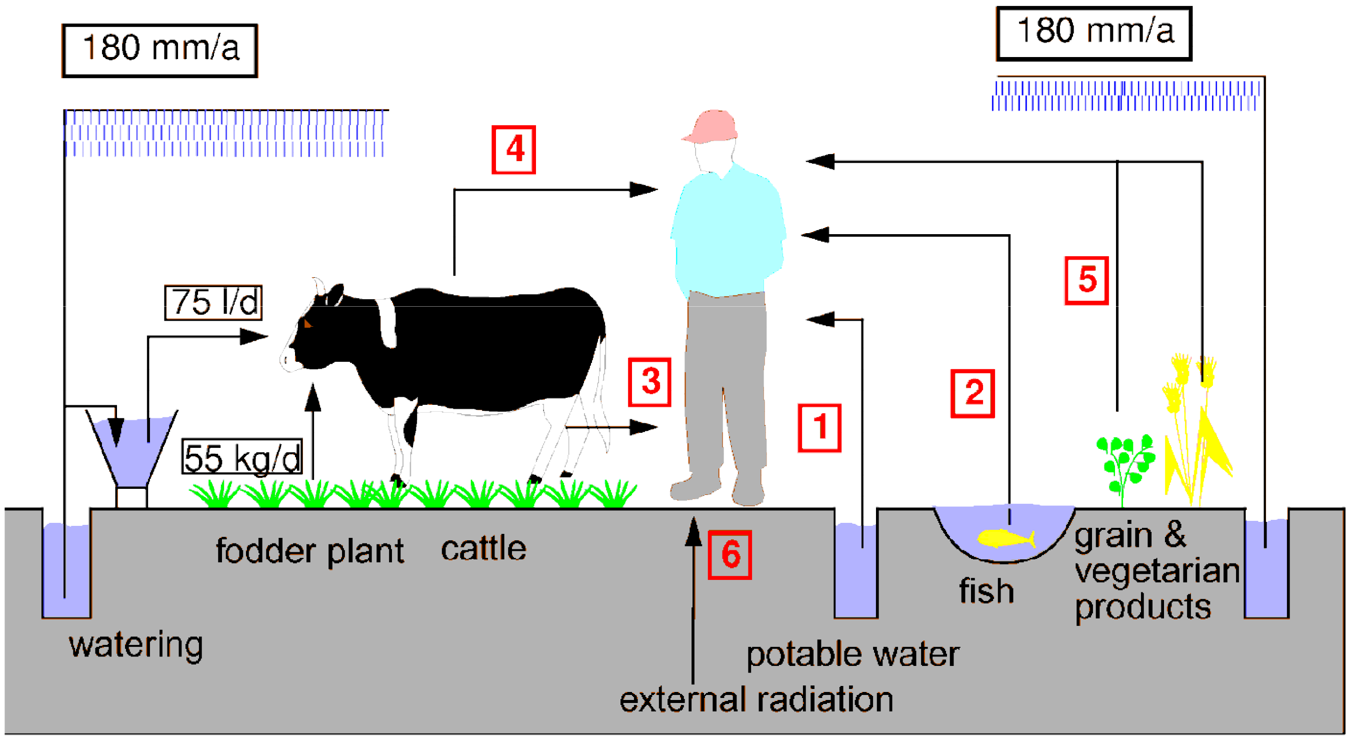
Comic not included in presentation for copyright reasons.

Bill Watterson, Calvin & Hobbes of June 9,1987

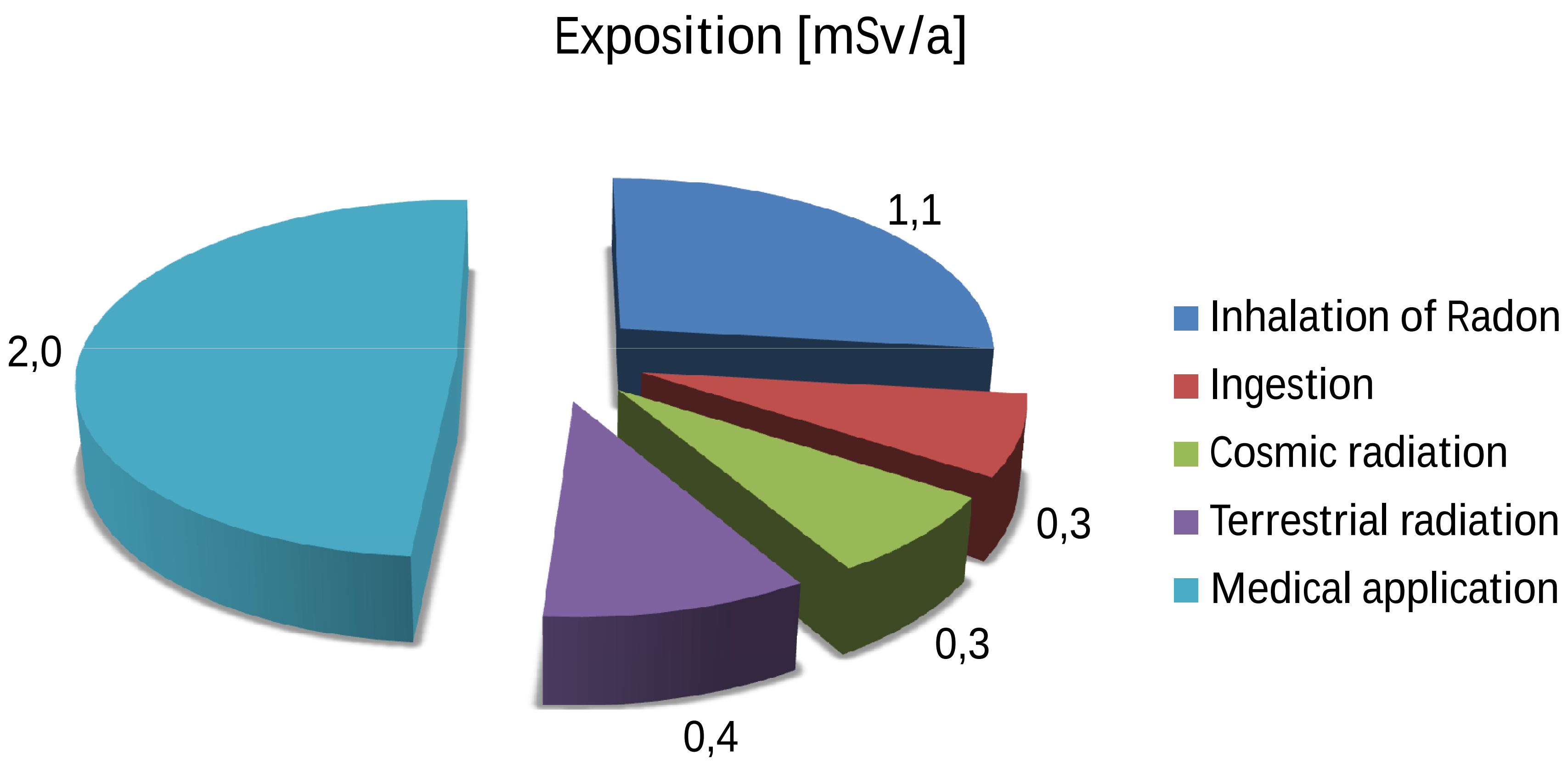
Safety assessment poses four key questions

- What might happen?
- When might it happen?
- What is the likelihood?
- What are the consequences?

Radionuclide exposure pathways



Mean radiation exposition of population in Germany



Mean natural radiation exposition: 2.1 mSv/a

Data from BfS

Past, present and future

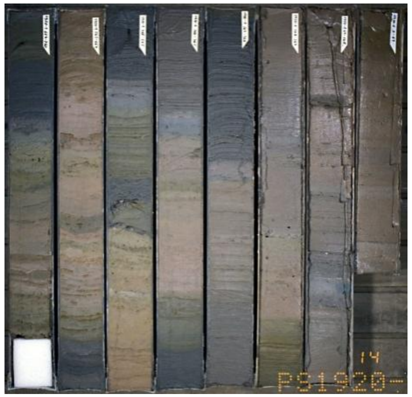
Climate

Durability of constructions

Geology

Human behaviour

1 000 000 a | 100 000 a | 10 000 a | 1 000 a | 100 a | present



Pictures: Wikimedia Commons

Challenges

Large scale system

Heterogeneous system properties

Spatial and temporal variable system properties

Complex interaction between different processes

Manifold of uncertainties

System is regarded for very long timescales

Safety assessment approach

Long-term safety assessment

Major element of the Safety Case

- Quantitative Analysis of the long-term development of the repository
  - Full repository system
  - Compartments and geotechnical components
- Aims
  - Assessment of repository safety
    - Calculation of indicators related to humans
    - Comparison of results with regulatory limits
  - Increase of system understanding
  - Optimisation of repository concept

No prognosis of the radiation exposition of future population!

Approach

- Site description
  - Geology
  - Hydrogeology
  - Hydrology (regional/local)
  - Biosphere
- Repository concept
- Geoscientific long-term prognosis of site
- Description of processes
  - Experimental results
  - Process modelling
  - Natural analogues

Many programmes use a FEP-catalogue

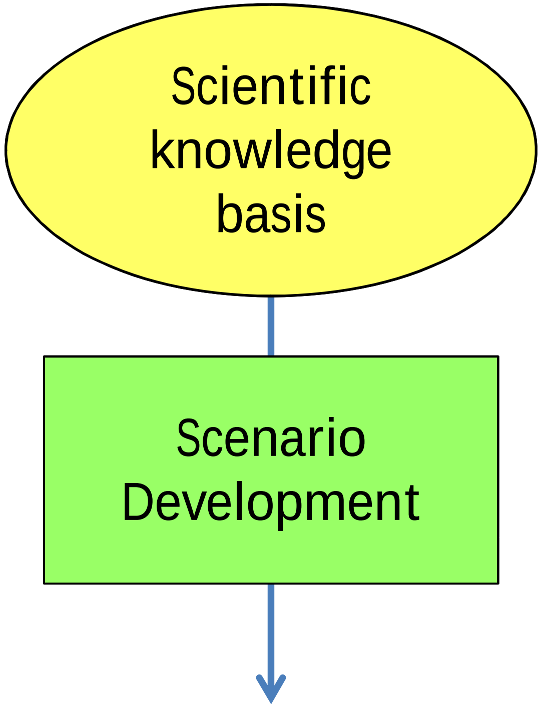
Scientific knowledge basis

Description of all relevant

- **F**eatures
- **E**vents
- **P**rocesses

Approach

Scenario



Description of all relevant **F**eatures, **E**vents, **P**rocesses

Description of site evolution

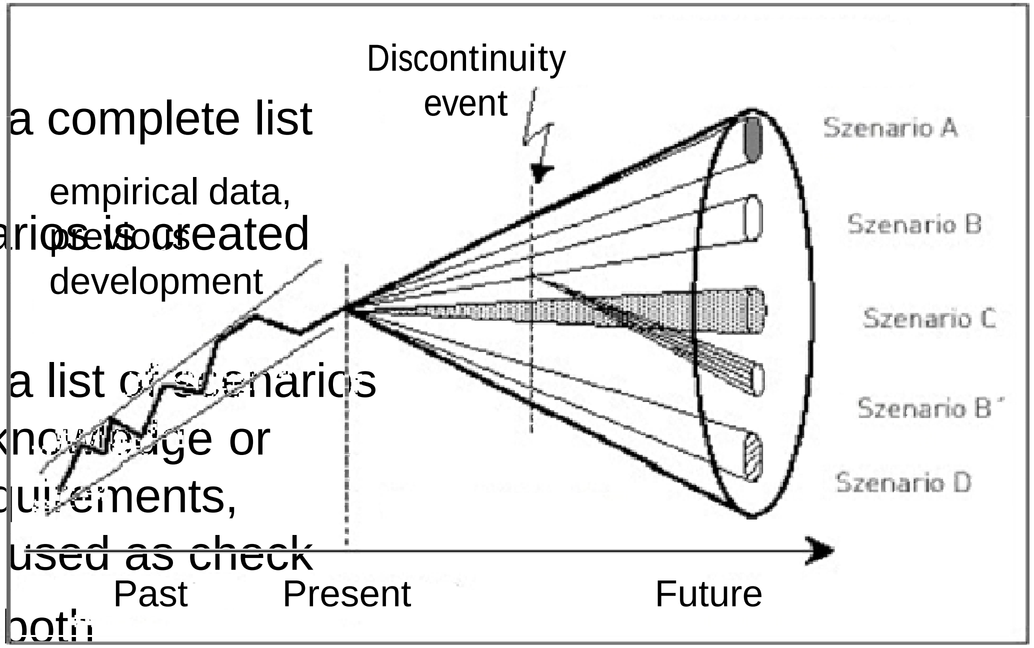
Use of scenarios

A scenario is a synthetic description of an event or series of actions and events

