Modelling Gas Migration in Compacted Bentonite: GAMBIT Club Phase 3 Final Report

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April 2004
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The conclusions and viewpoints presented in the report are those of author(s) and do not necessarily coincide with those of Posiva.
MODELLING GAS MIGRATION IN COMPACTED BENTONITE: GAMBIT CLUB PHASE 3 FINAL REPORT

This report describes the third phase of a programme of work to develop a computational model of gas migration through highly compacted water-saturated bentonite.

One difficulty with this endeavour is the definitive determination of the mechanism of the gas migration from the available experimental data. The report contains a brief review of the experimental data and their interpretation.

The model development work reported involves the investigation of two ways of enhancing a model proposed in the previous phase of the programme. This model was based on the concept that gas migration pathways were created by consolidating the clay fabric by application of gas pressure to create porosity through which the gas could flow.

The two developments of this model that are separately explored in this work are:

a) The incorporation of a proper treatment of the stress-strain behaviour of the clay in response to gas migration. The previous model had only considered stress effects through simple volume changes to the clay fabric.

b) The inclusion of a dual-porosity feature into the model in an attempt to address the role that the clay fabric might play in gas migration through the clay, in particular the role that pre-existing interstack voids might have in gas migration. The consideration of hysteresis effects was also included in this study.

As in previous GAMBIT Club work, the models are tested against the results of laboratory experiments.
KAASUNKULKEUTUMISEN MALLINTAMINEN KOMPAKTOIDUSSA BENTONITISSA: GAMBIT CLUB:n KOLMANNEN VAIHEEN LOPPURAPORTTI

Tässä raportissa kuvataan laskentamallia, jolla voidaan selvittää kaasun kulkeutumista suuren tiheyden omaavassa, veden kyllästämässä bentonitiissa.

Käytössä olleesta kokeellisesta aineistosta on ollut vaikeaa määrittää täsmällisesti kaasun kulkeutumisen mekanismia. Raportti sisältää lyhyen yhteenvedon kokeellisista tuloksista ja niiden tulkintoista.

Aikaisemmin esitetytä, vaiheen 2 mallia on parannettu kahdella vaihtoehtoisella tavalla. Vaiheen 2 mallissa oletettiin, että kaasunpaine puristaa kokon bentonittiittä avaten huokostilavuutta kaasun kulkeutumiselle.

Tässä työssä kehitetyt vaihtoehtoiset mallit olivat:

a) Kaasun kulkeutumisessa otettiin huomioon saven jännitys-muodonmuutos -ominaisuudet. Aikaisemmassa mallissa jännitystila oli yksinkertaisesti huomioitu saven rakenteen tilavuusmuutoksena.


Kuten aikaisemmissakin Gambit Club -selvityksissä malleja testattii laboratoriokokeiden tuloksilla.
EXECUTIVE SUMMARY

The GAMBIT Club was set up to support a programme of work on the development of a computational model of gas migration in highly compacted, water-saturated bentonite. The ultimate aim was the production of a model that (i) would adequately represent the principal features observed in experiments on gas migration through this bentonite, (ii) could be used to analyse and interpret experimental results, and (iii) would exist in a version suitable to assess the effects of bentonite barriers on the build-up of pressure and the escape of hydrogen gas from various disposal canister designs.

The work of Phase 3 of this programme is described in this report and builds on that carried out in two previous phases of the GAMBIT Club programme, in which a number of mechanisms and models of gas migration in compacted bentonite were considered.

The Phase 3 work reported consists of three main elements:

a) Review of the experimental data on gas migration through compacted bentonite;

b) An extension of a model developed during Phase 2 of the programme to include the effect of the full stress field on gas migration;

c) Investigation of the representation of clay fabric effects in the form of a distinction between inter- and intra-stack pore space in the clay and of a treatment of hysteresis effects.

The examination of the experimental data included consideration of whether the data was indicative of a particular mechanism for the gas flow. Three possible basic mechanisms have been proposed for gas invasion of water-saturated compacted bentonite:

a) Behaviour of the bentonite as a conventional porous medium, with the gas flow governed by conventional concepts of capillary pressure and relative permeability.

b) Microfissuring of the clay, in which small fissures are created or opened by the invading gas to provide the pathways for the gas to enter the clay.

c) Macroscopic fracturing of the clay to provide fracture pathways for gas flow.

It is possible that there is a spectrum of behaviour involving more than one of the above mechanisms simultaneously.

Examination of the experimental data has not produced a unique explanation of the experimental results in terms of these mechanisms, and areas of uncertainty are discussed in the report. These uncertainties constitute considerable difficulties in the development of models of gas migration in bentonite, because of the ambiguity that
results in the constitutive relationships needed for such models. However, it should be noted that the experimental data that has been collected does give a substantial degree of confidence that saturated compacted bentonite will function satisfactorily in relation to gas migration in as far as those aspects of its behaviour that are important for effective performance as a buffer material are concerned. In particular:

a) It has been shown that gas can pass through initially water-saturated bentonite buffers (although confirmation is needed that the pressure at which this occurs is acceptable).

b) Very little water is expelled from the buffer by migrating gas.

c) When resaturated, the buffer seems to reseal, with restoration of the hydraulic and transport properties that it possessed prior to the passage of gas.

In the Phase 2 GAMBIT Club work, a new “continuum model” of gas migration through bentonite was developed, called here the GAMBIT-GW model. The essence of this model is that gas cannot enter the clay until pathways have been created by a combination of squeezing water from and compressing water in the clay matrix. All the water resides in the clay matrix, which can change volume as indicated, in accordance with the swelling behaviour of the clay, thereby leaving voids that can be occupied by gas, but the gas cannot enter and displace water from the clay matrix itself. As well as gas migration, the model can also model water flow through the bentonite, some coupling between gas and water pressures, and resealing of gas pathways when the clay resaturates.

The GAMBIT-GW model contained only a highly simplified treatment of the mechanical response of the clay to the stresses induced by the applied gas pressure. It was considered desirable to investigate a more thorough treatment of the mechanical behaviour of the bentonite during gas migration. This was because of the possibility that gas migration might be sensitive to the stress state of the clay. For example, the stress field might influence the mode of gas migration and the direction that gas migration pathways might follow.

To extend the GAMBIT-GW model to include a proper treatment of the stress field in the bentonite, the original plan was to use a sophisticated pre-existing finite element modelling code, FEAT. This has a macro language facility, which allows the definition of specific elasto-plastic models and the coupling, in the case of porous materials, of the stress-strain behaviour with fluid flow through the medium. This had the potential to make use of constitutive models of deformation behaviour that had already been developed for bentonite. However, it was found that the FEAT model would not handle the propagation of gas through the bentonite. Analysis of the problem pointed to the fact that the quadratic finite elements used in FEAT, which are well suited to stress analysis, were not appropriate for simulating advance of the sharp front that was formed
at the leading edge of a gas pathway propagating through the bentonite. Essentially the
front developed oscillations which made the scheme unstable.

By consideration of an idealised version of the gas migration problem, an alternative
numerical scheme was developed based on linear elements and a particular integration
method which was guaranteed to be oscillation free in the idealised problem. This
numerical approach has been used in the ENTWIFE package to implement a gas
migration model that takes account of the stresses in the clay that develop as a
consequence of invasion by gas. The ENTWIFE code provides the facility for
automatically generating finite element computer code from a model specification in the
form of the model equations. This, in principle, allows different models to be easily
explored.

The model does not explicitly simulate fissure propagation, so for those experiments in
which this mechanism is indicated, the approach necessarily provides only a continuum
representation of the presence of fissures.

Other investigations of possible improvement to the GAMBIT-GW model, considered
separately from the refinement of the treatment of stresses discussed above, involved the
introduction of a dual porosity element into the model to provide a representation of the
possible influence of the clay fabric on gas migration. This was based on the distinction
that is sometimes drawn between interstack and intrastack porosity. Both are assumed to
be initially water filled. Gas invasion would occur through the larger interstack voids. In
the absence of experimental that could be used to characterise the mechanistic role that
clay fabric has in gas migration, modelling assumptions that were considered generally
plausible but had no other justification had to be made. The effect of adding additional
hysteresis to the model by providing for a time lag in the way that gas permeability
responded to changes that affected the permeability was also investigated.

In summary, the results of the attempts described here to extend the GAMBIT-GW
model introduced in Phase 2 of the GAMBIT Club project are as follows:

a) Careful analysis of the numerical requirements for modelling a sharp gas front
advancing through bentonite clay indicates that finite-element schemes based on
quadratic elements are not suitable and an alternative more robust numerical
approach has been devised.

b) Using this approach, a model of gas migration in which the full (elastic) stress-
strain behaviour of the clay is incorporated into the model, with gas entry being
determined by the relationship between gas pressure and the local effective
stress. This model has been implemented using the ENTWIFE program to
construct finite element computer code directly from the model equations, which
gives the flexibility, in principle, easily to explore different modelling options.

c) At present the constitutive relationships governing gas entry into saturated
bentonite and the relationships between gas pressure, water pressure, gas filled
porosity, and the stresses and strains in the clay are not established, but the creation of the ENTWIFE model provides a tool through which different possibilities can be explored in future work. This could be particularly valuable as more experimental data become available.

d) The model incorporating the full stress field has been used successfully to model a BGS experiment on gas migration through a highly compacted water-saturated bentonite sample constrained under isotropic stress. For this linear flow configuration, the new model gives agreement with experiment that is comparable with that obtained with the original GAMBIT-GO model. For this experiment, under isotropic stress conditions, it is perhaps to be expected that detailed representation of the full stress field in a model is not required to simulate the experimental results.

e) Difficulties have been experienced in applying the model to radially symmetric models of gas flow in cylindrical coordinates, both in the case of flow from a “central” source in a constant volume experiment, and the case of gas migration from a canister in a field-scale application.

f) Simulations of the radially symmetric models proceed successfully to model the evolution of the stresses within the bentonite as the applied gas pressure builds up to the point at which gas entry would occur. The stress distribution shows where gas entry would occur in the model.

g) However, the model fails at present in modelling the propagation of gas across the bentonite once it has started to enter the clay in the radially symmetric models. Despite the investment of considerable effort, it has not been possible to resolve the outstanding computational difficulties satisfactorily, and this has limited the investigation of the effects of varying the details of the conceptual model of gas migration in bentonite.

h) Incorporation of representations of the clay fabric into a derivative of the gambit-GW model by distinguishing between interstack and intrastack porosity did not provide any improvement in the ability to model experiments compared with the original GAMBIT-GW. The reason for this is that the connected interstack porosity added to the model dominates the gas migration behaviour, with the result that the model behaves more like a conventional two-phase porous medium flow model than one in which the porosity occupied by the gas is created by deformation and squeezing of water from the clay.

i) It is considered that further development of models of gas migration in bentonite is likely to depend on obtaining better characterisation of gas pathways in bentonite and of the couplings that exist in the clay between stress and strain, gas and water fluid pressures, and gas-filled porosity.
1 INTRODUCTION

This report describes work carried out by Serco Assurance as Phase 3 of the GAMBIT Club work programme on the modelling of gas migration in highly compacted, water-saturated bentonite. The work builds on that carried out in two previous phases of the GAMBIT Club programme [Nash et al., 1998; Swift et al., 2001].

The ultimate goal set out for the GAMBIT Club programme was the development of a computational model that (i) would adequately represent the principal features observed in experiments on gas migration through highly compacted bentonite, (ii) could be used to analyse and interpret experimental results, and (iii) would exist in a version suitable to assess the effects of bentonite barriers on the build-up of pressure and the escape of hydrogen gas from various disposal canister designs.

Phase 1 of the project [Nash et al., 1998] involved principally the development of a preliminary one-dimensional computational model of gas migration through compacted bentonite that was designed to test conceptual models of the process. The main features of this model were that:

a) Gas invasion was assumed to occur by the formation of microfissures that could propagate when the gas pressure reached a critical value. Creation of gas pathways by fracture propagation was described in the model.

b) Dilation of the gas pathways formed by fracture propagation was assumed to occur in response to changes in gas pressure, as such behaviour was implicated in the results of experiments on gas invasion of samples confined by a constant isotropic stress. The gas permeability was a function of the pathway dimensions.

c) The behaviour of the clay itself was represented simply by its mechanical and fracture resistance properties; neither water movement nor the swelling properties of the clay were modelled.

The mechanisms explored were suggested by the experimental data obtained by Horseman and Harrington [1997], and the results produced by the model were evaluated by comparison with the experimental "histories" obtained by these workers from controlled flow-rate gas injection experiments consisting of cycles of varying flow rates. The model was able to reproduce qualitatively the trends seen over the duration of the histories examined, and to reproduce quantitatively substantial parts of the histories. An inability to provide quantitative matches to complete histories, however, suggested that there were limitations to the model formulation (although there were also issues of experimental reproducibility, which might impinge on the degree of agreement that could reasonably be expected from comparisons between theory and experiment).
In the Phase 2 work [Swift et al., 2001], a number of refinements of the Phase 1 model were explored, including a model in which gas displaced water from pre-existing capillaries. More important from the point of view of the present Phase 3 work, was the development of a new “continuum model” of gas migration through bentonite, designated the “alternative” model at the time, but called here the GAMBIT-GW\(^1\) model. The motivations for the development of the alternative mode were twofold:

a) to represent some features of the experimental results that were not represented in the model developed in Phase 1;

b) to produce a model that was suitable for upscaling to 2-dimensional or 3-dimensional canister-sized models.

Features of the laboratory experiments that were not represented in the Phase 1 model investigation were:

a) flow of water through the bentonite;

b) coupling between the gas pressure and the water pressure as reported in some experiments [Horseman and Harrington, 1997; Harrington and Horseman, 2003];

c) resealing of the gas pathways after gas transport has finished and the clay is resaturated;

d) changes to the stress state of the clay, as for example produced by any dehydration of the clay that might occur.