Create visions of possible future evolutions that have a potential impact on the safety of the repository under consideration of experience, knowledge and probability

Scenario development:

- Bottom-up
  - Starting from a complete list of FEPs, a list of scenarios is created
- Top-down
  - Starting from a list of scenarios collected by knowledge or regulatory requirements, FEP-lists are used as check
- Combination of both



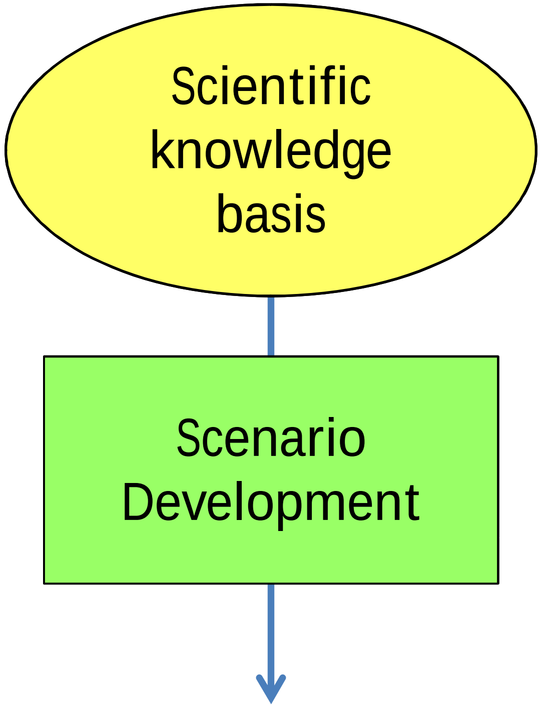
Graphic: Modified after Wikimedia Commons

Approach

Scenario

§ Description of site evolution
- expected evolution
- probable evolution
- less probable evolutions
- what-if cases

§ Stylized scenarios



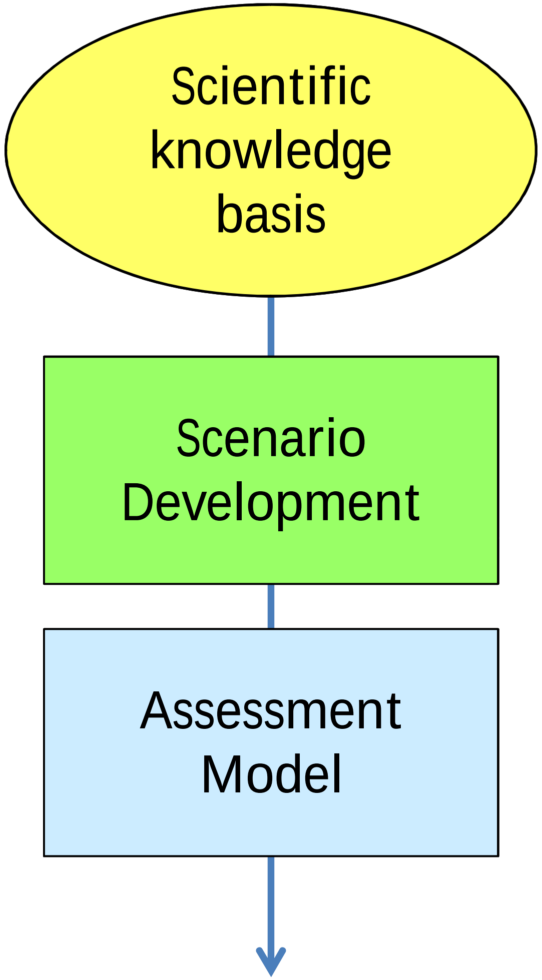
Description of all relevant **F**eatures, **E**vents, **P**rocesses

Description of site evolution

Approach

Model

- Includes various simplifications to reduce complexity of
  - Geometry
  - Processes
- Process Models
- Integrated Models



Description of all relevant **F**eatures, **E**vents, **P**rocesses

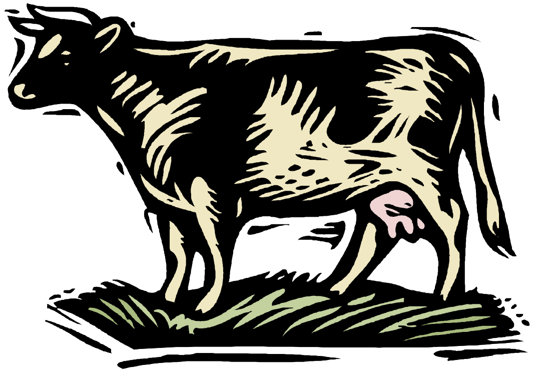
Description of probable and less probable evolutions including what-if cases

Representation of scenario

Simplifications to handle complexity in modelling

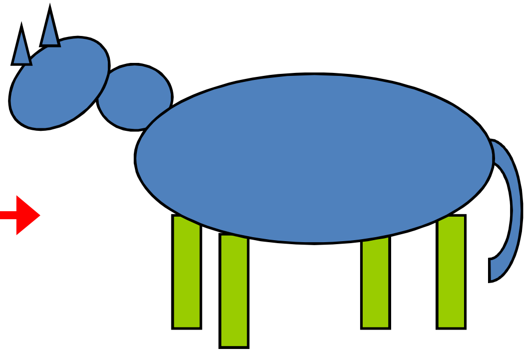
- Not all processes in real system can be described
- Computing time too high for thousands of simulations over Mio. of years

Realistic Model



Observation by experiment

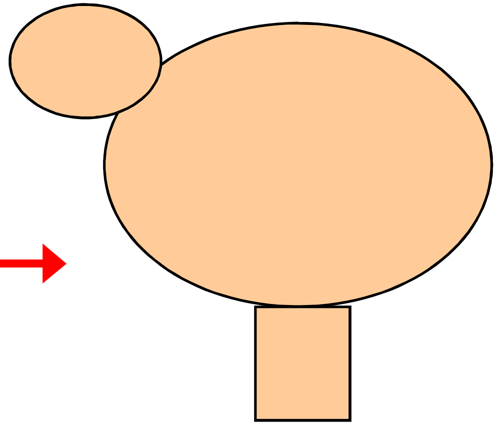
Process-Level Model



Mechanistic understanding

- High detail of description
- Long computing time
  - Subsystems
  - Short timespan
  - Few simulations

Integrated Model

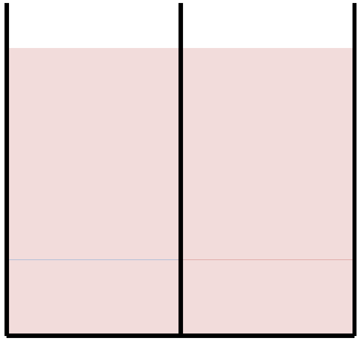


Abstraction describing behaviour

- Lower detail of description
- Short computing time
  - Total system
  - Full timespan
  - Large amount of simulations

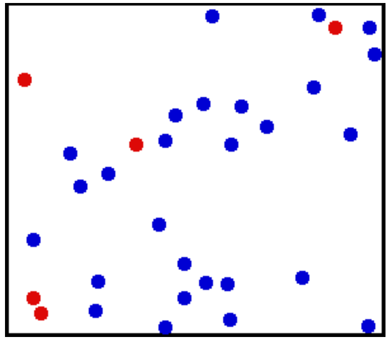
Example

Observation (Experiment)



Transport by diffusion

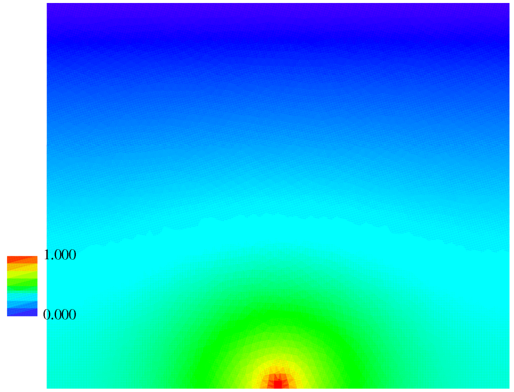
Mechanistic Model (Process-Level Model)



Brownian Motion

$$\frac{\partial \rho}{\partial t} = \frac{\partial^2}{\partial x^2} \cdot \int_{-\infty}^{+\infty} \frac{\Delta^2}{2\tau} \cdot \varphi(\Delta)\, d\Delta + \text{higher order even moments}$$

Phenomenological Model (Integrated Model)



Fick's law

$$J = -D \frac{\partial c}{\partial x}$$

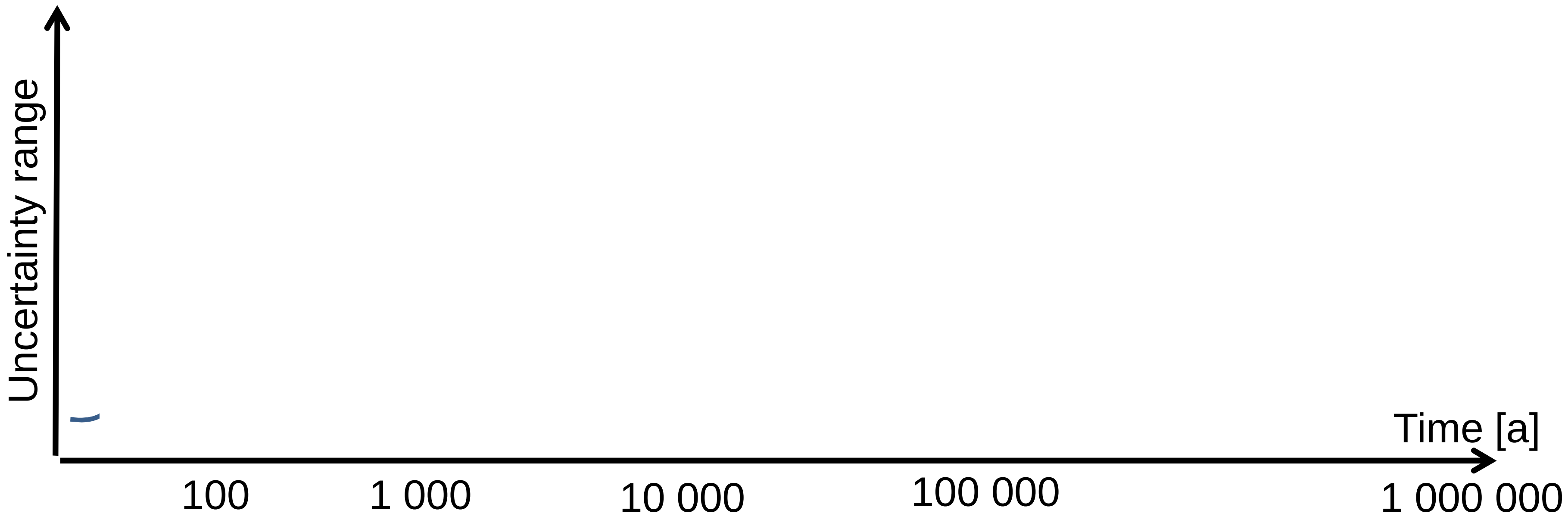
Animation: Wikimedia Commons

Qualitative temporal evolution of uncertainty of processes

Transient period

Disposal system stability

Geosphere evolution



Quantify by predictions with process models

Quantify by predictions with integrated models

Approach

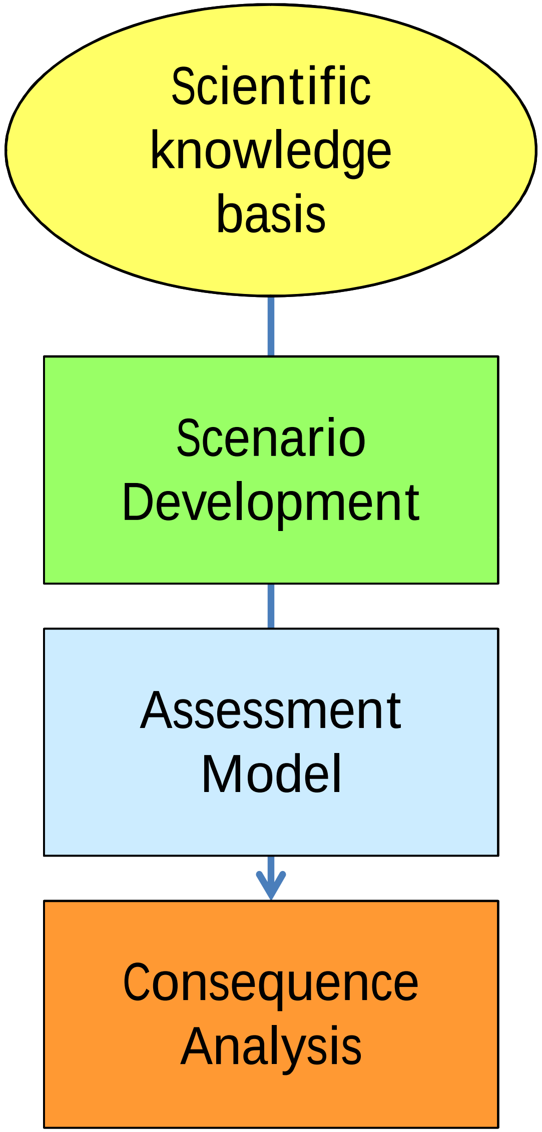
Consequence Analysis

Calculation of indicators

§ Safety indicators
  - Comparison with regulatory limit yields safety statement (dose / risk)