Although the Phase 1 modelling served the purpose of exploring mechanisms of gas migration in bentonite, it was anticipated that there would be difficulties in applying it to field-scale circumstances. In particular, the explicit representation of the propagation of multiple fissures carrying gas would become very complex in systems of more than one dimension. It was considered that it might not in any case be important to represent the detail of this pathway propagation in field-scale applications. Results obtained with the Phase 1 model suggest that, if gas pathway propagation occurs via fissuring of the clay, then this step will be rapid once the gas pressure threshold required to initiate fissuring has been exceeded, and therefore that it may not be necessary to model the detail of pathway propagation for performance assessment, which is generally concerned with events occurring on much longer time scales. Similarly, if gas migration is assumed to occur by displacement of water from capillary-like pathways,

\(^1\) The nomenclature is meant to signify that the model includes water flow through the bentonite as well as the gas whereas earlier GAMBIT Club models only dealt explicitly with gas flow.
then upscaling of this to a two- or three-dimensional model may require that the explicit representation of the capillaries be replaced by an effective permeability type of model.

The GAMBIT-GW model described in Phase 2 provides a representation of the missing features listed above, together with the essential features included in the Phase 1 model (see above), albeit that the representation of the changes to the clay stress state is very simple and considers only isotropic stresses. The model also attempts to provide a physical basis for the fact that, once created, gas pathways remain open even when the gas pressure has fallen substantially below the initial threshold for gas entry. The model should in principle be readily upscalable.

Using the models developed during the first two phases of the GAMBIT Club programme, it has proved possible to provide a reasonable representation of the main features seen in results from a series of laboratory experiments on gas invasion of compacted bentonite [Horseman and Harrington, 1997; Harrington and Horseman, 2003]. It is evident, however, that none of the conceptual models that have been explored so far provide a thoroughly quantitative description of the detailed experimental data. This indicates that there may be some deficiency in the modelling approaches, but it is not clear to what extent this is due to the deliberate approximations that have been made, or whether there is a significant fundamental feature of the behaviour of the clay that is missing from the models. The shortage of data covering a range of different conditions makes this assessment difficult, especially when results from different sources appear not to be consistent, and there is significant variability amongst data from a single source. The data available from various experimental programmes and their interpretation are summarised in Section 2.

The Phase 3 GAMBIT Club work described here was designed to explore some specific ways in which the models can be improved to better describe the experimental results. In view of the eventual need to upscale the modelling approaches to provide a computational tool that could be applied at the scale of deposition holes (or similar disposal configurations) it was planned to base these further developments on the GAMBIT-GW model developed during Phase 2.

One feature of the conceptual models that have been examined in Phases 1 and 2 of the GAMBIT Club programme is that only simplified treatments of the mechanical response of the clay to the stresses induced by the applied gas pressure (or other causes) have been investigated. The treatments included elastic dilation of a crack in the crack propagation model, the response of pathway dimensions to changes of gas pressure post breakthrough in the models with explicit representation of pathways, and the volumetric swelling behaviour of the clay in the macroscopic GAMBIT-GW model. A time dependence in the response to pressure changes investigated in the Phase 1 work, may perhaps be interpreted as a representation of creep in the clay. No attempt had been made to implement a detailed constitutive model of the mechanical behaviour of the clay, as this would have added substantial complexity to the model investigations, and it was considered that the simplified representations of mechanical responses that were
used were appropriate for the purpose of preliminary investigations of different conceptual models of gas migration.

However, GAMBIT Club members considered that it was now desirable to investigate a more thorough treatment of the mechanical behaviour of the bentonite during gas migration. This was because:

a) The conceptual understanding of gas migration in clay (for example involving some dilation of the clay) suggests that a sensitivity to the stress state of the clay might be expected (e.g. Horseman and Harrington [1993], Harrington and Horseman [2003], Rodwell et al. [1999]).

b) The international consensus expressed at the recent international workshop on gas generation and migration [NEA, 2001] was that gas migration in bentonite would be sensitive to the stress state of the material.

c) In upscaling a model of gas migration in bentonite to the scale of deposition holes it becomes important to consider the factors which might control the direction that is likely to be followed by gas migration pathways. The stress field is considered likely to be a factor having a strong influence on this direction as dilatation of the clay is expected to occur more easily normal to the lowest stress. Satisfactory treatment of the stress field may therefore become an important issue in upscaling, for reasons that make it less so in modelling laboratory experiments in which the gas flow direction is prescribed by the experimental geometry.

d) A more thorough treatment of the mechanical behaviour of the bentonite may facilitate possible future extension of the model to gas migration in argillaceous host rocks in which there may be a pre-existing anisotropic stress field.

The original intention had been to incorporate the GAMBIT-GW Phase 2 gas migration model into a pre-existing sophisticated finite-element stress analysis programme, the FEAT programme (Finite Element Analysis Toolbox). In the event, this approach turned out to be unsuccessful, for reasons explained in the Appendix, and an alternative approach utilising Serco Assurance’s ENTWIFE programme was adopted. This is described in Section 3.

Part of the planned Phase 3 work was to demonstrate that the Phase 2 GAMBIT-GW model, extended to include the proper treatment of stress behaviour indicated above, could be applied to field-scale situations. To this end, the model was to be applied to a model of gas migration through the bentonite buffer surrounding a canister in a deposition hole. The limited progress made on this work is described in Section 4.

Two other enhancements of the Phase 2 GAMBIT-GW model were to be investigated as part of the Phase 3 programme, separately, in this phase of the work, from the implementation of a full stress model discussed above. These were:
a) the introduction of a dual porosity model to provide a more realistic representation of the clay fabric; and

b) the implementation of a time dependence in the response of gas pathway dilation to changes in gas pressure.

The investigation of the potential of a dual porosity feature was motivated, in part, by the emphasis by a number of workers of the importance of the clay fabric and pre-existing pathways in the clay on gas migration behaviour. In particular, it was thought that it could be useful to introduce a distinction between interlayer (intrastack) water and interstack water. The main contribution to the permeability would come from the part of the clay structure containing interstack water, but the interlayer water would control the swelling behaviour. Gas would only flow through the interstack spaces. The water in the interstack spaces might have an actual pressure essentially the same as that of the external equilibrium water pressure, whereas that of the interstack water would be treated in the same way as in the existing model. In order to reflect the impermeability of the clay to gas until a threshold pressure was reached, it would have to be assumed that the interstack spaces were not connected until the gas pressure reached the threshold value (typically the swelling pressure). The opening of these pathways to gas would have to be a feature of a revised gas permeability model. The plan was to investigate these ideas more deeply to determine whether they would significantly improve the existing model.

The second enhancement to be investigated, the introduction of an explicit time delay between changes in gas pressure and changes in gas permeability (point (b) above) was intended to provide a representation of the hysteresis effects seen in the experiments. Such a feature had been incorporated into the Phase 1 modelling. The physical justification of such a feature is not clear at present; presumably it would be a consequence of some sort of creep in the mechanical behaviour of the clay.

The investigation of these two enhancements to the GAMBIT-GW model is described in Section 5.

The report concludes in Section 6 with a discussion of the results obtained.
2 INTERPRETATION OF GAS MIGRATION MECHANISMS FROM EXPERIMENTAL DATA

At various points during the course of the GAMBIT Club project, the experimental data available on gas migration through saturated bentonite has been reviewed. Attention has been focused particularly on the information that can be gleaned from the data about the mechanism of this gas migration. New data has been obtained during the course of the project by BGS and others. This section provides a summary of what it is considered can be inferred about gas migration mechanisms from the experimental data, noting where there are uncertainties and inconsistencies in the experimental data.

Three possible basic mechanisms have been proposed for gas invasion of water-saturated compacted bentonite:

a) Behaviour of the bentonite as a conventional porous medium, with the gas flow governed by conventional concepts of capillary pressure and relative permeability.

b) Microfissuring of the clay, in which small fissures are created or opened by the invading gas to provide the pathways for the gas to enter the clay.

c) Macroscopic fracturing of the clay to provide fracture pathways for gas flow. This differs from (b) by the scale of the fracturing; it is assumed that in the laboratory macroscopic fracturing would involve fracture lengths comparable to the sample size (e.g. typically cutting right across the sample), whereas microscopic fissuring would involve fissures that have lengths small compared to the sample size (and that the sample remains intact when removed from the experiment).

It may be that different mechanisms occur under different conditions, or that there is a spectrum of behaviour involving more than one of the above mechanisms simultaneously.

Subsection 2.1, following, outlines the experimental data that has been assembled by groups around the world on gas migration in bentonite. Some of this data was discussed in more detail in the report of the GAMBIT Club Phase 2 work [Swift et al., 2001]. The overall interpretation of this data in terms of the gas migration mechanisms that might operate is addressed in subsection 2.2.

2.1 Experimental Data on Gas migration in Bentonite

The main published sources of experimental data on gas invasion of compacted bentonite are listed in Table 2.1.
Table 2.1  Summary of Experiments on Gas Migration in Compacted Bentonite

<table>
<thead>
<tr>
<th>Authors</th>
<th>Bentonite</th>
<th>Dry Density (Mg m(^{-3}))</th>
<th>Flow geometry</th>
<th>Gas Flow Controls</th>
<th>Confining Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pusch and Forsberg [1983] (\dagger)</td>
<td>Mx80</td>
<td>(\sim 1.35 - 1.65^*)</td>
<td>Linear</td>
<td>Constant pressure / pressure increments</td>
<td>Constant volume oedometer</td>
</tr>
<tr>
<td>Pusch et al. [1985]</td>
<td>Mx80</td>
<td>(\sim 1.1 - 1.78^*)</td>
<td>Linear</td>
<td>Pressure increments</td>
<td>Constant volume oedometer</td>
</tr>
<tr>
<td>Horseman and Harrington [1997]</td>
<td>Mx80</td>
<td>1.5 - 1.7</td>
<td>Linear (axial) flow</td>
<td>Displacement of gas by water from an upstream reservoir.</td>
<td>Constant isotropic stress in flexible sleeve subject to external fluid pressure (8 - 22 MPa)</td>
</tr>
<tr>
<td>Horseman and Harrington [1997]</td>
<td>Mx80 paste</td>
<td>1.3 - 1.4</td>
<td>Point source and sink</td>
<td>Displacement of gas by water from reservoir.</td>
<td>Cylindrical pressure vessel with confining pressure (0.8 - 2.7 MPa) imposed on floating end cap</td>
</tr>
<tr>
<td>Tanai et al. [1997]</td>
<td>Kunigel VI, Fo-Co Clay</td>
<td>1.4 - 1.8</td>
<td>Linear</td>
<td>Pressure increments</td>
<td>Constant volume cylinder</td>
</tr>
<tr>
<td>Gallé [1998; 2000]</td>
<td>Fo-Co Clay</td>
<td>1.6 - 1.9</td>
<td>Linear</td>
<td>Pressure increments</td>
<td>Constant volume oedometer cell</td>
</tr>
<tr>
<td>Graham et al. [2002]; Hume [1999]</td>
<td>Avonlea</td>
<td>0.6 - 1.4</td>
<td>Linear</td>
<td>Pressure increments</td>
<td>Constant volume oedometer cell</td>
</tr>
<tr>
<td>Harrington and Horseman [2003]</td>
<td>Mx80</td>
<td>1.577, 1.582</td>
<td>Approximately radial from central source</td>
<td>Displacement of gas by water from an upstream reservoir.</td>
<td>Constant volume cylindrical vessel.</td>
</tr>
<tr>
<td>Harrington and Horseman [2003]</td>
<td>Mx80</td>
<td>1.596</td>
<td>Linear</td>
<td>Displacement of gas by water from an upstream reservoir.</td>
<td>Cylindrical pressure vessel with confining pressure (10 MPa) applied to floating end cap</td>
</tr>
<tr>
<td>Tanai [unpublished 2002]</td>
<td>Mx80</td>
<td>1.63</td>
<td>Linear</td>
<td>Constant gas pumping rate</td>
<td>Constant isotropic stress in flexible sleeve subject to external fluid pressure (? MPa)</td>
</tr>
</tbody>
</table>

\(\dagger\) Gas flow in these experiments may have occurred via diffusion of dissolved gas

* Estimated from saturated bulk density
There is also data, which is outside the scope of the present work, on bentonite-sand mixtures, and on other clays. The experiments have shown, in varying degrees, the following features:

a) A threshold pressure for gas entry. This has been related by some to the bentonite swelling pressure.

b) Apparently, the displacement of only small volumes of water.

c) Once gas flow is established, it continues to flow at pressures below the threshold pressure at which gas flow was initially established, but there is a “shut-in” gas pressure, below the threshold pressure but above the applied back pressure, at which gas ceases to flow.

d) Changes in pore-water pressure in response to the applied gas pressure.

e) Evidence of macroscopic fracturing events with radial flow from a central source.

The existence of a threshold pressure for gas entry seems first to have been reported by Pusch and coworkers [Pusch et al., 1985], but has subsequently been observed by most other workers. The most notable exception is found in the work of Graham et al. [2002] and Hume [1999], who claim that, if enough time is allowed, gas will flow at pressures only slightly above the backpressure.

Pusch et al. [1985] correlated the gas entry pressure with the bentonite swelling pressure for compacted clays, although the correlation was not clear cut, with the entry pressure ranging from 0.2-0.9 times the swelling pressure (which in some cases was estimated). In isotropically constrained experiments, Horsemann and Harrington [1997], found a much closer correlation between gas entry pressure and swelling pressure, or rather between gas entry pressure and total stress (assumed equal to swelling pressure plus the external equilibrium pore-water pressure) in their experiments with samples under constant isotropic stress. When the gas exceeds the total stress it could squeeze the clay, both compressing the clay components and forcing water from the clay. This could generate new pathways for gas invasion, either through the clay or between the clay and wall of its container. In these constant stress gas experiments, any rise of the gas pressure above the constant confining pressure could also expand or rupture the flexible confining sheath, and it was necessary to rule out this possibility of the gas bypassing the clay. The demonstration, after a gas migration experiment in a specimen held under constant isotropic stress, of the presence of gas within the clay suggested that gas flow through the clay had occurred.

Pusch and coworkers [Pusch et al., 1987; Pusch and Hökmark, 1990] explained the gas entry pressure as the capillary entry pressure for pre-existing pathways through the clay. Microstructural analysis showed the presence of a small porosity of voids within the
clay, although it is not clear that the connectivity of these voids was established (simple percolation theory arguments might suggest that they would not be connected unless there was some mechanism operating during their formation that required that they be connected). A more extensive theory has been developed of the structure of compacted smectite clays, embodying the presence of connected channels as the primary determinant of the flow properties of the clay [Pusch et al., 1990].

Horseman and Harrington [1997] suggest that gas migration in highly compacted bentonite requires fissuring of the clay; that is, there are no pre-existing connected pathways that will provide a route for gas flow.

Experiments in a $K_0$ geometry$^2$ under a confining axial stress of 10 MPa similarly showed [Harrington and Horseman, 2003]$^3$ a well-defined threshold pressure for gas breakthrough; this pressure was equal to the axial stress. This breakthrough pressure was of a similar size to the sum of the estimated swelling pressure and backpressure. No gas flow occurred with the gas pressure maintained constant at 8.8 MPa for a long period.

The experiments by Gallé [1998, 2000] and Tanai et al. [1997] also exhibited threshold pressures for gas flow that were comparable to the swelling pressures. In these experiments, the samples were confined in constant volume vessels. In more recent experiments Tanai [unpublished, 2001] has obtained results under constant isotropic stress conditions in which the differential threshold pressure for gas flow was above the swelling pressure.

Experiments carried out by Harrington and Horseman in a cylindrical constant volume cell, in which gas was introduced from a central filter and collected from an array of sink filters located around the external radius of the cylinder, led to much larger gas entry pressures. In the first test of this type [Harrington and Horseman, 2003], the swelling pressure plus back pressure was estimated to be about 10 MPa (results from a later experiment, discussed below, suggest that it might have been less than this), but the peak gas injection pressure was nearly twice this at about 19.4 MPa. Two other features of this test were

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$^2$ The term $K_0$ geometry is borrowed from soil science, in which it is used to refer to a soil in which no horizontal strain is allowed while the soil is compressed vertically. $K_0$ is actually the ratio of horizontal to vertical stresses under these conditions, the coefficient of earth pressure at rest (e.g. Mitchell [1993], Fredlund and Rahardjo [1993]).

$^3$ Note that the discussion provided here of the experiments reported in this reference for the $K_0$ and radial flow constant volume experimental set ups was based on pre-publication information. A more definitive characterisation and discussion of the experiments has since been provided by Harrington and Horseman [2003].
a) strong indications, from a small discontinuity in the pressure profile, the response of other sensors and subsequent examination of the sample, that macroscopic fracturing had occurred; and

b) evidence of very small “precursor” flows that took place when the pressure exceeded 13.7 MPa.

It may be [Swift et al., 2001] that the high threshold pressure for gas flow may be a consequence of the injection geometry (i.e. into a cylindrical cavity). The small precursor flows may be water displaced by consolidation of the clay.

The threshold pressure for gas flow in the second test in this geometry [Harrington and Horseman, 2003] exhibited a more complex behaviour:

a) There was a small outflow, inferred to be water, but this time at a gas pressure of 3-6 MPa.

b) At gas pressures of about 11 MPa, small flows (assumed to be mixed gas and water) were observed in all sink filters. With the pressure maintained at 11 MPa the flow remained at about 3 μL hr⁻¹ for about 50 days. Responses in stress sensors and in the porewater pressure suggested that some “flow-initiating” event occurred at the time that these flows were first observed. Further similar events were seen as the pressure was raised above 11 MPa.

c) Large gas flows (with production rates approximating the imposed injection rate) were not observed until a gas breakthrough event occurred when a gas injection pressure of 22 Pa was reached (but with an earlier transient flow spike at 16 MPa)

d) The events at 16 and 22 MPa injection pressure were associated with sensor responses that suggested that fracturing had occurred.

In this experiment, the swelling pressure was measured and had a value of 5.4 MPa, so that the excess pressures at which significant gas flow was observed were much higher than the swelling pressure.

Horseman and Harrington [Horseman and Harrington, 1997; Harrington and Horseman, 2003] have attempted to measure porewater pressures and radial and axial stresses in some of their gas and water flow experiments in order to improve the characterisation of the systems under investigation.

The character of the response of the porewater pressure to gas invasion of a bentonite sample was found to vary with experiment. In experiments on bentonite pastes [Horseman and Harrington, 1997], the porewater pressure was found in some, but not all cases, to closely follow the gas injection pressure. In experiments using compacted bentonite, the porewater pressure showed a clear but smaller response. For example, in
the most recent constant volume radial flow experiment, the porewater pressure, measured at a point outside the group of sink filters, mirrored the variation in the gas injection pressure, but with a lower value; the maximum gas injection pressure reached was about 22 MPa, whereas the maximum porewater pressure measured was about 13 MPa, occurring at the same time.

A porewater pressure response was also seen in the experiments in a $K_0$ geometry mentioned above [Harrington and Horseman, 2003], during both water flow and gas injection experiments. These results were discussed in the GAMBIT Phase 2 report [Swift et al., 2001]. An anomaly found with this response was that the porewater pressure did not appear to relax back to the applied back pressure.

The manner in which Horseman and Harrington [Horseman and Harrington, 1997; Harrington and Horseman, 2003] apply their upstream gas pressure, by pumping water into a gas-filled vessel to compress the gas, affords the opportunity to observe the evolution of the post-breakthrough gas pressure in this vessel. After breakthrough, the gas pressure drops smoothly towards a steady-state value below the breakthrough pressure. That is, gas flow continues at a pressure below the breakthrough pressure. If the pump is turned off (sometime after gas breakthrough has occurred), the gas pressure naturally drops further. However, the upstream gas-pressure does not continue to fall as far as the back pressure imposed at the downstream end of the sample; rather, it seems to asymptote slowly to some “shut in” value, well above the back pressure. It appears that there is some value of upstream gas pressure between the breakthrough pressure and the back pressure at which gas flow ceases. It is not clear what determines this value; it may be due to a capillary pressure or due to mechanical closure of pathways.

Graham et al. 2002] see no argument for the posited relationship between gas entry pressure and swelling pressure. For experiments on nearly water-saturated Avonlea bentonite$^4$, with the inlet gas pressure increased incrementally, they found very high entry pressures. On the other hand they found that, if only a modest gas pressure was applied for a long time, gas flow through the sample was established. The GAMBIT Club Phase 2 report [Swift et al., 2001] provides a discussion of these results. It is worth noting here that the rate of gas pressure increase used by Graham et al. 2002 in the experiments in which the gas pressure was incremented, was, at 2.4 MPa h$^{-1}$, about 100 times that adopted by Horseman and Harrington 1997, and also that the dry density of the bentonite used was significantly less than that used by workers reporting a relationship with swelling pressure.

Direct measurements of porewater displacement from bentonite samples by gas injection are limited. Those measurements that have been made show that only small

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$^4$ Experiments were also reported for lower water saturations, but current GAMBIT Club interest is in saturated samples.
amounts of water are displaced [Hume, 1999; Tanai, unpublished 2001]. No workers have reported substantial water displacement from samples, and the fact that not much water needs to be displaced to allow gas passage is widely accepted.

2.2 Implications of Experimental Data for the Mechanism of Gas Migration through Compacted Bentonite

It will be evident, from the above account of available experimental results on gas migration in bentonite, that the data does not point clearly to one mechanism of gas migration that can explain all the results. In the introduction to Section 2, three mechanisms of gas migration that have been proposed were noted:

a) Gas migration by displacement of water from the pores of the clay in accordance with conventional concepts of two phase flow in which the pore structure is essentially unchanged;

b) Gas migration through the creation of pathways by microfissuring; that is the creation of gas pathways by disturbance of the clay structure;

c) Gas migration by macroscopic fracturing of the clay sample.

It was noted that these may occur in combination and the mechanisms may vary with the conditions. However, there is not an obvious relationship between the observed gas migration behaviour and any particular system parameters.

As discussed in the previous subsection, there is very strong evidence that macroscopic fracturing does occur in the constant volume radial flow experiments carried out by Harrington and Horsemann [2003] at high gas injection pressures of 16-22 MPa compared with a back pressure of 1 MPa. There were also indications of small gas flows at lower pressures, particularly in the second experiment where they occurred at gas pressures above ~11 MPa. Responses on stress sensors indicated the occurrence of discrete events, presumed to be associated with the formation of fractures. It therefore appears that some fracturing occurred at pressures above 11 MPa.

In these constant volume experiments, gas flow through the sample does not occur until the gas pressure is well above the sum of the swelling pressure and the water back pressure (at least in the second experiment, for which the swelling pressure has been directly measured). This is in contrast to the earlier BGS experiments in samples constrained under isotropic stress or in a \(K_0\) geometry, in which substantial gas flows were established at a threshold pressure that was usually well defined and was approximately equal to the sum of the swelling pressure (sometimes estimated) and the water back pressure. If the clay is isotropic and initially in equilibrium, this sum is also the (initial) total stress in the clay. Once the gas pressure exceeds this pressure it is capable of consolidating the clay, by compression and particularly by squeezing some water from the clay. It is an assumption of the GAMBIT-GW Phase 2 model that this allows the creation of void space, which can form gas migration pathways. However,
the detailed mechanism and geometry of the deformation is not known; it may depend, for example, on the local stress field and on inhomogeneities in the clay that provide gas entry or fracture initiation sites (as necessary for the GAMBIT Phase 1 fracture propagation model). In some circumstances it could be the case that the application of the pressure may merely consolidate the clay without initially generating fractures (if the stresses become sufficiently large of course failure will occur). The fact that clay samples in the work by Hume [1999] were found to be shortened by ~5-11% after application of rapid increases in gas pressure suggests that applied gas pressures can cause consolidation. Of course, consolidation of the clay will raise the swelling pressure of the clay, perhaps making gas entry more difficult.

In the tests at constant isotropic stress, the global stress in the clay cannot rise in the same way as in the constant volume experiments. This may result in a different response of the clay to the application of gas in the two situations. The $K_0$ geometry provides an intermediate situation.

Other workers have, however, also apparently carried out gas migration tests in constant volume vessels [Tanai et al., 1997; Gallé, 1998, 2000] and found that gas migration does occur above a threshold gas pressure closely associated with the swelling pressure (plus back pressure). The work by Graham et al. [Graham et al., 2002; Hume, 1999] is anomalous in showing high gas threshold pressures from the application of rapidly (relative to other studies) increasing gas pressures, but no threshold to the sustained application of constant gas pressures that were much lower than the threshold pressures in the increasing gas pressure experiments.

It is possible that the differences between the radial and linear geometries, or the small size of the gas source term in the radial flow geometry may be significant. It would be easier in linear geometries for the gas to creep between the clay and its jacket, once the pressure was high enough to consolidate the clay, than in the radial flow geometry.

Arguments that gas migration occurs via water displacement from pre-existing pathways generally involves recourse to a picture of the clay fabric. There does not seem to be any disagreement that the basic elements of the clay fabric are particles consisting of stacks of clay platelets separated by tightly bound interstitial water. It is a change in thickness of these water layers that controls the swelling behaviour of bentonite clays. Between these particles there will be less tightly bound intrastack water, and perhaps soft clay gels formed by the foliation of clay gels into the interparticle pore space. The possible role of clay gels on gas migration has not been widely considered, except in the work of Pusch et al. [1990], who consider that it is the water-filled pathways through these gels (which may be compressed by the gas pressure) that provide the route for gas migration. The crucial question is what is the size and connectivity of these pathways in order to decide whether they can (without dilation) provide a credible route for gas migration. In highly compacted bentonite, it has been suggested [Horsemans and Harrington, 1997] that there is little to distinguish interstack from intrastack voids.
If gas migration does occur through pre-existing pathways, then the existence of an entry pressure for gas migration would arise from the gas-water capillary pressures for the channels. For large entry pressures this does require that the channels are very small; for example, a 10 MPa excess gas pressure for entry into a sample corresponds to a circular capillary of radius about 15 nm. To provide a typical gas permeability of $\sim 10^{-20}$ m$^2$ after breakthrough would then require a density of capillaries of about $5 \times 10^{11}$ m$^{-2}$, assuming they behaved as smooth parallel capillaries (since they would in fact be tortuous, a rather larger number would be needed, but this is a detail beyond the accuracy of these estimates). This would be about $10^9$ capillaries in a typical 5 cm diameter experimental sample. While this is a very large number it is not apparently physically impossible; it would correspond to an average separation between pathways of about 3 μm, which is conceivable given the small particle sizes in bentonite, and the gas filled porosity would be about $4 \times 10^{-4}$. However, it would result in a radically different conceptual picture of the nature of gas migration pathways in bentonite from one in which a relative small number of pathways are created by the gas pressure. With the very large number of pathways implied by the displacement of water from capillaries model, the conceptual model accords very closely with that of conventional continuum porous medium flow models. (Note that a similar picture is obtained if the pathways are considered to be elliptical in cross-section, with a large eccentricity.)

The erratic, intermittent downstream flows often seen in experiments would seem to indicate that flow is occurring through a relatively small number of pathways; if a very large number of pathways were involved it would be expected that fluctuations in individual flows would be subsumed into a smooth overall flow (unless the flows in separate channels were strongly coupled in some way).

The way that the bentonite closes to gas flow may also be pertinent to understanding the mechanism of gas migration. There now seems good evidence that if water is passed through a bentonite sample that has previously sustained gas flow (established from an initially saturated state), then the initial resistance to gas flow is restored. That is the pathways that were opened to gas are resealed; this could occur, for example, by swelling of the clay or restoration of capillary barriers.