§ Performance indicators
  - increase of system understanding
  - optimisation of repository concept

§ Iterative process



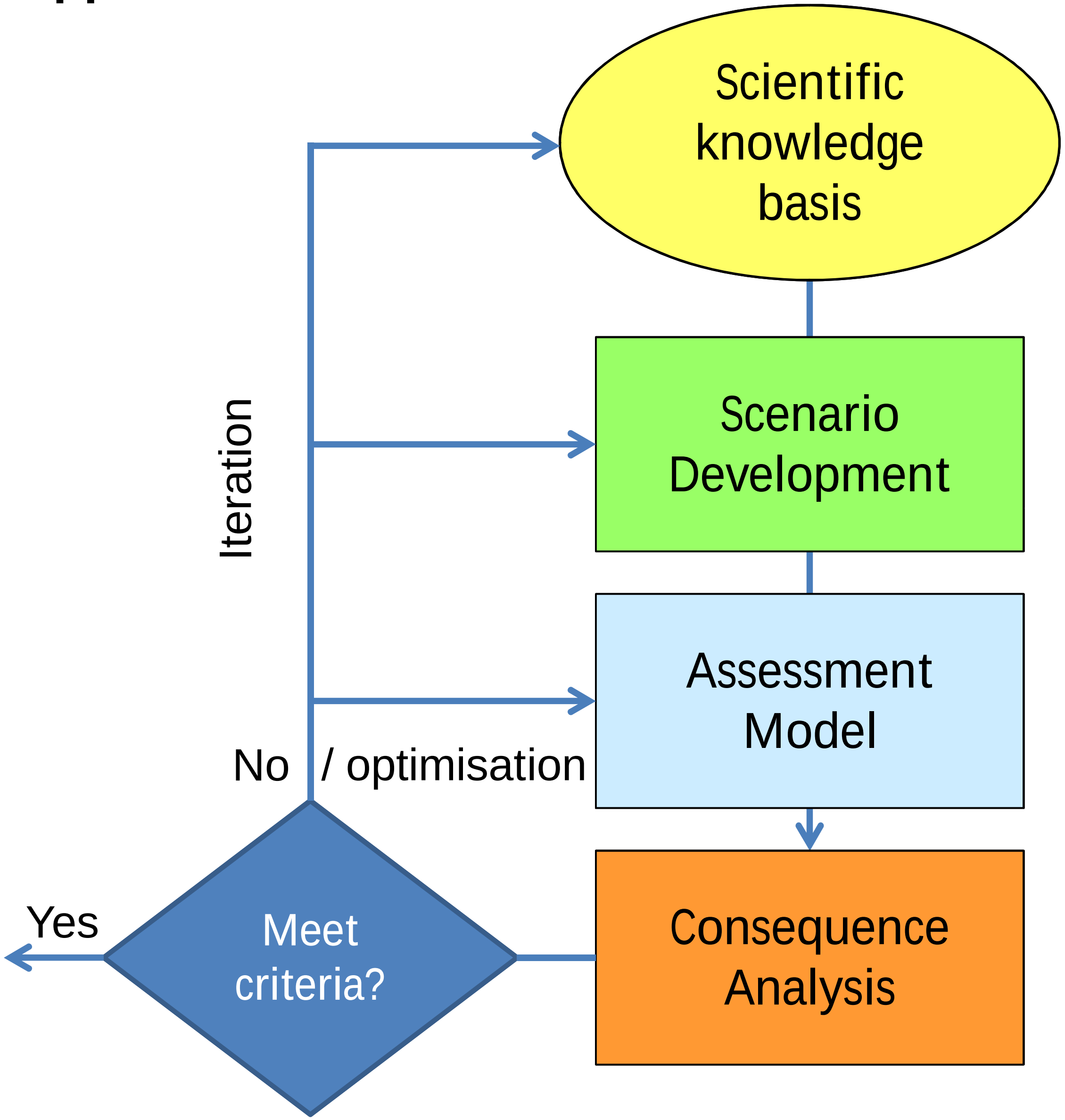
Description of all relevant **F**eatures, **E**vents, **P**rocesses

Description of probable and less probable evolutions including what-if cases

Representation of scenario

Calculation of indicators and comparison with limits

Approach



Description of all relevant **F**eatures, **E**vents, **P**rocesses

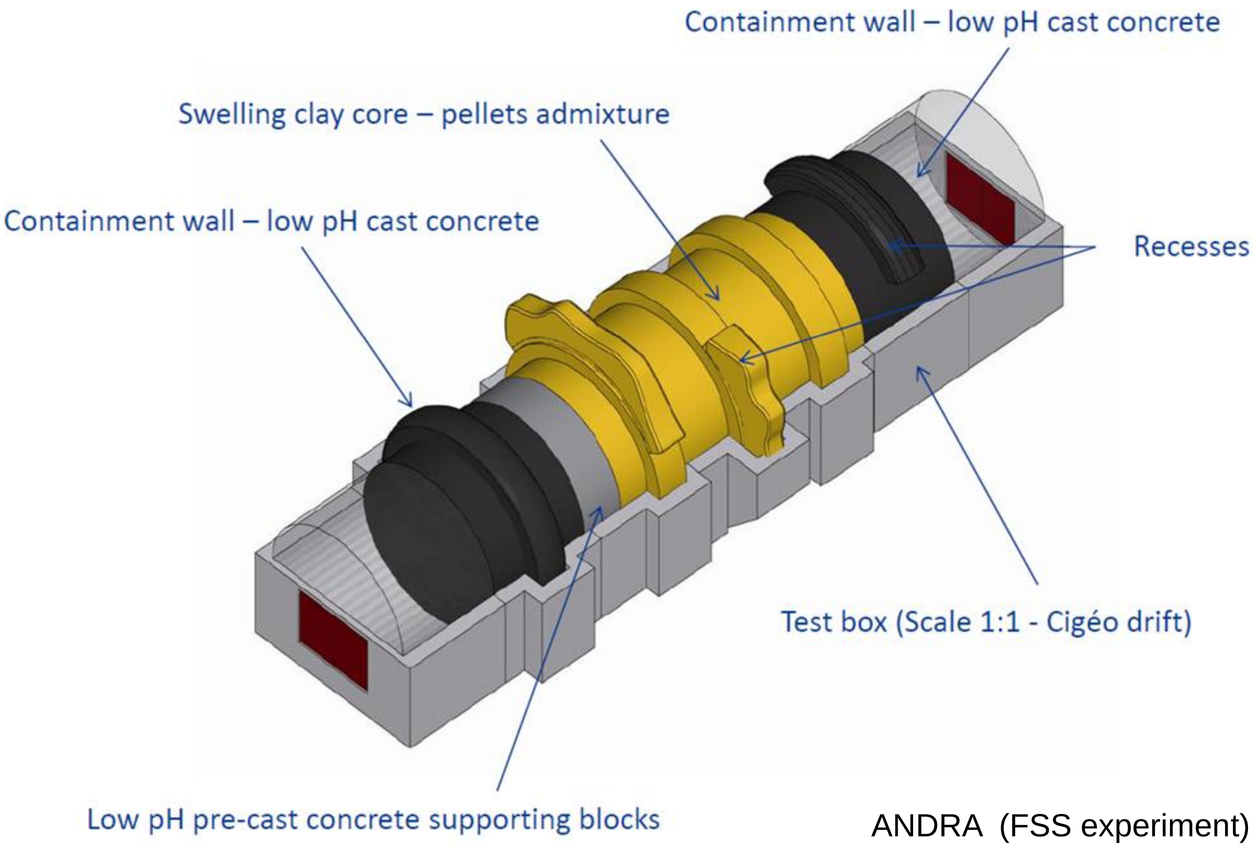
Description of probable and less probable evolutions including what-if cases

Representation of scenario

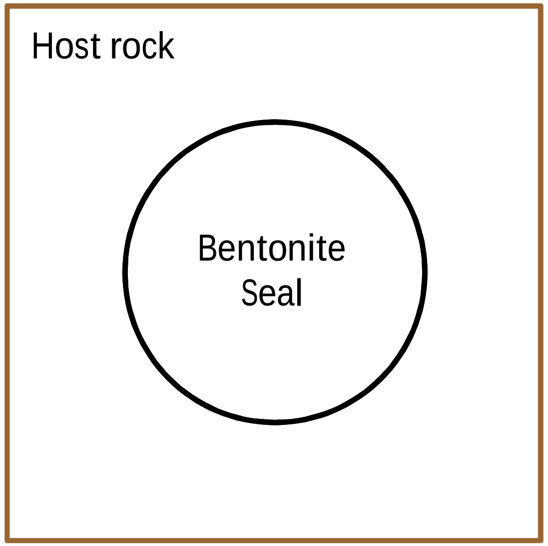
Calculation of indicators and comparison with limits

Process modelling of sealings

Coupling of processes – Example: Resaturation of a clay sealing



ANDRA (FSS experiment)



Coupling of processes – Example: Resaturation of a clay sealing

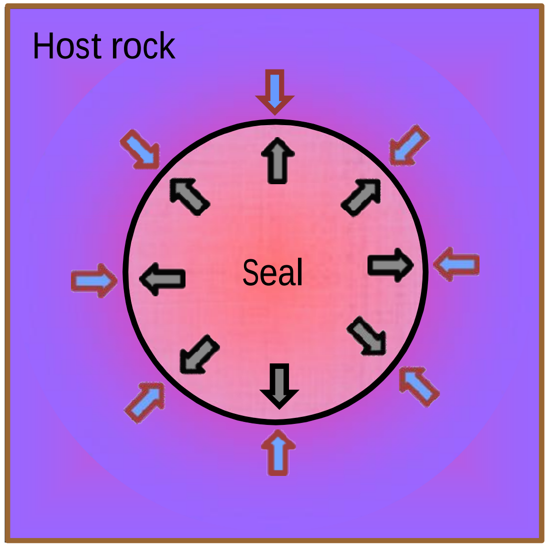
Thermal, **H**ydraulic, **M**echanical **C**hemical Processes