The existence of the “shut-in” behaviour, that is a cessation of gas flow, when the upstream pressure is reduced sufficiently below the initial breakthrough requires some explanation. This shut-in pressure is typically substantially below the initial breakthrough pressure, and gas continues to flow at pressures above this. If the breakthrough event is associated with a fracture opening mechanism, then conventional hydraulic fracturing theory would suggest that the fracture would close when the pressure dropped below the initial fracture opening pressure. This does not occur (unless the breakthrough pressure is much bigger than the fracture opening pressure because fracture propagation takes very much longer than predicted). This was a difficulty with the GAMBIT Club Phase 1 fracture propagation model that was only overcome using heuristic arguments about possible adjustments of the fissure geometry. Part of the motivation for the Phase 2 GAMBIT-GW model was to provide at least a
self-consistent model for observed behaviour based on the idea that pathway opening required the squeezing of water from the clay matrix, and the pathways could not reseal until this water was replaced. This provided an explanation of why the pathways remained open at pressures below the breakthrough pressure. It did not, however, provide an explanation of the shut-in pressure.

Horseman and Harrington [1997] consider that the shut-in pressure may represent the capillary pressure of the gas-carrying channels. If this is the case, it is not clear why gas migration does not occur once this pressure is reached rather than needing to reach a much higher threshold pressure for gas breakthrough. It is possible that if it is a capillary pressure that controls shut in, then this might be the capillary pressure of dilated pathways created by the migrating gas, rather than the capillary pressure associated with pore sizes in the fully water-saturated bentonite before gas migration. Resealing of pathways through capillary effects requires the movement of water into the narrowest portions of the gas channels in order to close them off. It is interesting to speculate about where this water might come from. In the BGS experiments, gas is passed from the top to the bottom of the clay samples. This means that after gas breakthrough water will be flushed from the outlet sintered disks and pipework as gravity segregation will cause the gas to sit on top of the water initially in these parts of the apparatus. It will not therefore be possible for liquid water to imbibe from outside the sample to reseal pathways. Closing off of pathways by the establishment of water films across the pathways will therefore require either the redistribution of water within the bentonite or the condensation of water vapour from the wet gas passing through the clay. Given the large change in the gas pressure difference across the clay between breakthrough and shut-in, some redistribution of the water seems plausible, although whether this would involve the redistribution of water films remaining in the gas channels or the movement of water from the clay matrix into the gas channels is unclear (suction in the clay following the release of gas pressure would seem to act to prevent the latter). Note that measurements of capillary pressure hysteresis in conventional porous materials are normally carried out with the fluids involved in contact with the sample surfaces.

It is of interest to consider the effect of the downstream boundary condition on the nature of gas flow from the clay and potentially on the way that gas channels might be shut-in. The back pressure applied at the downstream boundary (~1 MPa in the BGS experiments) is well below the pressure at which gas flow apparently ceases. This means that at the boundary itself, pathways should not be open. Assuming that there is a real shut-in pressure, this explains the intermittent nature of the downstream gas flows: when gas breaks through its pressure at the downstream boundary will drop to close to the applied back pressure, which is below the shut-in pressure, causing the gas pathway to close; the gas pressure will build up locally behind this closure point until it reaches a value at which it can force the channel open again; this cycle is then repeated. This explanation of the intermittent or “burst-type” downstream flow was put forward by BGS workers in the context of experimental work on gas migration in Boom Clay [Volckaert et al., 1995]. Whether this intermittent closing of the paths involves
mechanical opening and closing of the pathways, or a capillary type mechanism in which water films are displaced and reform, is not determined by the evidence available.

In all the GAMBIT Club modelling studies, it is a feature of the calculated results that most of the change in gas pressure in a flowing gas stream occurs very close to the downstream boundary; that is, for most of the length of the sample the gas pressure is close to the upstream gas pressure, but it drops sharply to the value of the applied back pressure (or this value plus some user supplied notional capillary pressure) close to the downstream end of the sample. It would be interesting to know whether this is also the situation in a real system, or whether it is an artefact of the modelling.

It would be helpful to the resolution of the uncertainties in the possible contribution of different mechanisms to gas migration in bentonite if experiments could be devised that were able to identify the geometric characteristics of the gas pathways formed through compacted bentonite, and in particular the numbers of distinct pathways formed.
3 EXTENSION OF THE PHASE 2 GAMBIT-GW GAS MIGRATION MODEL TO INCLUDE TREATMENT OF THE STRESS TENSOR

This section describes the extension of the GAMBIT-GW model, which was developed during the Phase 2 work, to include a proper representation of stresses in the clay. This will be designated the GAMBIT-GWS model. The mathematical formulation of this extended model is described in subsection 3.1, and its numerical implementation in subsection 3.2. Results from the application of the extended model to the simulation of certain laboratory experiments on gas migration in compacted bentonite are presented in subsection 3.3.

3.1 Mathematical Formulation

It is helpful to develop the theory by considering first the coupled mechanical deformation of and flow through a porous medium for the case in which only a single fluid phase is present, in practice water. This theory was developed originally by Biot [1941], and is summarised in the next subsection. The extensions necessary for Biot’s theory to be applicable to gas invasion of water-saturated bentonite are presented in subsection 3.1.2. The relationship of the resulting generalised model to the simpler GAMBIT-GW model is described in subsection 3.1.3.

3.1.1 Single-phase Flow through a Deformable Porous Medium

This section summarises Biot’s [1941] model of consolidation. The model consists of:

a) Force balance equations, which determine the equilibrium state of a small element of the porous medium.

b) Macroscopic stress-strain relations, which are the generalisation of Hooke’s Law to the case of an isotropic elastic body with a pore fluid.

c) A continuity equation for the pore fluid, in which the fluid velocity is determined by Darcy’s Law.

For completeness, these equations are listed in the rest of this subsection.

Force balance equations

The stresses in the rock satisfy equations of equilibrium\(^5\):

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\(^5\) Throughout this section the Einstein summation convention will be adopted (i.e. repeated appearance of a tensor index implies a summation).
\[
\frac{\partial}{\partial x_j} \sigma_{ij} + \rho X_i = 0. \tag{3.1}
\]

Here:
- \(x_i\) is the spatial co-ordinate [m];
- \(\sigma_{ij}\) is the stress tensor [Pa];
- \(\rho\) is the density of the body [kg m\(^{-3}\)];
- \(X_i\) is the body force per unit mass [m s\(^{-2}\)].

**Generalised Hooke’s Law**

Hooke’s Law for an isotropic elastic material,

\[
\Delta \varepsilon_{ij} = \frac{1 + \nu}{E} \Delta \sigma_{ij} - \frac{3\nu}{E} \frac{\Delta \sigma_{ii}}{3} \delta_{ij}, \tag{3.2}
\]

has been generalised to the case in which a pore fluid is present [e.g. Biot, 1941; Rice and Cleary, 1976; Palciauskas and Domenico, 1989]:

\[
\begin{align*}
\Delta \varepsilon_{ij} &= \frac{1 + \nu}{E} \Delta \sigma_{ij} - \frac{3\nu}{E} \frac{\Delta \sigma_{ii}}{3} \delta_{ij} + \frac{1}{3H} \Delta p_w \delta_{ij} \\
\frac{\Delta V_p}{V} &= \frac{1}{H} \Delta \sigma_{ii} + \left( \frac{1}{R} - \phi \beta_w \right) \Delta p_w
\end{align*} \tag{3.3}
\]

Here:
- \(\varepsilon_{ij}\) is the strain tensor [-];
- \(\nu\) is Poisson’s ratio [-];
- \(E\) is Young’s modulus [Pa];
- \(H, R\) are material properties [Pa];

---

\(^6\) The natural stress, \(\sigma_{ij}\), defined as force per unit area, where the area at the beginning of the time-step is taken, can be distinguished from the engineering stress, \(\sigma_{ij}^{e}\), which is defined in terms of the original area (i.e. at \(t = 0\)). The distinction is unimportant for small deformations.

\(^7\) The natural strain, \(\varepsilon_{ij}\), which is defined in terms of displacement, \(u_i\), from position at the beginning of the time-step, also can be distinguished from the engineering strain, \(\varepsilon_{ij}^{e}\), where the cumulative displacement vector, \(U_i\), is defined from the position at \(t = 0\).
$p_w$ is the pressure of the pore fluid [Pa];

$V_p$ is the volume of the pore space in a small element [m$^3$];

$V$ is the volume of the porous material in a small element [m$^3$];

$\phi$ is the volume of the pore space per unit volume of the porous material (i.e. $\phi = V_p / V$; strictly, one ought to distinguish between the *kinematic* and *total* porosity) [-];

$\beta_w$ is the compressibility of the pore fluid [Pa$^{-1}$].

Note that:

a) The convention adopted is that stresses are reckoned positive when tensile. To have displacements follow the same pattern (i.e. for positive displacements to correspond to positive stresses) displacements are reckoned positive when in the positive direction of the axes. This is opposite to the normal convention in geomechanics, but is the normal convention in treatises on elasticity.

b) The generalised Hooke’s Law has been written in incremental form to allow for the possibility that the material properties may depend on scalar invariants of the stress/strain state.

There are a number of equivalent formulations of Equation (3.3). For example,

\[ \Delta \varepsilon_j = \frac{1 + \nu}{E} \Delta \sigma_j - \frac{3\nu}{E} \Delta \sigma_{ij} \delta_j + \frac{1}{3H} \Delta p_w \delta_j \]

\[ \frac{1}{V} \Delta \left( \frac{\rho_w V_p}{\rho_w} \right) = \frac{1}{H} \Delta \sigma_{ij} + \frac{1}{R} \Delta p_w \]  \hspace{1cm} (3.4)

and

\[ \Delta \varepsilon_j = \frac{1 + \nu}{E} \Delta \sigma_j - \frac{3\nu}{E} \Delta \sigma_{ij} \delta_j + \frac{1}{3H} \Delta p_w \delta_j \]

\[ \Delta \phi = \left( \frac{1}{H} - \frac{1 - 2\nu}{E} \right) \Delta \sigma_{ij} \delta_j + \frac{1}{R} \Delta p_w \] \hspace{1cm} (3.5)

can be derived. Here:

$\rho_w$ is the density of the pore fluid [kg m$^{-3}$],

\[ \rho_w = \rho_o \exp \left[ \beta_w (p_w - p_o) \right] . \]  \hspace{1cm} (3.6)

**Continuity equation for the pore fluid, and Darcy’s Law**

The continuity equation for the pore fluid in a deformable medium is \cite{deMarsily1986}:
\[
- \frac{1}{\rho_w} \frac{\partial}{\partial x_i} (\rho_w q_i) = \frac{\phi}{\rho_w} \frac{D p_w}{Dt} + \frac{1}{1 - \phi} \frac{D \phi}{Dt} - \frac{\phi}{\rho_s} \frac{D \rho_s}{Dt},
\]

where the filtration velocity, \( q_i \), is determined by Darcy’s Law:

\[
q_i = -\frac{k_{wij}}{\mu_w} \left( \frac{\partial p_w}{\partial x_j} + \rho_w g \delta_{ij} \right).
\]

Here:
- \( q_i \) is the filtration velocity [m s\(^{-1}\)];
- \( \frac{D}{Dt} \) is the material derivative\(^8\) with respect to time [s\(^{-1}\)];
- \( \rho_s \) is the density of the solid grains (in practice, the solid grains usually can be assumed to be incompressible - see below) [kg m\(^{-3}\)];
- \( k_{wij} \) is the permeability tensor for the pore fluid [m\(^2\)];
- \( \mu_w \) is the viscosity of the pore fluid [Pa s];
- \( g \) is the acceleration due to gravity (the 3\(^{rd}\) axis is assumed vertical) [m s\(^{-2}\)].

**Biot’s model of consolidation**

Biot’s [1941] model of consolidation is obtained by combining Equations (3.3) and (3.7):

\[
- \frac{1}{\rho_w} \frac{\partial}{\partial x_i} (\rho_w q_i) = \left( -\frac{K}{H^2} + \frac{1}{R} \right) \frac{D p_w}{Dt} + \frac{K}{H} \frac{D \epsilon_{ij}}{Dt} + \frac{1}{Q} \frac{D p_w}{Dt} + \alpha \frac{D \epsilon_{ij}}{Dt}.
\]

Here:
- \( K \) is the bulk modulus of the porous material, \( K = \frac{E}{3(1 - 2v)} \) [Pa];
- \( Q \) [Pa\(^{-1}\)], \( \alpha \) [-] are parameters introduced by Biot [1941].

---

\(^8\) The material derivative is the variation of a property in unit time interval at a point that moves with the solid grain [Batchelor, 1967]. If the velocity of the solid grain is small, the material derivative can be approximated by the ordinary time derivative.
Simplification for incompressible grains

If the solid grains are \textit{incompressible}, an assumption that usually can be justified, then the change in the volume of a small element of the porous medium is equal to the change in pore volume of the element:

\[
\Delta \varepsilon = \frac{\Delta V_p}{V} .
\]  

(3.10)

Hence, it can be shown that the generalised Hooke’s Law (i.e. Equation 3.3) simplifies as follows:

\[
\Delta \varepsilon = \frac{1 + \nu}{E} \Delta \sigma - \frac{3\nu}{3K} \Delta \sigma \delta_y + \frac{1}{3K} \Delta p_w \delta_y
\]

\[
= \frac{1 + \nu}{E} \Delta \sigma + p_w \delta_y \]

\[
\Delta V_p = \Delta \varepsilon
\]

(3.11)

In this case, the stress-strain relations are seen to depend only on the effective stress tensor:

\[
\sigma_{\text{eff}} = \sigma + p_w \delta_y .
\]  

(3.12)

Note that:

a) The definition of the effective stress tensor, \( \sigma_{\text{eff}} \), has this form because of the assumption that stresses are reckoned positive when tensile.

Biot’s [1941] model of consolidation (i.e. Equation 3.9) also simplifies:

\[
- \frac{1}{\rho_w} \frac{\partial}{\partial x_i} (\rho_w q_i) = \phi \beta_w \frac{Dp_w}{Dt} + \frac{DE_{\text{eff}}}{Dt} .
\]  

(3.13)

3.1.2 Two-phase Flow through a Deformable Porous Medium

This subsection extends Biot’s [1941] model to the case of two-phase flow through a deformable porous medium. It will be assumed that the solid grains are \textit{incompressible}. As before, the model consists of:

a) Force balance equations, which determine the equilibrium state of a small element of the porous medium (i.e. Equation 3.1).

b) Macroscopic stress-strain relations that are the generalisation of Equation (3.11) for a porous medium with both a liquid phase and a gas phase.
Continuity equations for the pore fluids (i.e. liquid phase and gas phase), in which the fluid velocities are determined by Darcy’s Law.

There are two parts to extending Biot’s [1941] model for the case of two-phase flow: first, a dependence on the pressure of the gas phase has to be included in the macroscopic stress-strain relation (i.e. Equation 3.11); secondly, continuity equations for the pore fluids have to be developed.

**Generalised Hooke’s Law**

If the solid grains are *incompressible*, then the obvious generalisation (see Appendix A) of the constitutive equations (i.e. Equation 3.11) to the case of two-phase flow is:

\[
\Delta \varepsilon_{ij} = \frac{1 + \nu}{E} \Delta \sigma_{ij} - \frac{3\nu}{E} \frac{\Delta \sigma_{ii}}{3} \delta_{ij} + \frac{1}{3K} \Delta p_v \delta_{ij} + \frac{1}{3H_m} (\Delta p_g - \Delta p_w) \delta_{ij}.
\]  

\[
\frac{\Delta V_p}{V} = \Delta \varepsilon_{ii}.
\]  

(3.14)

Here:

- \(H_m\) is the modulus of elasticity for the porous material with respect to a change in matric suction, \(p_g - p_w\) [Pa];
- \(p_g\) is the pressure of the gas phase [Pa].

Equation (3.14) is supplemented by an additional constitutive equation for the volume occupied by the gas phase:

\[
\frac{\Delta (S_g V_p)}{V} = \frac{1}{H_m} \left( \frac{\Delta \sigma_{ii}}{3} + \Delta p_w \right) + \frac{1}{R_m} \left( \Delta p_g - \Delta p_w \right),
\]  

(3.15)

or, equivalently,

\[
\phi \Delta S_g = \left( \frac{1 - S_g}{H_m} \right) \left( \frac{\Delta \sigma_{ii}}{3} + \Delta p_w \right) + \left( \frac{1}{R_m} - \frac{S_g}{H_m} \right) \left( \Delta p_g - \Delta p_w \right).
\]  

(3.16)

Here:

- \(S_g\) is the volumetric saturation of the gas phase, which is related to \(S_w\), the volumetric saturation of the liquid phase, by \(S_g = 1 - S_w\) [-];
- \(R_m\) is the volumetric modulus of the gas phase with respect to a change in matric suction, \(p_g - p_w\) [Pa].

It is convenient in these equations to introduce different elastic moduli, defined by:
\[
\frac{1}{H_m} = \frac{1}{H_m} - \frac{S_g}{K} \\
\frac{1}{R_m} = \frac{1}{R_m} - \frac{S_g^2}{K} .
\]  

(3.17)

Hence, Equations (3.14) and (3.16) respectively become:

\[
\Delta e_{ij} = \frac{1 + \nu}{E} \Delta \sigma_{ij} - \frac{3\nu}{E} \Delta \sigma_{ij} \delta_{ij} + \frac{1}{3K} S_g \Delta p_w \delta_{ij} + \frac{1}{3K} S_g \Delta \phi \delta_{ij} \\
+ \frac{1}{3H_m} (\Delta p_g - \Delta p_w) \delta_{ij} ,
\]

(3.18)

\[
\frac{\Delta V_p}{V} = \Delta e_{ij} 
\]

and

\[
\phi \Delta S_g = \frac{1}{H_m} \left( \frac{\Delta \sigma_{ij}}{3} + \Delta p_w \right) + \left( \frac{1}{R_m} - \frac{S_g}{H_m} \right) (\Delta p_g - \Delta p_w) .
\]

(3.19)

The response of a clay to changes in either the applied stress or the pressure of a pore fluid will be determined completely by its elastic moduli, that is \( \nu, E, H_m \) and \( R_m \).

The choice of functions to represent these elastic moduli is a modelling decision, albeit one motivated both by physical insight and by experiment, and is discussed further below.

**Continuity equation for the liquid phase**

The continuity equation for the pore water (i.e. Equation 3.7) generalises to:

\[
- \frac{1}{\rho_w} \frac{\partial}{\partial x_i} (\rho_w q_i) = S_w \phi D \rho_w + \frac{\phi D S_w}{Dt} + S_w D \phi ,
\]

(3.20)

where the filtration velocity, \( q_i \), is determined by Darcy’s Law (i.e. Equation 3.8).

Note that:

1. \( k_{w,i} \), which depends on the scalar invariants of the stress / strain state, now can depend also on \( S_w \). Conventional models assume that \( k_{w,i} \) depends only on \( \phi \) and \( S_w \).

By combining Equations (3.14), (3.15) and (3.20), an alternative, more intuitive form of Equation (3.20) is obtained:
Continuity equation for the gas phase

Below some critical stress / pressure, there will be no free gas present in the bentonite, but gas will dissolve in the pore water and diffuse through the porous material. At higher stress / pressure the gas will flow as a distinct phase. The latter flow obeys equations that are similar to those for the liquid phase. These two types of flow are discussed below, and then a continuity equation for the gas phase is derived.

Allowing for the presence and transport of dissolved gas represents an extension to the original GAMBIT-GW model, but as well as providing the capability to model a process that sometimes may be important, it also is convenient computationally in managing the transition from no free gas to free gas.

(i) Dissolved gas phase

The flow of the dissolved gas phase is described by:

\[-\frac{\partial}{\partial x_i} \left( \rho_a q_i \right) = \frac{1}{V} \frac{D(\rho_a S_w V_p)}{Dt} .\]  (3.21)

\[
\frac{\partial}{\partial x_j} \left( c q_i - D_{ij} \frac{\partial c}{\partial x_j} \right) = \frac{1}{V} \frac{D(c S_w V_p)}{Dt} .\]  (3.22)

Here:

- \( c \) is the molar concentration, defined as moles of dissolved gas per unit volume of solution [mol m\(^{-3}\)];
- \( D_{ij} \) is the dispersion tensor [m\(^2\) s\(^{-1}\)].

Note that, most generally:

\[D_{ij} = S_w \frac{d_m}{\tau} \delta_{ij} + (a_L - a_T) \frac{q_i q_j}{\sqrt{q_i q_i}} + a_T \frac{q_i q_j}{\sqrt{q_i q_i}} \delta_{ij} .\]  (3.23)

Here:

- \( d_m \) is the molecular diffusion coefficient [m\(^2\) s\(^{-1}\)];
- \( \tau \) is the tortuosity [-];
- \( a_L \) is the longitudinal dispersion length [m];
- \( a_T \) is the transverse dispersion length [m].

In clay the first term on the right-hand side of Equation (3.23) is likely to be dominant; that is, it should be possible to assume that \( a_L \) and \( a_T \) are zero.

\( c \) can be related to \( p_g \) by Henry’s Law:
\[ p_g = H_g c \]  \hspace{1cm} (3.24)

Here:

\( H_g \) is Henry’s constant [Pa mol\(^{-1}\) m\(^3\)].

This equation can be used to define \( p_g \), even if there is no free gas phase. In particular, using Henry’s law in Equation (3.22) gives:

\[-\frac{\partial}{\partial x_i} \left( p_g q_i - S_w \frac{d}{\tau} \frac{\partial p_g}{\partial x_i} \right) = \frac{1}{V} \frac{D \left( p_g S_w V_p \right)}{Dt} . \]  \hspace{1cm} (3.25)

(ii) \textbf{Free gas phase}

The flow law for the free gas phase, analogous to that for the liquid phase, is:

\[-\frac{\partial}{\partial x_i} \left[ -\rho_g \frac{k_{g,ij}}{\mu_g} \left( \frac{\partial p_g}{\partial x_j} + \rho_g \delta_{ij} \Delta \sigma_{ij} \right) \right] = \frac{1}{V} \frac{D \left( \rho_g S_g V_p \right)}{Dt} . \]  \hspace{1cm} (3.26)

Here:

\( \rho_g \) is the density of the gas [kg m\(^{-3}\)];

\( k_{g,ij} \) is the permeability tensor for the gas phase [m\(^2\)];

\( \mu_g \) is the viscosity of the gas [Pa s];

\( p_g \) is the pressure of the gas [Pa].

Note that:

a) \( \rho_g \) is related to \( p_g \) by the equation of state for an ideal gas:

\[ \rho_g = \frac{M_g}{R_g T} p_g . \]  \hspace{1cm} (3.27)

Here:

\( M_g \) is the molar mass of the gas [kg mol\(^{-1}\)];

\( R_g \) is the ideal gas constant [J K\(^{-1}\) mol\(^{-1}\)];

\( T \) is the temperature [K].

b) The most general form of the permeability tensor for the gas phase, where \( k_{g,0} \), \( k_{g,1} \), and \( k_{g,2} \) may depend on the scalar invariants of the stress / strain state, is:

\[ \Delta k_{g,ij} = k_{g,0} \delta_{ij} + k_{g,1} \Delta \sigma_{ij} + k_{g,2} \Delta \sigma_{ij} \Delta \sigma_{ij} . \]  \hspace{1cm} (3.28)
Conventional models assume that $k_{g,ij}$ depends only on $\phi$ and $S_g$.

(iii) Combined dissolved and free gas flow

Finally, it is possible to combine Equations (3.25) and (3.26), giving:

$$
-\frac{\partial}{\partial x_i} \left[ \frac{M_g}{H_g} \left( p_g q_i - S_w \phi \frac{d_m}{\tau} \frac{\partial p_g}{\partial x_j} \right) - \rho_g \frac{k_{g,ij}}{\mu_g} \left( \frac{\partial p_g}{\partial x_j} + \rho_g g \delta_{j3} \right) \right] = D \left[ \frac{p_g}{V} \left( \frac{S_w M_g}{H_g} + S_g \frac{M_g}{R_g T} \right) V_p \right].
$$

(3.29)

Physical properties of bentonite clay

At this point a mathematical framework has been created to describe the migration of gas through bentonite. However, in order to complete the specification of the model there are some decisions still to be taken, mainly to do with the choice of functional forms for the elastic moduli and the permeability tensor for the gas phase.

(i) Elastic moduli

The response of a clay to changes in either the applied stress or the pressure of a pore fluid is completely determined by its elastic moduli, that is $\nu$, $E$, $\tilde{H}_m$ and $\tilde{R}_m$.

Since the volume occupied by the gas phase is small (i.e. deformations of the bentonite are small), both Poisson’s ratio, $\nu$, and Young’s modulus, $E$, will be taken to be constant. Values have been measured in experiments on saturated bentonite [Börgesson et al., 1995; 1996].

Considering the other elastic moduli (i.e. $\tilde{H}_m$ and $\tilde{R}_m$), if Equations (3.18) and (3.19) are to apply also in the case when there is just a pure liquid phase (i.e. the equations reduce to Equation 3.11 in the limit $S_w \to 1$), then there has to be a gas entry condition, $\Gamma$, which depends only on the scalar invariants of the stresses, such that

$$
p_g < \Gamma \quad \Rightarrow \quad \text{no free gas phase}
$$

$$
p_g > \Gamma \quad \Rightarrow \quad \text{is a free gas phase},
$$

(3.30)

with the property that:

$$
p_g < \Gamma \quad \Rightarrow \quad \frac{1}{\tilde{H}_m} = \frac{1}{\tilde{R}_m} = 0.
$$

(3.31)
Now, the form of Equations (3.18) and (3.19), as well as experience with the GAMBIT-GW model [Swift et al., 2001], suggests it may be appropriate always to set:

$$\frac{1}{H_m} = 0 \quad .$$

(3.32)

This choice, in particular, would mean that:

$$\Delta \varepsilon_{ij} = \frac{1 + \nu}{E} \Delta \sigma_{ij} - \frac{3\nu}{E} \frac{\Delta \sigma_{jj}}{3} \delta_{ij} + \frac{1}{3K} S_w \Delta p_w \delta_{ij} + \frac{1}{3K} S_g \Delta p_g \delta_{ij} \quad ,$$

(3.33)

which is a simple generalisation of the corresponding single-phase constitutive relation (i.e. Equation 3.11). It also would mean that a change in gas saturation depends only on a change in matric suction, which is consistent with the GAMBIT-GW model.

A form for the remaining elastic modulus, $\tilde{R}_m$, was deduced by the following argument:

a) If the gas saturation is zero, $S_g = 0$, and if the gas pressure is less than the gas entry condition, $p_g < \Gamma$, then $1/\tilde{R}_m = 0$ (see Equation 3.31).

b) As the gas pressure increases, the bentonite should fail. A typical failure criterion is that the gas pressure must exceed the sum of the minimum principal effective stress and the tensile strength of the clay [Jaeger and Cook, 1975]. In the GAMBIT-GW model, this criterion has been implemented as:

$$\frac{1}{\tilde{R}_m} = \frac{1}{\bar{R}_i} \sum_{i=1}^{3} \theta[p_g - (\sigma_i - p_w + \tau_s)] \quad .$$

(3.34)

Here:

$\bar{R}_i$ is a parameter that is characteristic of the bentonite [Pa];

$\theta$ is the Heaviside step function, defined by $\theta(x) = \begin{cases} 0.0 & \text{if } x < 0 \\ 0.5 & \text{if } x = 0 \\ 1.0 & \text{if } x > 0 \end{cases}$

$\sigma_i$ is the $i^{th}$ principal component of the stress tensor [Pa];

$\tau_s$ is the tensile strength of the bentonite [Pa].