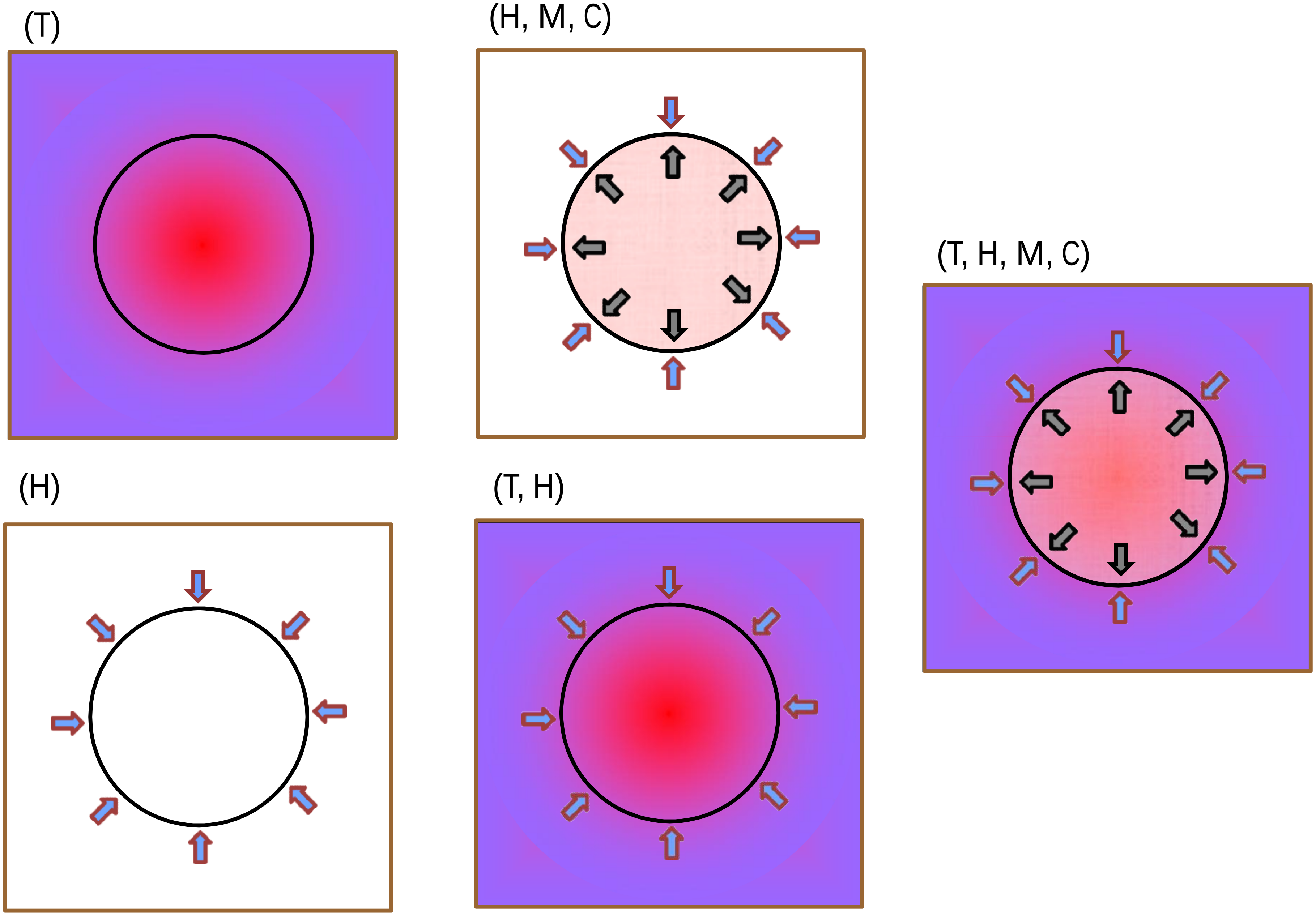
Inflow of water from host rock (H)
Change of thermal conductivity ð (T)

Rise of temperature (T)
Expansion of water ð (H)

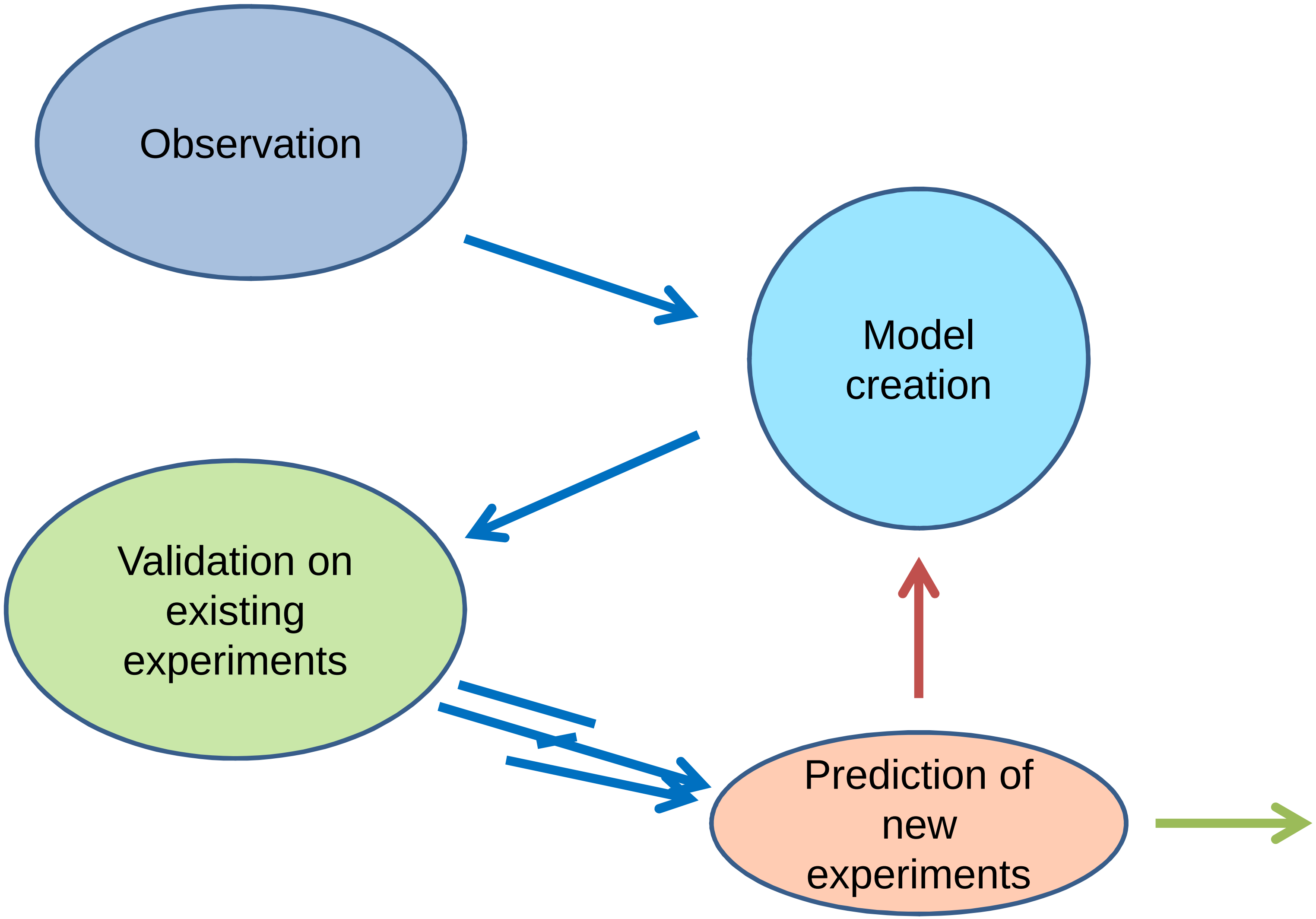
(H) ð Uptake of water by Bentonite which is not in chemical equilibrium (C)
Change of Bentonite composition
Change of Bentonite permeability ð (H)

(H, C) ð Swelling of Bentonite (M)
Increase of swelling pressure
Change of permeability of EDZ ð (M, H)




(T)
(H, M, C)
(T, H, M, C)
(H)
(T, H)

Validity of models



Process-level modelling codes used in DOPAS

- Commercial:
  - Particle Flow Code (PFC™) (M) http://www.itascacg.com/software/pfc
  - 3DEC™ (M) http://www.itascacg.com/software/3dec
  - ALGOR (M) http://www.algor.com
  - FEFLOW (H) http://www.mikepoweredbydhi.com/products/feflow
- Research (Free):
  - EQ3/6 (C) https://missions.llnl.gov/energy/technologies/geochemistry
  - PhreeqC (C) http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc
  - Code_Bright (T,H,M) https://www.etcg.upc.edu/recerca/webs/code_bright
  - OpenGeoSys (H) http://www.opengeosys.org
- Company owned:
  - CLOE (H,M)

Remark: Codes might have additional capabilities (THMC) that haven't been used in DOPAS

Processes modelled in DOPAS

- Hydraulic modelling
  - Temporal evolution of seal permeability
  - Flow rates of fluid through the seal with time
  - Temporal evolution of the pore saturation
  - Pore pressure of fluids in the seal
- Hydraulic / Mechanical modelling
  - Temporal evolution of the sealing porosity
  - Total pressure of the seal
- Mechanical modelling
  - Mechanical stress and load of the seal
- Chemical Modelling
  - Mineral phase changes in sealing material

Integrated performance assessment modelling of sealings

Integrated performance assessment modelling

- No total system performance assessment is performed in DOPAS

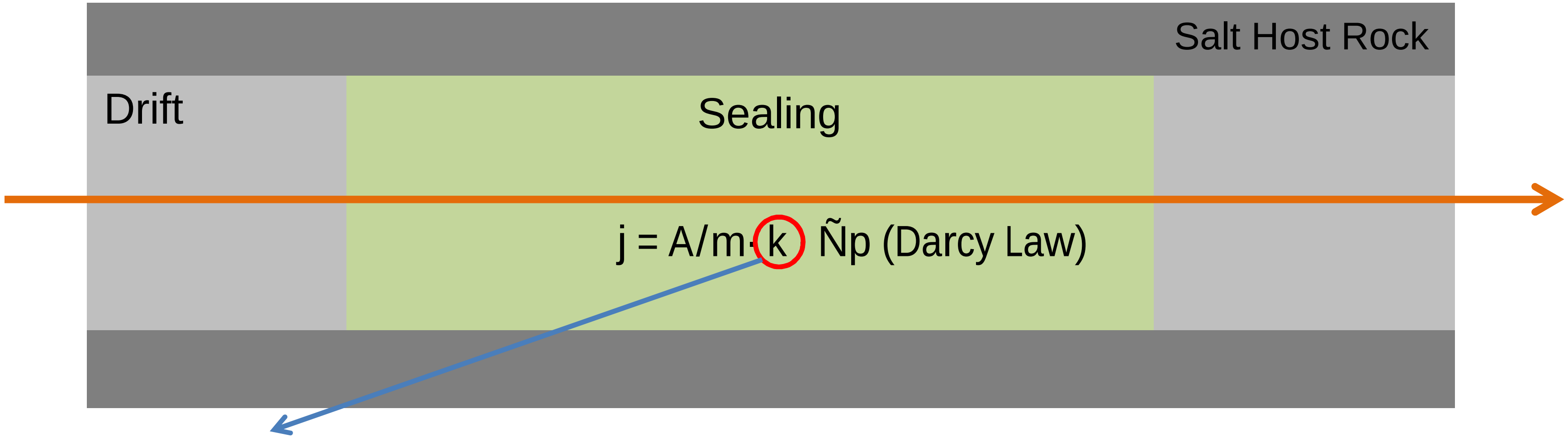
...but

- Development of integrated performance assessment models
  - Using experimental results
  - Using process modelling
- Modelling of sub system (sealing) using integrated assessment code

Aim:

- Better representation of sealing in integrated assessment code
- Reduction of uncertainty

Sealing in integrated PA: So far…

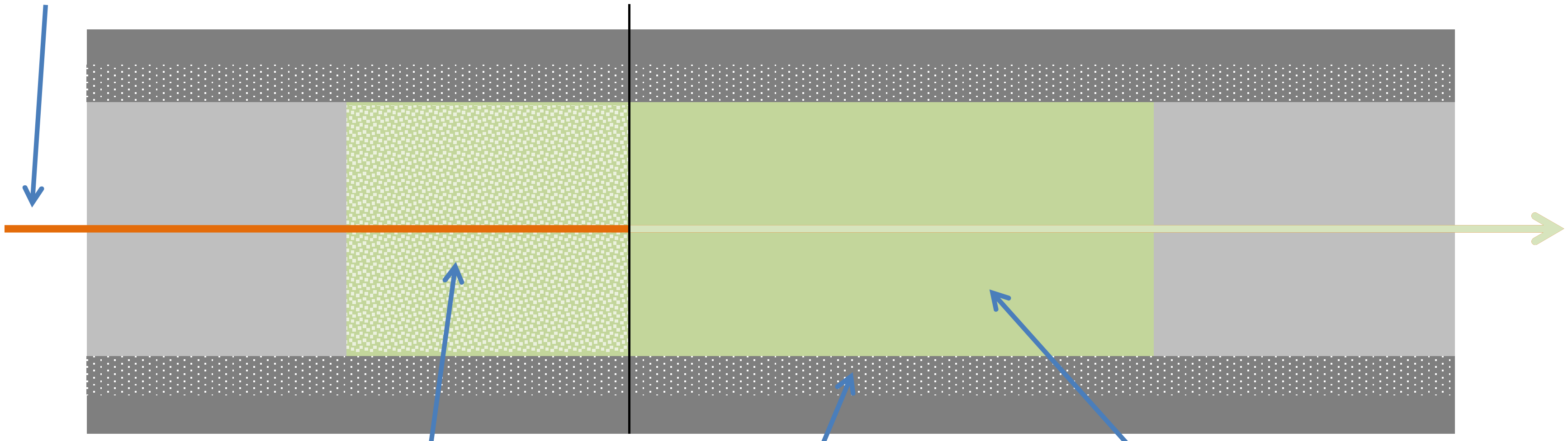


Permeability: k

- uniform average value across cross section of sealing
- stepwise constant in time
- conservative values are used to match assumptions

Sealing in integrated PA: Closer to reality?