This corresponds to choosing the gas entry condition to be:

$$\Gamma = \min_i (\sigma_i - p_w + \tau_s) \quad .$$

(3.35)

c) The interface between gas and liquid may be unstable (see Appendix B, which presents the classic analysis of this instability). In order to have control over this
potential instability, Equation (3.34) was modified to include a term that looks like surface tension:

\[
\frac{1}{R_m} = \frac{1}{R_1} \sum_{i=1}^{3} \theta \left[ p_g - (\sigma_i - p_w + \tau_s) - \Sigma \kappa \right],
\]

(3.36)

where:
- \( \Sigma \) is a numerical parameter, used to control any instability at the interface between gas and liquid [Pa m];
- \( \kappa \) is the curvature of a contour of the gas pressure \(^9 [\text{m}^{-1}] \).

It was hoped this term might be used to stabilise the gas pathway as it propagates through the clay, but in practice it did not help control the numerical instabilities found in some simulations, so for all the results reported \( \Sigma = 0 \) Pa m.

d) The gas saturation should continue to evolve for as long as gas is present in the bentonite, even after the gas pressure has fallen below the condition for gas entry. This behaviour was modelled by adding another term to Equation (3.36), giving:

\[
\frac{1}{R_m} = \frac{1}{R_1} \sum_{i=1}^{3} \theta \left[ p_g - (\sigma_i - p_w + \tau_s) - \Sigma \kappa \right] + \frac{1}{R_2} \theta \left( S_g - S_g^* \right).
\]

(3.37)

Here:
- \( \tilde{R}_2 \) is a parameter that is characteristic of the bentonite [Pa];
- \( S_g^* \) is an irreducible gas saturation [\( \cdot \)].

e) Finally, previous experiences of modelling the migration of gas in bentonite [e.g. Nash et al., 1998] suggest that the gas saturation (actually, the ‘permeability’ for the gas phase) should evolve with an exponential dependence on matric suction, \( p_g - p_w \). Therefore, the form for the elastic modulus \( \tilde{R}_m \) was taken to be:

\[
\frac{1}{R_m} = \frac{1}{R_1} \sum_{i=1}^{3} \theta \left[ p_g - (\sigma_i - p_w + \tau_s) - \Sigma \kappa \right] + \frac{1}{R_2} \theta \left( S_g - S_g^* \right) S_g.
\]

(3.38)

\(^9\) The curvature, \( \kappa \), of a contour of the gas pressure, i.e. \( p_g(x, y) = \text{constant} \), is given by

\[
\kappa = \left( \frac{\partial^2 p_g}{\partial x^2} \left( \frac{\partial p_g}{\partial y} \right)^2 - 2 \frac{\partial^2 p_g}{\partial x \partial y} \frac{\partial p_g}{\partial x} \frac{\partial p_g}{\partial y} + \frac{\partial^2 p_g}{\partial y^2} \left( \frac{\partial p_g}{\partial x} \right)^2 \right) \left( \frac{\partial^2 p_g}{\partial x^2} + \frac{\partial^2 p_g}{\partial y^2} \right)^{-3/2}.
\]
To summarise, it is proposed that:

a) The usual elastic moduli, that is \( \nu \) and \( E \), should be taken as constants;

b) The modulus \( \tilde{H}_m \) should satisfy \( 1/\tilde{H}_m = 0 \);

c) The modulus \( \tilde{R}_m \) should be modelled by Equation (3.38).

This choice of functions to represent the elastic moduli is somewhat arbitrary, although hopefully motivated both by physical insight and by experiment. A different choice of functions might be possible, and experiment must be the arbiter as to which is the more accurate description of the behaviour of bentonite.

(ii) **Permeability tensor for the gas phase**

Another modelling decision concerns the permeability tensor for the gas phase.

It has been argued that the most general form of the permeability tensor for the gas phase is:

\[
\Delta k_{g,ij} = k_{g,0} \delta_{ij} + k_{g,1} \Delta \sigma_{ij} + k_{g,2} \Delta \sigma_y \Delta \sigma_{jl},
\]

(3.39)

where \( k_{g,0} \), \( k_{g,1} \), and \( k_{g,2} \) may depend on the scalar invariants of the stress / strain state. Conventional models assume that \( k_{g,ij} \) depends only on \( \phi \) and \( S_g \).

The question arises as to what controls the direction in which a gas pathway propagates through bentonite. It may be that the gas entry condition (Equation 3.35), with its explicit dependence on the local state of stress in the clay, determines the direction; alternatively, it may be that an anisotropic permeability tensor is needed. In this preliminary model, it will be assumed that:

\[
k_{g,ij} = \theta(S_g - S_{g_c}) k_0 S_g^2 \delta_{ij} \quad \Rightarrow \quad k_{g,0} = \Delta \theta(S_g - S_{g_c}) k_0 S_g^2, \quad k_{g,1} = 0, \quad k_{g,2} = 0.
\]

(3.40)

Here:

\( S_g \) is a critical gas saturation [\(-\)];

\( k_0 \) is a parameter that is characteristic of the bentonite [m\(^2\)].

This choice is consistent with the GAMBIT-GW model [Swift et al., 2001], which assumes that the permeability of the gas phase is for flow along capillaries.
Summary

A conceptual model of gas migration in bentonite has been developed. In particular the model consists of:

a) Force balance equations, Equation (3.1);

b) Macroscopic stress-strain relations, Equations (3.18) and (3.19);

c) Continuity equations for the liquid (Equation 3.21) and the gas (Equation 3.29).

This model has to be supplemented by physical assumptions regarding, for example, the elastic moduli (Equations 3.32 and 3.38) and the permeability tensor for the gas phase (Equations 3.39 and 3.40).

3.1.3 Relationship to the GAMBIT-GW model

This subsection explains how the GAMBIT-GWS model (developed in subsection 3.1.2) may be related to the GAMBIT-GW model [Swift et al., 2001] (a short summary of the main features of the latter model is given in subsection 5.1). It will be shown that the GAMBIT-GW model can be regarded as a special case of the GAMBIT-GWS model in which the treatment of stress has been very much simplified.

The GAMBIT-GW model can account for bulk volume changes of the clay through an empirical dependence of the volume on the stress. However, this was found to have a small effect on results obtained using the GAMBIT-GW model, and so only the constant volume case is considered below.

Stress sub-model

Assuming that ‘constant volume’ means the volumetric strain everywhere is zero, Equation (3.18) (using also Equation 3.32) becomes:

$$\Delta \varepsilon_v = \frac{1}{K} \frac{1}{3} \Delta \sigma_v + \frac{1}{K} S_w \Delta p_w + \frac{1}{K} S_g \Delta p_g$$,

$$= 0$$, \hspace{1cm} (3.41)

and when there is no ‘free’ gas present, this equation simplifies to:

$$\Delta \varepsilon_v = \frac{1}{K} \Delta \left( \frac{\sigma_v}{3} + p_w \right)$$.

$$= 0$$ \hspace{1cm} (3.42)

Equation (3.42) implies that prior to gas entry the effective stress, $\sigma_v/3 + p_w$, remains constant.
In comparison:

i)  *The GAMBIT-GW model assumes that initially the mean stress in the clay, \( \sigma_0/3 \), is a uniform value, calculated from the sum of the swelling pressure (which is a function of the initial porosity) and the applied water pressure. This mean stress is used to determine if gas can enter the clay.*

ii)  *After gas entry the GAMBIT-GW model sets the mean stress equal to the gas pressure, and the mean stress vanishes as an independent variable.*

**Volume change sub-model**

Equation (3.19) (using also Equation 3.32) becomes:

\[
\phi \Delta S_g = \frac{1}{\tilde{R}_m} \Delta (p_g - p_w)
\]  

(3.43)

where the elastic modulus \( \tilde{R}_m \) is given by Equation (3.38).

*In the GAMBIT-GW model gas-filled porosity is created by a change in matric suction, \( p_g - p_w \). In particular, before gas entry, identified by the test \( p_g < -\sigma_0/3 \), the gas-filled porosity is unchanging and zero, but after gas entry the gas-filled porosity is calculated from:*

\[
\frac{\alpha}{e^2} = p_g - p_w
\]  

(3.44)

*Here, \( e \) is the void ratio:*

\[
e = \frac{S_w}{\left( \frac{1}{\phi} - 1 \right)}
\]  

(3.45)

*Since, at constant volume, the total porosity is taken to be constant, Equation (3.44) can be written in incremental form as:*

\[
\phi \Delta S_g = \frac{1}{\gamma \left( p_g - p_w \right)} S_w \Delta \left( p_g - p_w \right)
\]  

(3.46)

*In this equation \( \frac{1}{\tilde{R}_m} = \frac{1}{\gamma \left( p_g - p_w \right)} S_w \) is approximately a constant value.*

There clearly are a couple of differences between the two models:
a) The GAMBIT-GWS model uses effective stress to determine if gas can enter the clay, whereas the GAMBIT-GW model uses total stress.

b) After gas breakthrough, the GAMBIT-GWS model assumes:

\[ \phi \Delta S_g \sim \frac{1}{R_g^2} \phi (S_g - S_{g,J}) S_g \Delta (p_g - p_w) \]

but the GAMBIT-GW model assumes:

\[ \phi \Delta S_g \sim \frac{1}{R_g^2} \Delta (p_g - p_w). \]

**Flow sub-model**

Finally, it is possible to relate the continuity equations for the pore fluids (i.e. liquid phase and gas phase) in the GAMBIT-GWS model and in the GAMBIT-GW model.

First, note that the various volume measures used in the GAMBIT-GW model can be related to those in the GAMBIT-GWS model as follows:

\[ \phi_g = \frac{S_g V_p}{V} \]
\[ \phi_{wc} = \frac{S_w V_p}{V - S_g V_p} \]
\[ \phi_w = (1 - \phi_g) \phi_{wc} = \frac{S_w V_p}{V} \]
\[ e = \frac{S_w V_p}{V - V_p} \]
\[ \phi_s = 1 - \frac{V_p}{V} \]

where

- \( \phi_{wc} \) is the water porosity in the water-clay system considered separately,
- \( \phi_g \) is the gas porosity,
- \( \phi_s \) is the solid volume fraction,

as described for the GAMBIT-GW model in subsection 5.1.

Assuming that the volumetric strain, \( \Delta V/V \), is zero, the equation for conservation of the pore water (i.e. Equation 3.21) becomes:
If the permeability tensor for the pore fluid is a constant, scalar quantity, and any effects of the acceleration due to gravity can be ignored, then this equation is the same in both the GAMBIT-GWS model and the GAMBIT-GW model.

Similarly, the equation for conservation of the gas phase (i.e. Equation 3.29), assuming in addition that:

a) \( k_{g,j} \) is a scalar quantity, that is \( k_{g,j} = k_{g,0} \delta_{ij} \);

b) \( H_g \) is infinite, that is no gas dissolves in the pore water;

becomes:

\[
- \frac{\partial}{\partial x_j} \left( - \rho_g \mu_g k_{g,0} \frac{\partial p_g}{\partial x_j} \right) = \frac{1}{V} \frac{D(\rho_g S_g V_p)}{Dt} = \frac{D(\rho_g \phi_g)}{Dt} .
\]  

This equation is the same in both models, provided that \( k_{g,0} = C_1 (S_{g} - C_2)^2 \), where, using notation from the GAMBIT-GW model, \( C_1 \) and \( C_2 \) are constants defined by:

\[
C_1 = \frac{1}{\sqrt{8\pi n_c}} \frac{V_p}{V} ,
\]
\[
C_2 = \frac{1}{\sqrt{8\pi n_c}} \phi_{gc} .
\]

3.2 Numerical Implementation using ENTWIFE

The GAMBIT-GWS model, described in subsection 3.1.2, was implemented using the Serco Assurance computer program ENTWIFE.

At the outset of this study the intention was to implement the GAMBIT-GWS model using a pre-existing sophisticated finite-element program called FEAT (Finite Element Analysis Toolbox). FEAT is designed to solve coupled problems in stress analysis, fluid flow, including flows in porous media, and heat transfer. In the UK nuclear industry, both British Energy and BNFL Magnox have used FEAT extensively. However, the attempt to incorporate the GAMBIT-GWS model into FEAT (see Appendix C) was unsuccessful.
An alternative approach, using the program ENTWIFE, is described in this section.

### 3.2.1 ENTWIFE

ENTWIFE is a finite-element program that was developed originally to study fluid flows of relevance to the UK nuclear industry, and to the fast reactor programme in particular. Many fluid flows in the fast reactor programme were influenced strongly by buoyancy, and the particular numerical difficulties associated with these flows provided the impetus for the development of some of the features in ENTWIFE. The program, in particular, has a number of facilities that allow difficult non-linear problems to be analysed. One of the characteristic features of a non-linear problem is that it is possible to find multiple steady-state solutions. ENTWIFE has algorithms for analysing problems of this kind that can assess the stability of a given steady-state solution to determine if the solution might be observed experimentally, and can identify the conditions under which the number of solutions (‘bifurcation points’) might change.

These algorithms are quite sophisticated, and require the solution of systems of equations that are extensions of those governing the physical model [Cliffe et al., 2000]. The implementation of the algorithms requires the analytic computation of various functional derivatives of the equations before the results can be coded in Fortran. The analytic computations in principle are straightforward, involving only standard techniques from differential calculus. However, in practice they are time consuming and prone to human error. This would not have been an issue if ENTWIFE had been used to solve only one set of equations, since the computations would have had to be done only once. However, there was a need to apply the algorithms in ENTWIFE to a number of different problems, each with its own set of equations. Therefore, the difficulties associated with the analytic computations had to be addressed.