Inflowing solution is not in chemical equilibrium with sealing material

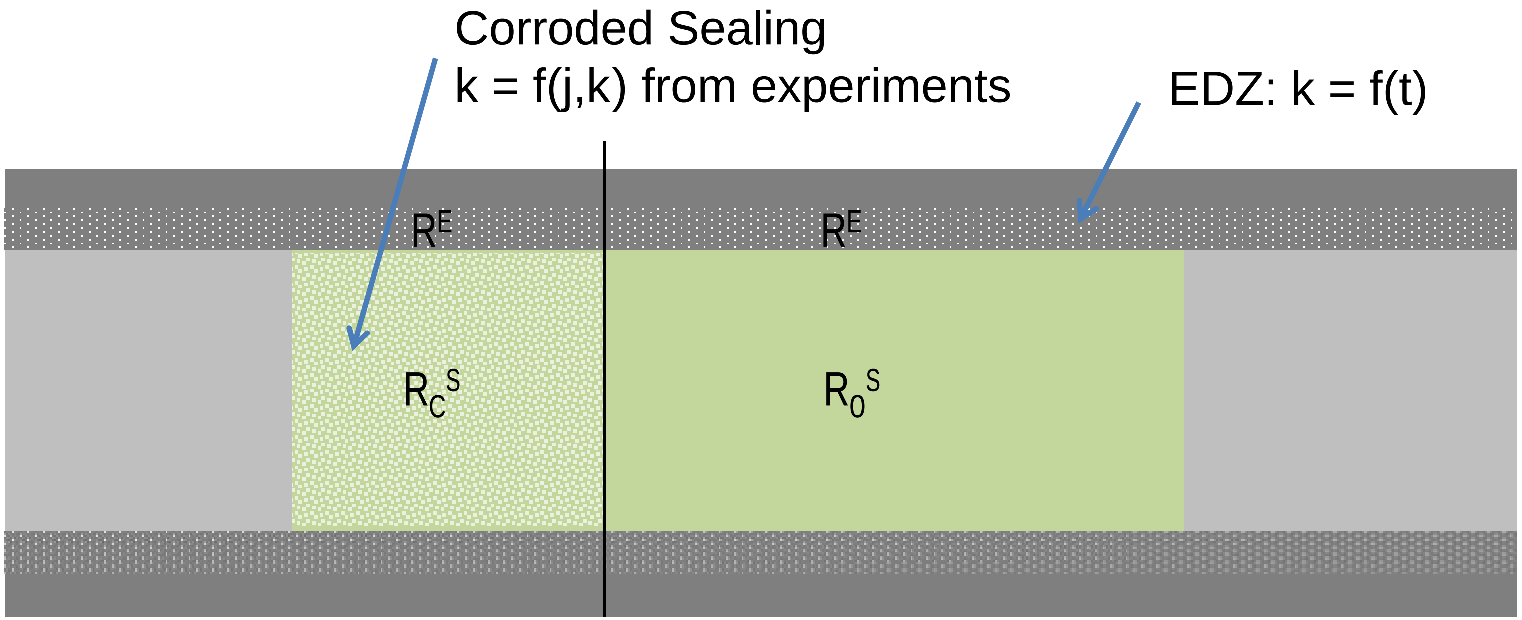


Sealing material is disturbed
→ permeability is increasing

Original sealing material

Excavation disturbed Zone (EDZ) around sealing with increased permeability

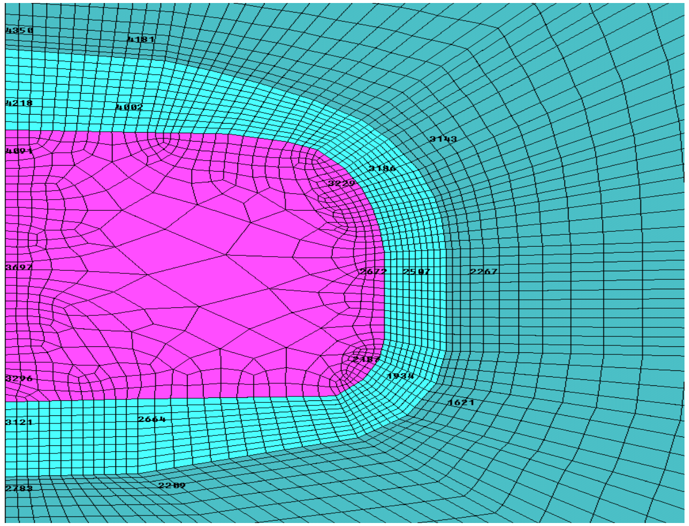
Sealing in integrated PA: New!

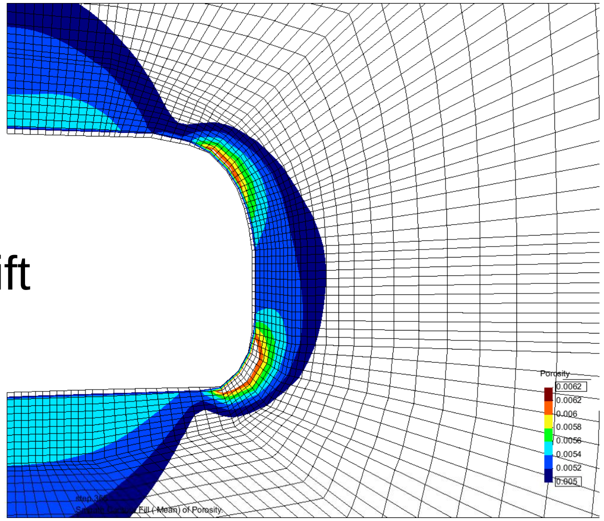


$$R = R_C + R_0 = \frac{R_C^E R_C^S}{R_C^E + R_C^S} + \frac{R_0^E R_0^S}{R_0^E + R_0^S} = \frac{R_C^E R_C^S \left(R_0^E + R_0^S\right) + R_0^E R_0^S \left(R_C^E + R_C^S\right)}{\left(R_C^E + R_C^S\right) \times \left(R_0^E + R_0^S\right)}$$

$$R_0^S = \frac{m_C L_0}{A^S k_0^S}, \quad R_0^E = \frac{m_C L_0}{A^E k_0^E}, \quad R_C^S = \frac{m_0 L_C}{A^S k_C^S}, \quad R_C^E = \frac{m_0 L_C}{A^E k_C^E}$$

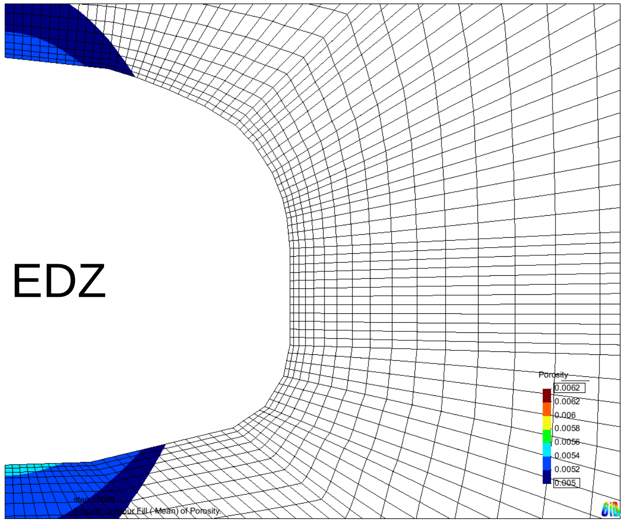
Process modelling (I): Mechanical modelling of EDZ (drift seal)



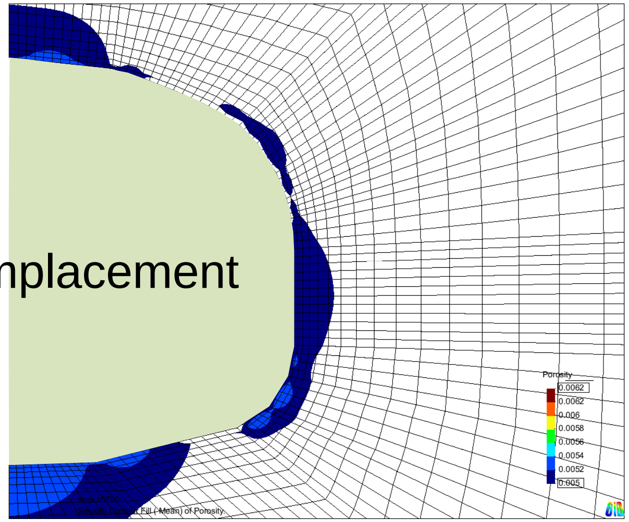


Open drift

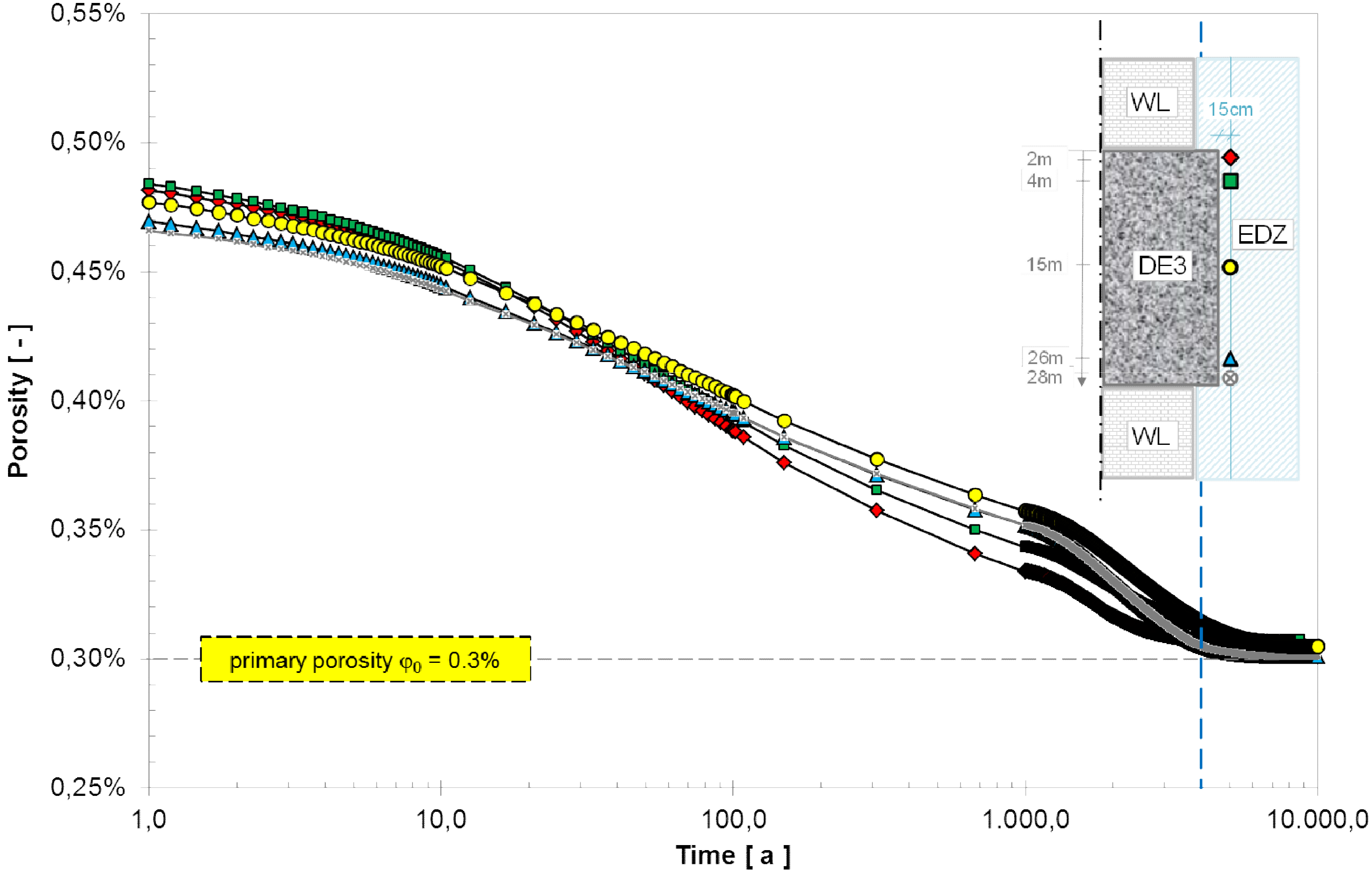
Cutting of EDZ



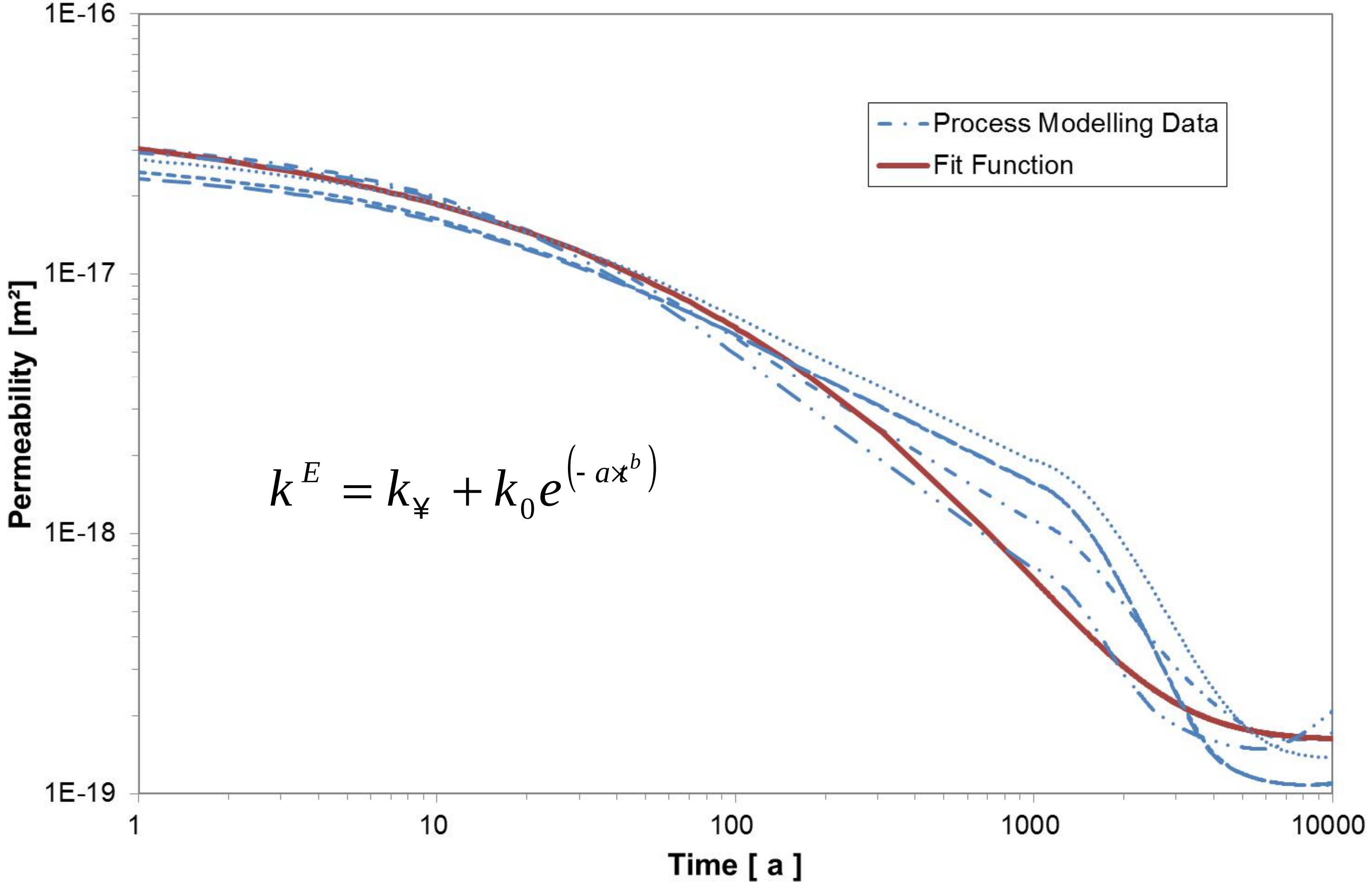
After seal emplacement



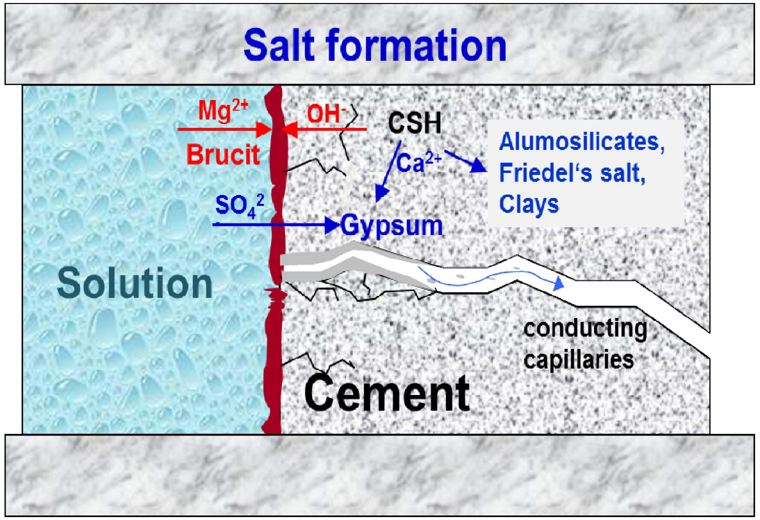
Process modelling (I): Mechanical modelling of EDZ (shaft seal)