Two crucial observations were made which influenced the subsequent development of ENTWIFE. The first observation was that the techniques used to solve the various extended systems of equations could be implemented in a way that separated the complexities inherent in the algorithms from the details of the equations being solved. Thus, the algorithms could be programmed once and for all, and then applied to different problems via a straightforward interface to sets of Fortran subroutines which depended only on the equations to be solved and not on the algorithm. The second observation was that the Fortran subroutines for a specific problem could be generated automatically using a symbolic computer algebra tool. This circumvented the difficulties associated with the analytic computations referred to above [Cliffe and Tavener, 2000].

There are a number of commercial, symbolic computer algebra tools that can carry out all of the necessary computations, and even produce the Fortran subroutines. In particular, ENTWIFE has a pre-processor with an interface to either Mathematica or Maple (two commercial programs that support symbolic computer algebra).
A new problem is described using either Mathematica or Maple to input the ‘weak form’ of the equations governing the physical model. (The input format closely resembles standard mathematical notation; e.g. the Mathematica input file for the GAMBIT-GWS model is given in the Appendix D.) Next, the pre-processor is run to produce the relevant set of Fortran routines, which are compiled and included in ENTOIFE at run time. The process is both efficient, in terms of time required to code up a new problem, and reliable.

The pre-processor, using symbolic computer algebra, makes ENTOIFE an extremely powerful tool for investigating new physical models; this feature of ENTOIFE proved particularly valuable when implementing the GAMBIT-GWS model.

ENTOIFE has several other features relevant to this study, and these are now described:

a) A wide range of finite-element types (i.e. more than 50) is available. It is easy to change the element and the interpolation scheme being used for the variables in a problem.

b) The Gauss scheme used to evaluate the integrals appearing in the weak form can be changed. ENTOIFE has a number of Gauss schemes available, and it is easy to implement new schemes.

c) ENTOIFE has a number of different algorithms for ‘time stepping’. For example, Crank-Nicholson and backward Euler methods are available, as well as Gear’s method. Gear’s method [Byrne and Hindmarsh, 1975] uses backward differences, and adjusts dynamically both the order of the difference method and the time step size in an attempt to minimise the computational time needed to achieve a given accuracy. Error estimation is carried out using a predictor-corrector technique.

d) The user interface to ENTOIFE is via the TGIN input language, which is also used by other Serco Assurance computer programs (e.g. NAMMU). Grids can be generated easily, and the program has a range of output options.

ENTOIFE is developed under an ISO9001 approved quality system.

3.2.2 Development of numerical approach

In this subsection, the development of a numerical approach to solve the GAMBIT-GWS model is described.

An initial attempt was made to implement the GAMBIT-GWS model using the computer program FEAT (see Appendix C). FEAT:

a) Uses the standard Galerkin version of the finite-element method, as far as possible (i.e. the same finite-element basis functions are used both to
approximate the dependent variables in the problem and to act as test functions in the weak form of the equations).

b) Has a limited range of finite-element types, which are suited to its usual domain of application. Variables, for the most part, are approximated using continuous quadratic interpolation.

When the underlying problem is sufficiently well behaved, accurate answers are obtained using these high order methods.

The standard Galerkin finite-element method may be thought of as equivalent to ‘central differencing’ in a finite-difference method. A characteristic of the standard Galerkin method is that it gives excellent results provided the problem is well behaved and, crucially, the grid is fine enough to resolve the features present in the solution. If these conditions do not hold then the method can give poor results. Typically, unphysical oscillations (‘wiggles’) appear in the results. Under many circumstances the ‘wiggles’ are not troublesome, and simply indicate that the results are inaccurate. This point of view was advocated strongly by Gresho and Lee [1981], and, by and large, is the philosophy underlying programs such as FEAT and ENTWIFE.

However, there are circumstances in which the ‘wiggles’, to which the standard Galerkin method is susceptible, can be a problem. For a highly non-linear problem, the unphysical oscillations can lead to spurious non-linear feedback, causing numerical instability and, possibly, unphysical values of variables (e.g. negative gas pressure in the GAMBIT-GWS model). The symptoms of this are that either it proves impossible to obtain a converged solution, or, in a transient calculation, the time step becomes smaller and smaller in order to meet the specified accuracy criterion. Either behaviour is undesirable. In some cases it is possible to refine the grid to the point where the standard Galerkin method again performs well, but in others the grid required would be so fine as to be prohibitively expensive.

The lack of success in incorporating the GAMBIT-GWS model into FEAT is, it is thought, due to the shortcoming of the standard Galerkin method described above. Any finite-element program based on the standard Galerkin method would have encountered the same difficulties. The rest of this subsection explicates where the numerical problems in the GAMBIT-GWS model lie, and describes a numerical method to overcome the problems.

GAMBIT-GWS is a complicated mathematical model, being a coupled system of equations governing the non-linear mechanical response of the clay, regarded as a porous elastic medium, and the flows of water and gas in the clay. The complete system of equations is too complicated to allow an analytical treatment, which is why a numerical approach is required in the first place. However, this means it is difficult to analyse the source of numerical difficulties when they are encountered. Therefore, here the GAMBIT-GWS model is simplified. Of course, in making the simplification some
of the essential features of the problem are lost, but the object of the exercise is not to produce a good approximation to the model, but rather to identify the source of the numerical difficulties encountered.

A key observation is that the GAMBIT-GWS model is just an extension of Biot’s poroelastic model, for which the standard Galerkin finite-element method performs well. Figures 3.1 and 3.2, for example, show a comparison of finite-element results obtained using ENTWIFE and an exact analytic solution to Biot’s poroelastic model. The problem considered is consolidation of a one-dimensional column of a saturated porous medium. The column is initially at equilibrium, and then a constant load is applied to the top surface. It is assumed that the load is applied via a porous plug, so that pore water can drain freely from the top of the column. The bottom of the column is impermeable. The load squeezes water out through the top surface, and the column ‘consolidates’ as a result. *Jaeger and Cook [1976]* give the analytic solution for this problem.

Figure 3.1 compares numerical and analytical results for the displacement of the top of the column, and Figure 3.2 compares the pressure at the bottom of the column. It is clear that the finite-element results are in good agreement with the analytical results. (There are some discrepancies in Figure 3.2 at large times, when the pressure has decreased almost to zero. Noting that logarithmic scales are used, the discrepancies are small and not significant.)

*Figure 3.1* Comparison of ENTWIFE results (green +) for the displacement of the top of a consolidating one-dimensional column of a saturated porous medium with the analytic solution (red line).
The fact that the standard Galerkin finite-element method performs so well for Biot’s poroelastic model suggests that in the GAMBIT-GWS model the source of the numerical difficulties lies in the gas equation, and its couplings to the mechanical response of the clay and to the flow of water. Therefore, a simplified model of the gas transport was abstracted from the GAMBIT-GWS model. It must be stressed that the purpose was not to produce a simplified version of the GAMBIT-GWS model for use in modelling experiments, but to encapsulate the essential numerical difficulties in a simple model that could be studied both numerically and theoretically.

**Simplified model of the gas transport**

The simplified model of the gas transport is:

\[
\frac{\partial p_g}{\partial t} = \frac{\partial}{\partial x_i} \left( k(p_g) \frac{\partial p_g}{\partial x_i} \right)
\]

(3.51)

For small values of the gas pressure, \( p_g \), the function \( k \) should just equal the diffusion coefficient of the gas in the liquid phase, but for large values of the gas pressure \( k \) should represent the flow of ‘free’ gas, so that:

\[
k(p_g) \approx p_g k_g
\]

(3.52)
where \( k_g \) is the gas permeability. The full prescription for \( k \) is:

\[
\begin{align*}
k(p_g) &= D & \text{for } p_g < p_1 \\
k(p_g) &= D \left( 1 - f \left( \frac{p_g - p_1}{p_2 - p_1} \right) \right) + p_g k_g \left( \frac{p_g - p_1}{p_2 - p_1} \right) & \text{for } p_1 \leq p_g \leq p_2 , \quad (3.53) \\
k(p_g) &= p_g k_g & \text{for } p_2 < p_g
\end{align*}
\]

where \( f \) is any monotonically increasing function, defined on the interval \([0,1]\), such that:

\[
\begin{align*}
f(0) &= 0 & f'(0) &= 0 \\
f(1) &= 1 & f'(1) &= 0 . \quad (3.54)
\end{align*}
\]

Thus, Equation (3.51) represents the movement of gas by diffusion through the pore water for values of \( p_g \) below a lower threshold value, \( p_1 \), and represents the flow of ‘free’ gas for values of \( p_g \) above an upper threshold value, \( p_2 \). The exact details of the transition region, \( p_1 \leq p_g \leq p_2 \), will subsequently be shown to be unimportant, which is why the function \( f \) has not been specified more fully.

In the GAMBIT-GWS model, the transition to ‘free’ gas flow occurs when the gas pressure exceeds a value that is determined by the effective stress field. For gas pressures above the threshold, the permeability to gas depends on the saturation, which, in turn, depends on the history of the stress field, and the pressures in the liquid and gas phases. The simplified model does not capture the detail of these complicated interactions, but does have the essential feature that when the gas pressure exceeds a threshold the gas can flow much more quickly. It is the rapid change in \( k \) as a function of gas pressure close to the threshold that is thought to be the source of the numerical difficulties in the GAMBIT-GWS model.

(Note that a number of other simplifications have been made in Equation 3.51, e.g. neglecting variations in the porosity and the advection of dissolved gas in the water.)

**Solution of the simplified model**

Under fairly mild assumptions, a class of solutions to Equation (3.51) can be obtained.

Consider Equation (3.51) in one dimension but referred to a moving frame of reference. In particular, define a new co-ordinate, \( y \), given in terms of \( x \) and \( t \) by:

\[
y = x - vt , \quad (3.55)
\]

where \( v \) is the velocity of the moving frame. In terms of \( y \), Equation (3.51) becomes:
\[
\frac{\partial p_g}{\partial t} = v \frac{\partial p_g}{\partial y} + \frac{\partial}{\partial y} \left( k(p_g) \frac{\partial p_g}{\partial y} \right) .
\]  
(3.56)

Solutions to this equation for which \( p_g \) does not depend on time are sought\(^{10}\), that is:

\[
0 = v \frac{\partial p_g}{\partial y} + \frac{\partial}{\partial y} \left( k(p_g) \frac{\partial p_g}{\partial y} \right) .
\]  
(3.57)

This equation can be integrated once to give:

\[
v p_g + k(p_g) \frac{\partial p_g}{\partial y} = c_1 ,
\]  
(3.58)

where \( c_1 \) is an arbitrary constant.

Assume next that far ahead of the travelling wave the gas pressure is constant, and its value, \( p_0 \), is below the threshold value \( p_1 \). It follows that:

\[
v p_0 = c_1 ,
\]  
(3.59)

and so Equation (3.58) can be written as:

\[
v(p_g - p_0) + k(p_g) \frac{\partial p_g}{\partial y} = 0 .
\]  
(3.60)

This equation can be integrated to give the solution in implicit form, as:

\[
y = \int \frac{k(p_g)}{v(p_0 - p_g)} dp_g .
\]  
(3.61)

Ahead of the wave, the solution takes the form:

\[
\ln \left( \frac{p_g - p_0}{p_1 - p_0} \right) = - \frac{v}{D} (y - y_1) ,
\]  
(3.62)

and behind the wave, the solution is:

\[
p_g - p_2 + p_0 \ln \left( \frac{p_g - p_0}{p_2 - p_0} \right) = \frac{v}{k_g} (y_2 - y) ,
\]  
(3.63)

\(^{10}\) If such solutions exist, they would correspond to profiles of gas pressure that move at velocity \( v \) without changing their shape. Such solutions are called travelling waves.
where the co-ordinate system has been chosen such that the gas pressure at \( y = y_1 \) is the lower threshold value, \( p_1 \), and at \( y = y_2 \) is the upper threshold value, \( p_2 \). \( y_1 \) and \( y_2 \) are connected by:

\[
y_2 - y_1 = \frac{p_2}{p_1} \int_{p_1}^{p_2} \frac{k(p_g)}{v(p_0 - p_g)} dp_g .
\]  

(3.64)

For large negative values of \( y \), i.e. far behind the travelling wave, Equation (3.63) shows that the gas pressure is proportional to \( y \). If the gas permeability is large, the gradient in gas pressure behind the travelling wave is small and is given approximately by:

\[
\frac{\partial p_g}{\partial y} \approx -\frac{v}{k_g} \left( \frac{p_2 - p_0}{p_2} \right) \quad \text{for } y < y_2 .
\]  

(3.65)

Thus, there is indeed a travelling wave solution to Equation (3.51). This corresponds to gas moving into a region where the gas pressure is below the threshold for the formation of gas porosity. Behind the travelling wave the gradient in gas pressure is approximately constant, and the speed of the wave is:

\[
v = -k_g \left( \frac{p_2}{p_2 - p_0} \right) \frac{\partial p_g}{\partial y} .
\]  

(3.66)

If such a travelling wave is to occur, the boundary conditions at the inlet must be compatible with a constant pressure gradient in the region behind the wave. Even if this condition were not satisfied one still would expect to see a wave move across the region, but with a velocity that depends on the boundary condition.

The following observations can be made about the travelling wave solution presented above:

a) The speed of the travelling wave does not depend on the diffusion coefficient, \( D \), of the gas in the liquid phase.

b) The speed of the travelling wave does not depend on the detail of the variation of \( k \) with \( p_g \) in the transition region, \( p_1 \leq p_g \leq p_2 \). The only effect of changing this dependence is to shift the origin, \( y_2 \), for the variation of \( p_g \) behind the travelling wave in Equation (3.63).

c) The travelling wave solution is very ‘steep’ in the transition region, \( p_1 \leq p_g \leq p_2 \). The abruptness of the change in \( p_g \) depends on the ratio of the gas permeability, \( k_g \), to the diffusion coefficient, \( D \), of the gas in the liquid phase, and this can be very large indeed.
It now is clear where the difficulties with the standard Galerkin finite-element method lie. When gas is injected into a sample of clay that initially does not have any ‘free’ gas, a pressure wave moves through the clay. This wave has a very sharp front as the gas pressure, \( p_g \), increases in the transition region, \( p_1 \leq p_g \leq p_2 \). The distance over which this increase takes place is proportional to the ratio of the gas permeability, \( k_g \), to the diffusion coefficient, \( D \), of the gas in the liquid phase, which can be very small indeed, typically \( 10^8 \). It would be virtually impossible to resolve this front, even if adaptive meshing techniques were employed. When trying to resolve this front with the standard Galerkin finite-element method, large, unphysical oscillations are produced that lead to numerical instability. In short, the problem is too hard for the standard Galerkin finite-element method.