EDZ behaviour used in integrated model

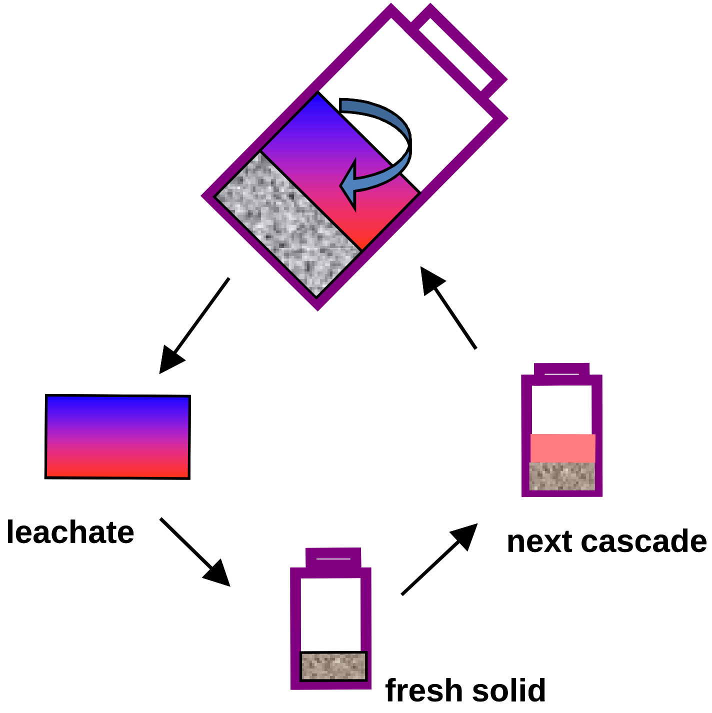


Process modelling (II): Geochemical modelling of material dissolution

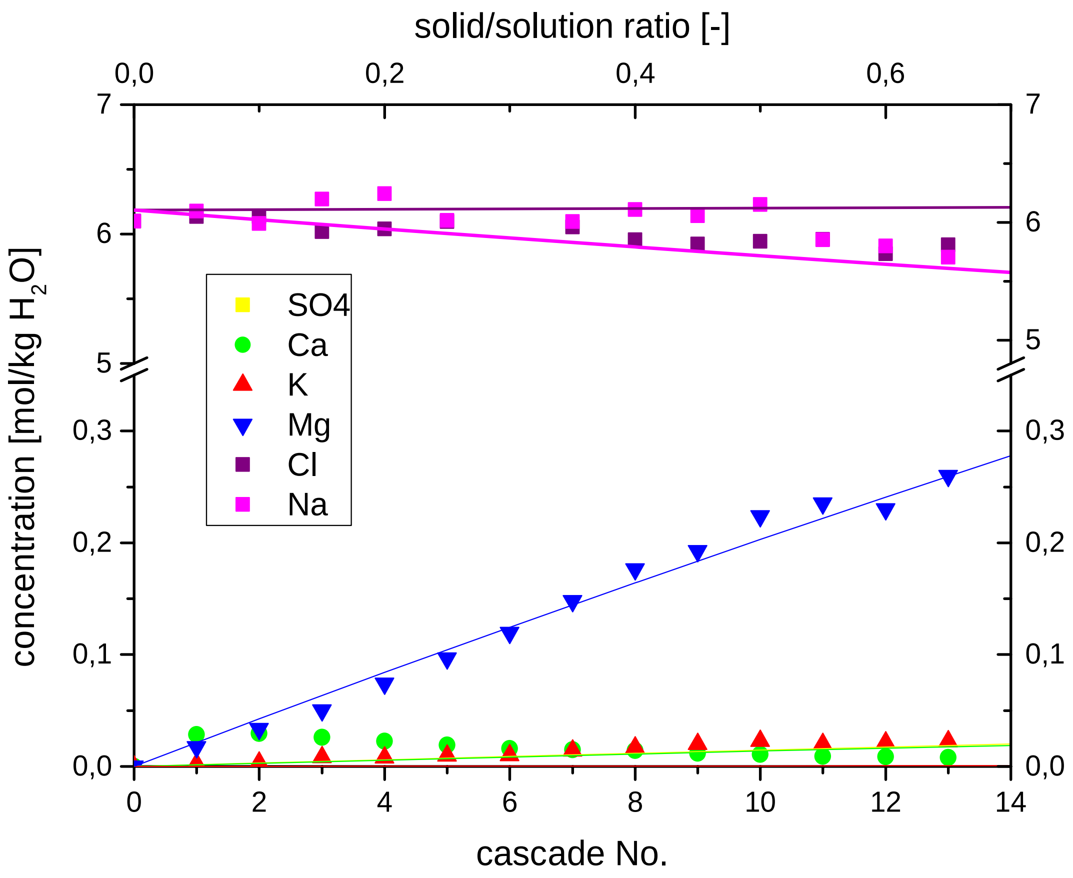


Process modelling (II): Geochemical modelling of material dissolution

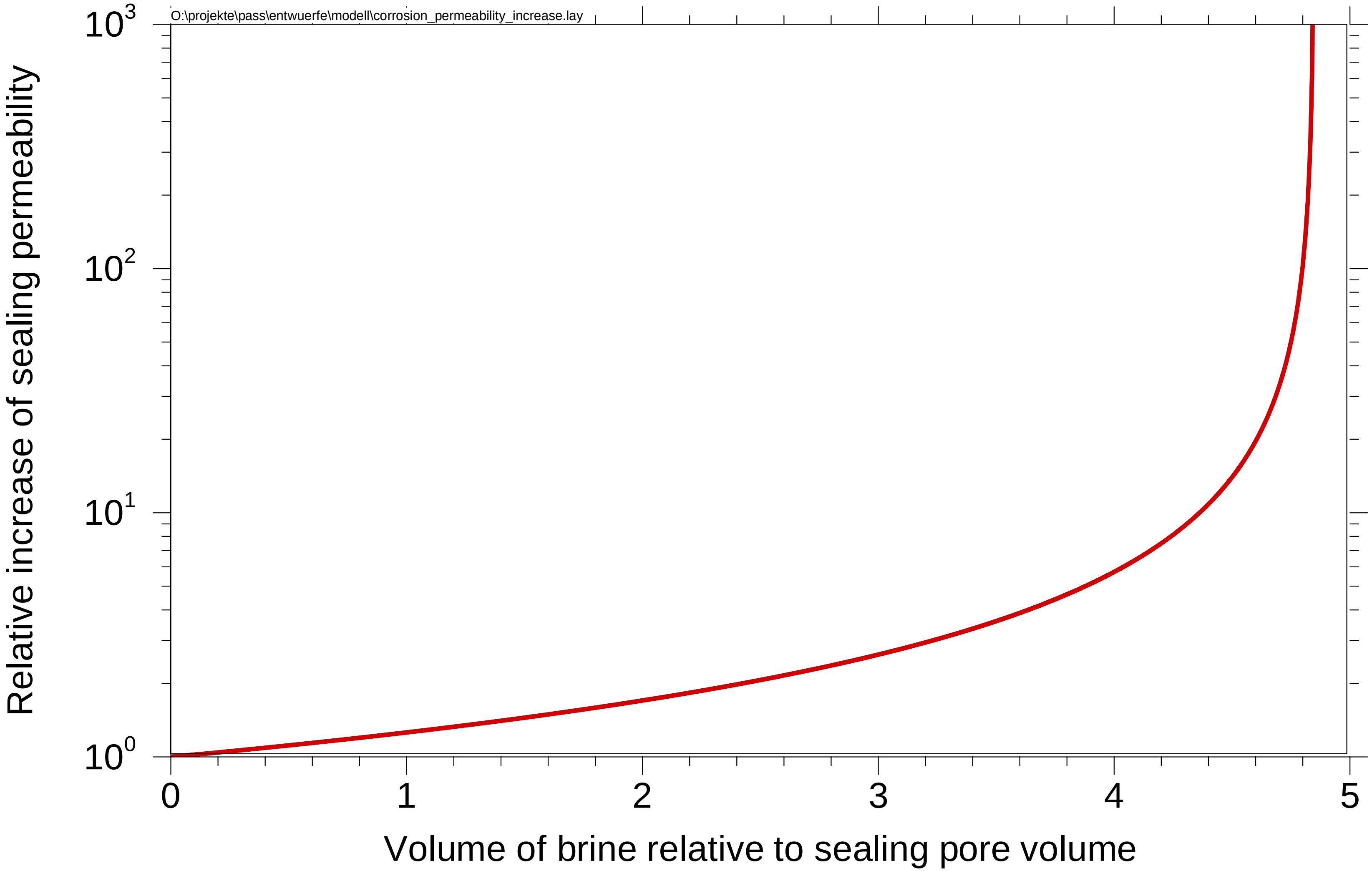
Experiment



Process modelling on experimental data



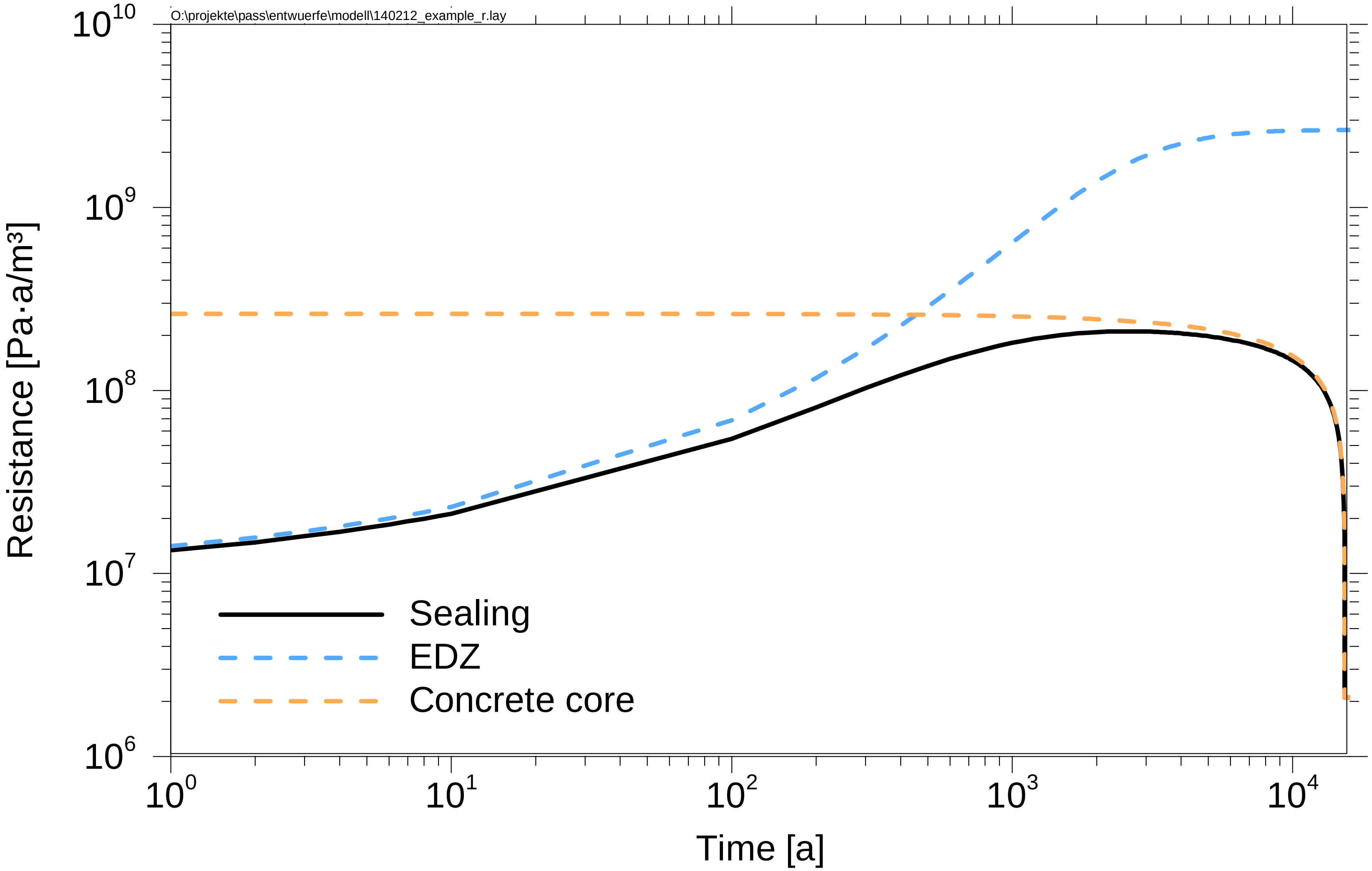
Material behaviour used in integrated model



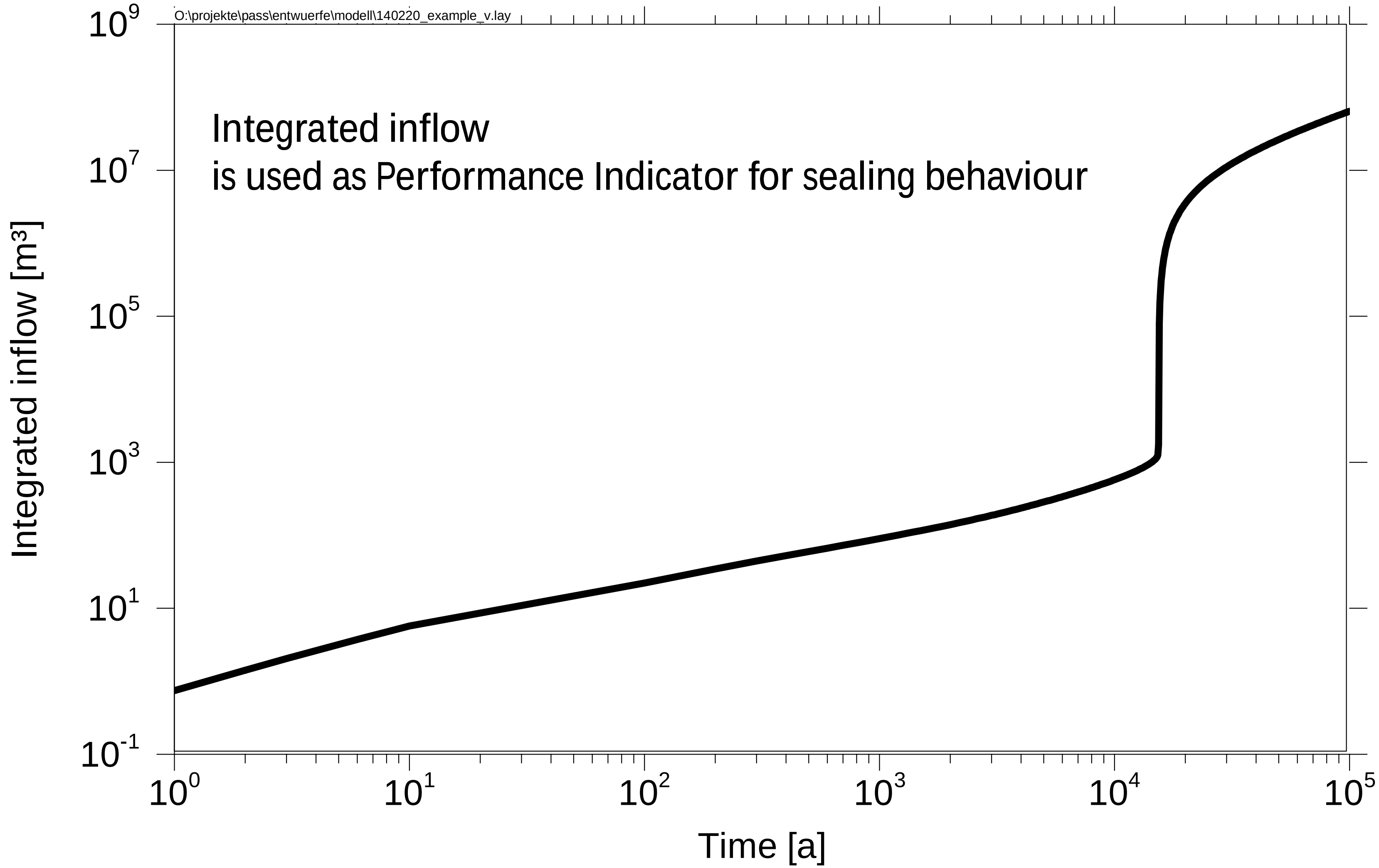
Integrated model: Illustrative example calculation

Parameter		Value
Length of the sealing	[m]	30
Diameter of the sealing	[m]	7
Hydraulic pressure at sealing	[MPa]	10
Viscosity of brine m	[Pa s]	$5.3 \cdot 10^{-3}$
Porosity of salt concrete material f	[-]	0.2
Initial permeability of salt concrete material	[m^2]	$5 \cdot 10^{-19}$
Permeability of corroded salt concrete material	[m^2]	$1 \cdot 10^{-14}$
Corrosion capacity of the brine $k_{L,V}$	[l/l]	1
Extension of the EDZ	[m]	1
EDZ initial permeability k_0	[m^2]	$4.5 \cdot 10^{-17}$
EDZ long-term permeability k_∞	[m^2]	$1.6 \cdot 10^{-19}$
EDZ fitting parameter a	[-]	0.4
EDZ fitting parameter b	[-]	0.35

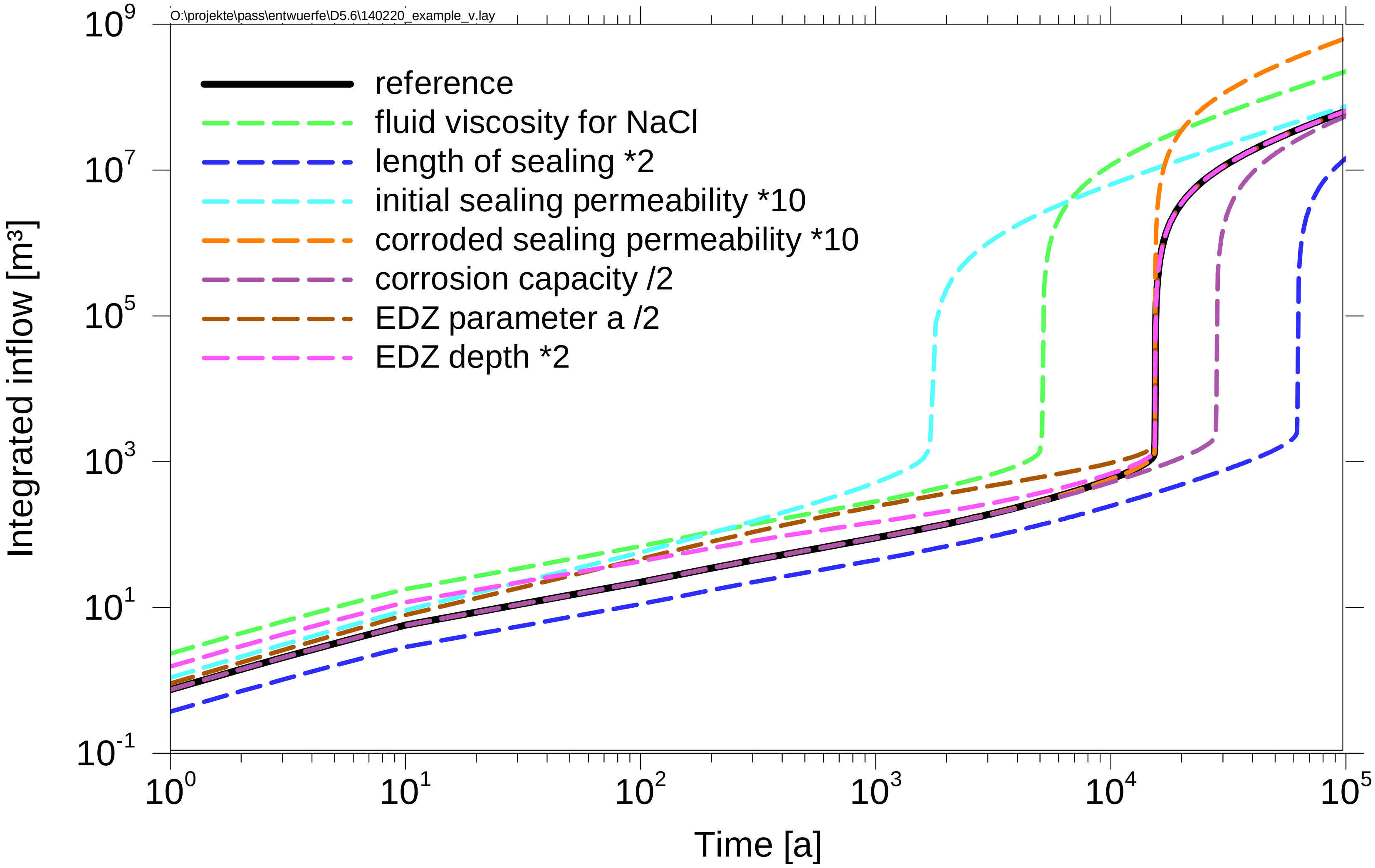
Integrated model: Hydraulic resistance of a sealing



Integrated model: Integrated inflow



Integrated model: Parameter variations



Managing Uncertainties

Type of uncertainties

§ Epistemic

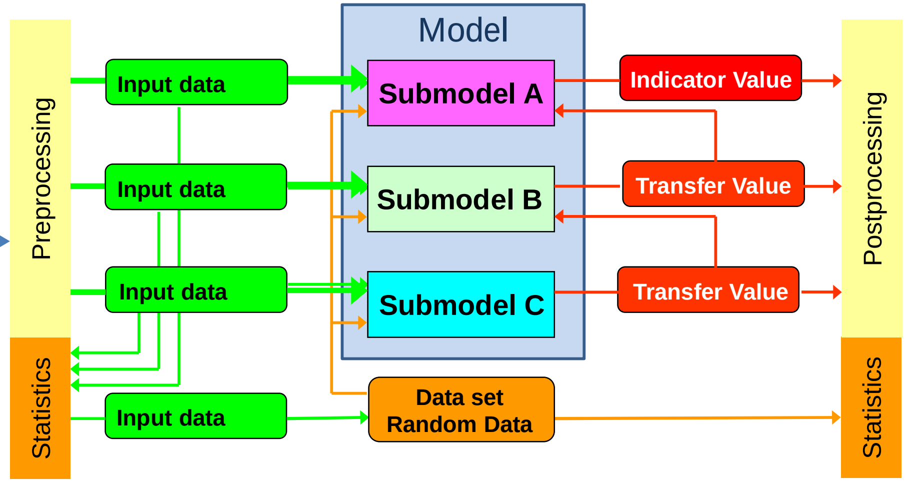
- Knowledge based
- Reducible
  - Parameter uncertainties
  - Model uncertainties

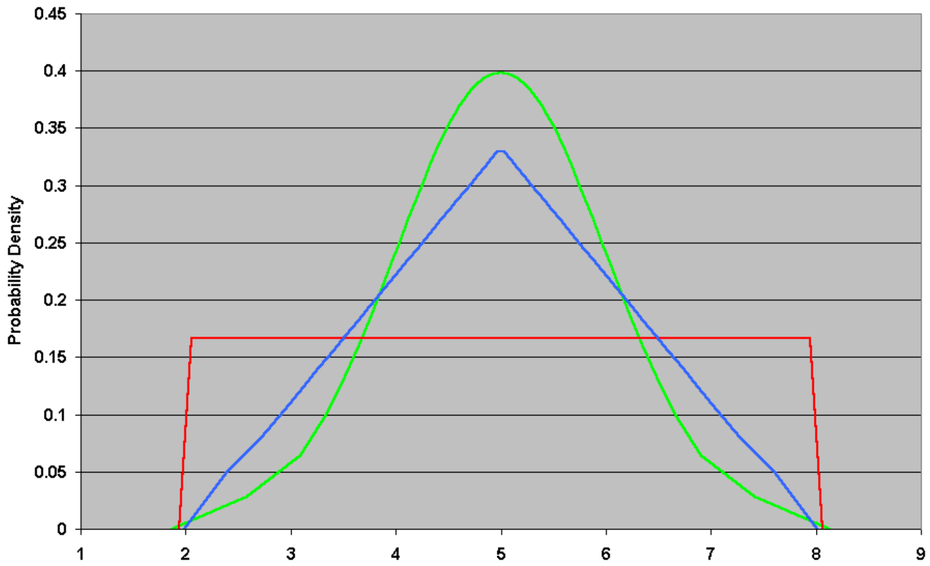
§ Aleatoric

- Random
- Irreducible
  - Scenario uncertainties

Managing Uncertainties

- § Mitigation
  - Reduce by better characterisation
- § Argument
  - Qualitative argument
  - Uncertainty not important
- § Assessment
  - Estimate/quantify uncertainty
  - Probabilistic Assessment
  - Monte Carlo Simulations
    - Large number of runs
    - Probabilistic varied parameters

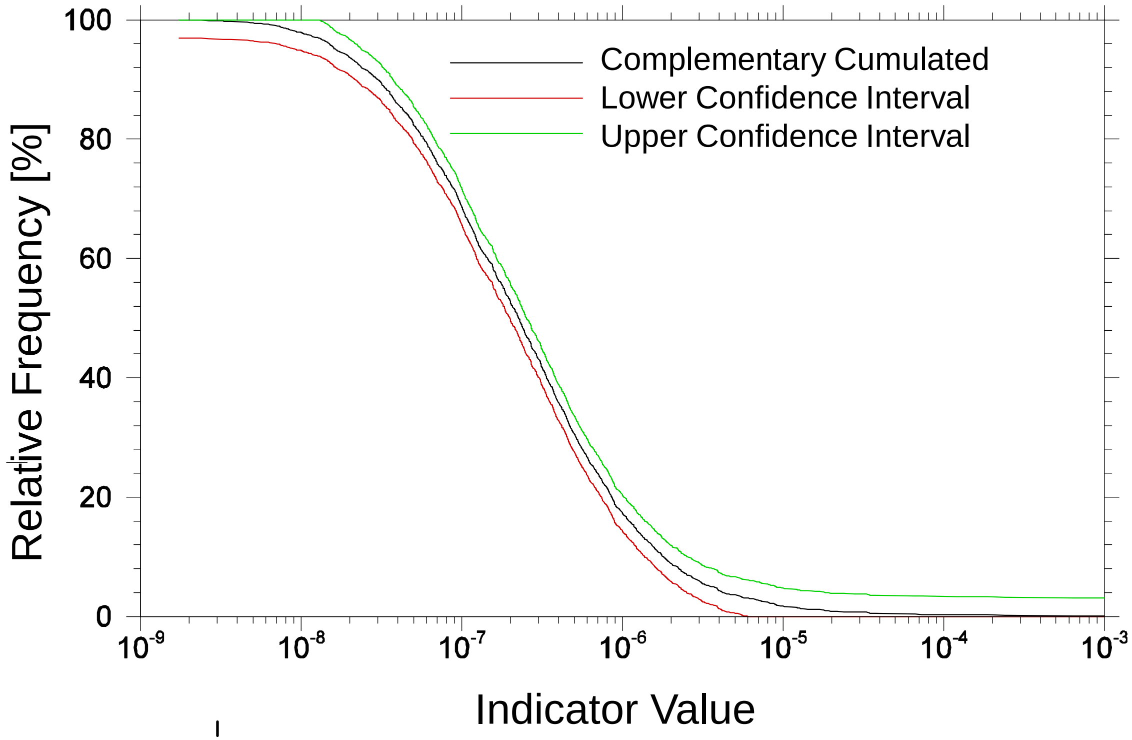


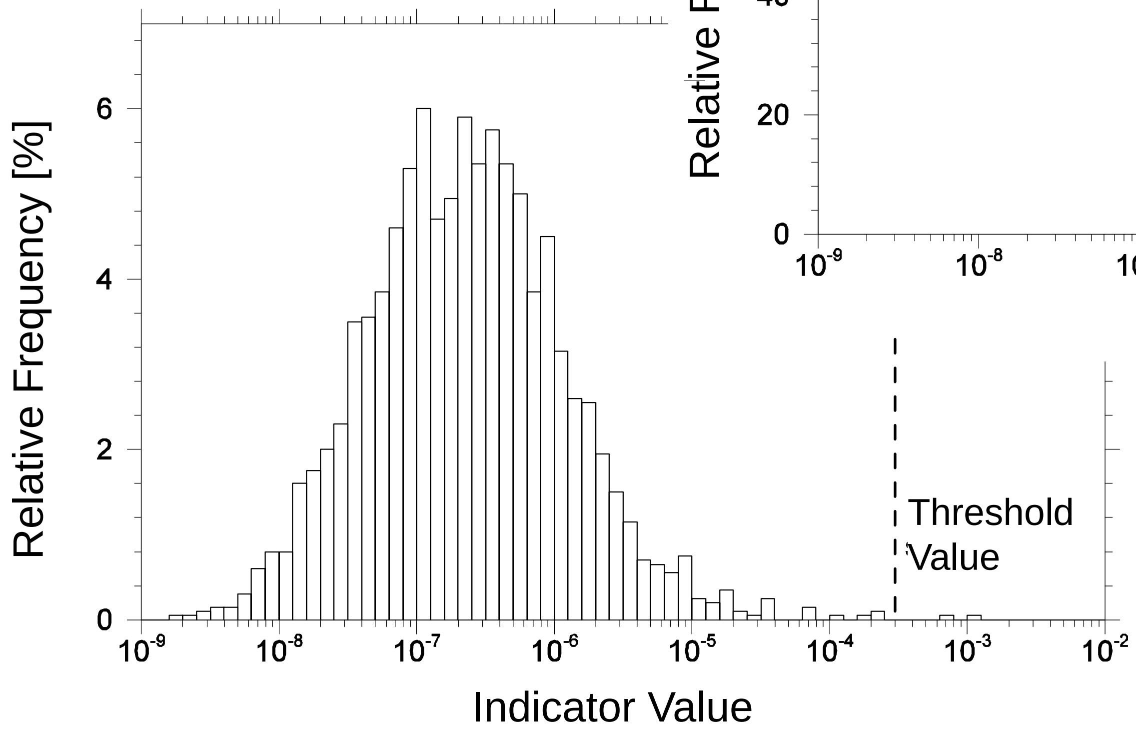


Probabilistic Monte-Carlo-Analysis of large number of simulations

Uncertainty analysis:

Statistical assessment of uncertainty and confidence interval of result





Figures show schematic examples not related to DOPAS

Probabilistic Monte-Carlo-Analysis of large number of simulations

Sensitivity analysis

- Identification of parameters which contribute most to uncertainty
- Arbitrary example not related to DOPAS:

	Parameter	Spearman Test	Rank Correlation	FAST	EFAST
1	Initial permeability	1	1	1	1
2	Mg-content of solution	2	2	2	2
3	...	3	3	3	3
4	...	4	4	4	4
5	...	6	6	6	6
6	...	5	5	5	11

§ Copyright notice

- This material can only be used for non-commercial use
- If no reference given, pictures in the presentation by GRS

§ References for further reading:

- For further reading look at the final reports of the Integrated Project PAMINA which was part of the 6th framework programme of the European Commission. The material van be found here: http://www.ip-pamina.eu
- An overview can be found in the

"*European Handbook of the state-of-the-art of safety assessments of geological repositories*"

which can be downloaded here:
http://www.ip-pamina.eu/downloads/pamina1.1.4.pdf

Acknowledgement

The research leading to these results has received funding

from the European Atomic Energy Community's (Euratom) Seventh Framework Programme FP7/2007-2013, under Grant Agreement No. 323273 for the DOPAS project

and under contract no. 02E11142 from the German Federal Ministry of Economic Affairs and Energy (BMWi).