However, since the speed of the travelling wave is insensitive to how the gas pressure varies near the front, it should be possible to develop a numerical method that captures the front in a few finite elements and that still has the front moving at the correct speed.

**Maximum principle**

Equation (3.51) belongs to the class of non-linear parabolic differential equations for which it is possible to show powerful maximum principles hold. In a classical reference for the subject, Protter and Weinberger [1967] describe many results of this kind. The main result of relevance here (i.e. Theorem 12), can, for the one-dimensional case, be stated as follows:

\[
\begin{align*}
\text{For any solution, } p_g, \text{ to Equation (3.51), the maximum and minimum values must occur either at the initial time or on the boundary.}
\end{align*}
\]

This maximum principle shows that the solution to Equation (3.51) should not suffer from spatial oscillations or unphysical negative values of gas pressure.

The key to designing a good numerical method for this problem is to ensure that the discretisation preserves the maximum principle of the original equation. A discrete maximum principle would stop the solution from suffering unphysical spatial oscillations, and it should be possible to get the speed of the gas front right because it is insensitive to how the gas pressure varies near the front.


Consider the discretisation of Equation (3.51) on a regular mesh in one dimension. Let the gas pressure at node \( i \) and time \( n \) be denoted by \( p^{n}_{i} \). For a numerical method that uses linear finite-elements and \( m \) time levels, the equation at node \( i \) for the time-step that advances the solution to time \( n \) can be written as:
For a problem with rapid variations in the variables that are difficult to resolve, higher order methods often are not as accurate as lower order methods, and therefore only linear finite-elements will be considered here. A higher order discretisation of Equation (3.51) would involve terms in $p_{i-2}^n$, $p_{i+2}^n$, etc.)

The **Discrete Maximum / Minimum Principle** theorem may be stated as follows:

Let $p_i^n$ be the solution to the discretisation (i.e. Equation 3.67) arising from Equation (3.51). If at each point $(i, n)$ of the space-time mesh the coefficients in Equation (3.67) satisfy the following three conditions:

a) All of the coefficients except $\alpha_{i,n}$ are non-positive;

b) At least one of the coefficients is strictly negative;

c) The sum of all of the coefficients is zero;

then the maximum and minimum values of $p_i^n$ are attained either at the initial time or on the boundary.

This theorem is a simple extension of Theorem 3.5 in the book by *Braess* [1977]. (The proof is not given here.)

The equations arising from the standard Galerkin finite-element method do not satisfy the conditions of this theorem, and that is the cause of its poor performance. (The problem is that the discretisation of the time derivative involves the gas pressure at neighbouring spatial points; essentially, the discrete form of this term is related to the finite-element mass matrix.) What is required is a numerical method in which the discretisation of the time derivative involves the gas pressure only at node $i$ (i.e. a method with a diagonal mass matrix). This can be achieved by using the nodal integration scheme to produce the discrete equations, rather than the standard Gaussian integration scheme. The nodal integration scheme only requires the basis function at the nodal points, and this means that it gives rise to a discretisation with a diagonal mass matrix. On a uniform mesh in one-dimension, the nodal integration scheme, when combined with a first-order backward Euler time-stepping scheme, gives the following discrete equations:
\[
0 = \lambda \left( p_i^n - p_{i-1}^{n-1} \right) \\
- \left( k \left( p_{i-1}^n \right) + k \left( p_i^n \right) \right) p_{i-1}^n \\
+ \left( k \left( p_{i-1}^n \right) + 2k \left( p_i^n \right) + k \left( p_{i+1}^n \right) \right) p_i^n \\
- \left( k \left( p_i^n \right) + k \left( p_{i+1}^n \right) \right) p_{i+1}^n
\]

(3.68)

where:

\[
\lambda = \frac{8 \Delta x^2}{\Delta t}.
\]

(3.69)

It is easy to verify that the conditions of the **Discrete Maximum / Minimum Principle** theorem are satisfied by the discretisation given in Equations (3.68) and (3.69). It is also possible to show (although the algebraic details become messy) that the theorem applies:

a) In two-dimensions;

b) When non-uniform meshes are used; and

c) When \( k \) is replaced by a positive-definite, second-rank tensor.

Note that the ostensibly more accurate Crank-Nicholson time-stepping algorithm does not satisfy the conditions of the theorem unless the time-step is sufficiently small (for the test cases discussed below, that was found to be very small indeed), and therefore is not expected to perform well.

To summarise, the discretisation of Equation (3.51) using:

a) Linear finite-elements;

b) The nodal quadrature scheme; and

c) A first-order backward Euler time-stepping scheme;

satisfies the discrete maximum / minimum principle. This scheme does not suffer from the spatial oscillations of the standard Galerkin finite-element method, and so is much more robust. For realistic values of the parameters no numerical scheme can be expected to resolve the details of the behaviour near the gas pressure front, but it turns out that this scheme is otherwise surprisingly accurate.

**Test cases**

The results for a set of test cases will now be described. All the calculations were carried out on a one-dimensional grid of length 1 m. The gas pressure was initially set to 1 Pa everywhere, and at the left-hand boundary of the mesh the gas pressure gradient
was set to a value that would lead to a speed for the travelling wave of 10 m$^{-1}$. The upper threshold value of the gas pressure, $p_t$, was set to 10 Pa. The function $f$ appearing in the specification of $k$ was represented by a quintic polynomial satisfying Equation (3.54). Transient calculations were performed using a first-order backward Euler predictor-corrector method, in which the time-step was chosen to maintain a relative accuracy of $10^{-3}$. The other parameters varied from case to case.

For the first run, the values of the diffusion coefficient of the gas in the liquid phase and the gas permeability were set to $10^{-2}$ ms$^{-2}$ and $10^2$ m$^2$ respectively; the lower threshold value of the gas pressure, $p_l$, was set to 9.5 Pa. A mesh of 100 finite-elements was used.

Figure 3.3 shows profiles of the gas pressure at time intervals of 0.01s.

![Pressure profile](image)

**Figure 3.3** Gas pressure profiles at time intervals of 0.01s.

The profiles all look very similar, and appear to move about $1/10^6$ of the length of the grid in an interval of 0.01s, which is consistent with the theory presented above.

To measure the speed more accurately, the position at which the pressure was equal to 5 Pa was determined for each profile. The results are shown in Figure 3.4.
Listance travelled by the gas pressure front as a function of time. The dots are the computed values, and the straight line is a best fit to these values to determine the speed of the wave.

These results confirm that the travelling wave is indeed moving with constant speed to a good approximation. A straight line fit to the data, also shown in Figure 3.4, has slope 9.984 ms\(^{-1}\), which gives an error for the computed front speed of 0.16%. It appears that the front is captured over two or three finite-elements, which is not adequate to resolve the details of the variation in gas pressure. Nevertheless, the speed of the gas front is in remarkably good agreement with the analytical value.

A number of further calculations were carried out to check that the travelling wave speed was independent of:

a) The diffusion coefficient of the gas in the liquid phase;

b) The gas permeability (provided the gas pressure gradient at the inlet was suitably adjusted);

c) The lower threshold value of the gas pressure, \( p_L \); and

d) The number of finite-elements in the mesh.

To check for grid independence, additional calculations were performed with 200 finite-elements for all cases, and with 25 and 50 finite-elements for the first case.

In all cases, the error was much less than 1%, confirming that the numerical scheme used predicts the travelling wave speed to a high degree of accuracy over a wide range of parameters. The results of all the calculations are summarised in Table 3.1.
Table 3.1 Summary of Test Calculations Performed Using a Nodal Quadrature Scheme for the Simplified Model of Gas Transport.

<table>
<thead>
<tr>
<th>Run</th>
<th>$D$</th>
<th>$k_g$</th>
<th>$p_i$</th>
<th>Number of Elements</th>
<th>% Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$10^{-2}$</td>
<td>$10^0$</td>
<td>9.5</td>
<td>100</td>
<td>0.16</td>
</tr>
<tr>
<td>2</td>
<td>$10^{-2}$</td>
<td>$10^0$</td>
<td>9.5</td>
<td>200</td>
<td>0.22</td>
</tr>
<tr>
<td>3</td>
<td>$10^{-4}$</td>
<td>$10^0$</td>
<td>9.5</td>
<td>100</td>
<td>0.13</td>
</tr>
<tr>
<td>4</td>
<td>$10^{-4}$</td>
<td>$10^0$</td>
<td>9.5</td>
<td>200</td>
<td>0.15</td>
</tr>
<tr>
<td>5</td>
<td>$10^{-2}$</td>
<td>$10^0$</td>
<td>9.9</td>
<td>100</td>
<td>0.53</td>
</tr>
<tr>
<td>6</td>
<td>$10^{-2}$</td>
<td>$10^0$</td>
<td>9.9</td>
<td>200</td>
<td>0.50</td>
</tr>
<tr>
<td>7</td>
<td>$10^{-2}$</td>
<td>$10^2$</td>
<td>9.9</td>
<td>100</td>
<td>0.01</td>
</tr>
<tr>
<td>8</td>
<td>$10^{-2}$</td>
<td>$10^2$</td>
<td>9.9</td>
<td>200</td>
<td>0.01</td>
</tr>
<tr>
<td>9</td>
<td>$10^{-4}$</td>
<td>$10^3$</td>
<td>9.9</td>
<td>100</td>
<td>0.05</td>
</tr>
<tr>
<td>10</td>
<td>$10^{-4}$</td>
<td>$10^3$</td>
<td>9.9</td>
<td>200</td>
<td>0.06</td>
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<tr>
<td>11</td>
<td>$10^{-2}$</td>
<td>$10^0$</td>
<td>9.5</td>
<td>50</td>
<td>0.20</td>
</tr>
<tr>
<td>12</td>
<td>$10^{-2}$</td>
<td>$10^0$</td>
<td>9.5</td>
<td>25</td>
<td>0.04</td>
</tr>
</tbody>
</table>

Given the difficulty of the problem, it seems that the numerical scheme developed here performs remarkably well, and can be used with confidence for the full GAMBIT-GWS model.

3.3 Further Numerical Issues

At this stage a conceptual model of gas migration in bentonite (subsection 3.1.2) and a numerical approach for tracking a sharp gas front as it propagates (subsection 3.2) have been developed.

Next the GAMBIT-GWS model was implemented using the Serco Assurance computer program ENTWIFE (Release 7.2). Further numerical issues that arose in the course of the implementation included:

a) The Heaviside step function, $\theta(x)$, that appears repeatedly in the definition of the elastic modulus $\tilde{R}_m$ (see Equation 3.38) had to be smoothed. The following smooth approximation to $\theta$ was used:

$$\theta(x) = \frac{1}{1 + \exp\left(-\frac{2x}{\varepsilon}\right)}, \quad (3.70)$$
where \( \varepsilon \) is a parameter that gives the scale over which \( \theta \) ‘switches on’.

b) The equation for the evolution of gas saturation, \( S_g \), (see Equation 3.19) was better scaled, and also avoided problems due to \( S_g \) going out of range, if the independent variable was chosen to be \( G \), where:

\[
S_g = \frac{1}{1 + \exp(-2G)} .
\]  

(3.71)

c) The equation for the evolution of the gas permeability, \( k_g \), (see Equations 3.39 and 3.40) was better scaled if it was rewritten using the logarithm of the gas permeability tensor.

d) A ‘reservoir’ boundary condition had to be developed. This boundary condition applies over that part of the bentonite surface where gas is injected, and sets:

\[
\frac{\partial (p_g V_R(t))}{\partial t} = F_{in}(t) - F_{out} .
\]  

(3.72)

Here:

\( V_R \) is the volume of gas in the ‘reservoir’ [m\(^3\)];
\( F_{in} \) is the flow of any gas added to the ‘reservoir’ [J s\(^{-1}\)];
\( F_{out} \) is the flow of gas out of the ‘reservoir’ into the clay [J s\(^{-1}\)].

\( V_R \) and \( F_{in} \) are assumed to have a known dependence on time; \( F_{out} \) is calculated by carrying out a surface integral of the flux of gas into the bentonite:

\[
F_{out} = \int\limits_{\Omega} dA \cdot \mathbf{f}
\]

\[
-\mathbf{f} = \frac{R_g T}{H_g} \left( p_g q_i - S_w \phi \frac{d_m}{\tau} \frac{\partial p_g}{\partial x_i} \right) - \frac{k_{g,ij}}{\mu_g} \left( \frac{\partial p_g}{\partial x_j} + \rho_g \frac{\partial \rho_g}{\partial x_j} \right).
\]  

(3.73)

Here:

\( \Omega \) is the part of the clay surface that is in contact with the ‘reservoir’;
\( dA \) is an area element with normal directed outwards (i.e. from the clay to the ‘reservoir’) [m\(^2\)];
\( \mathbf{f} \) is the flux of gas (see Equation 3.29) [J m\(^{-2}\) s\(^{-1}\)].

\[\text{11} \] The flow is written in this form to avoid repetitious appearance of the factor \( R_g T \) in the equations. The molar flow in is simply \( F_{in}/R_g T \). Similarly for the molar flow out.
In addition, a set of graphical output options was developed. The commands:

- DRAW LINE GRAPH, used to draw a line graph showing the spatial variation of a scalar between two points in the model;
- PLOT CONTOURS, used to plot contours of a scalar;
- PLOT GRID, used to plot the finite-element grid;
- PLOT TENSORS, used to plot a tensor field;
- PLOT TIME EVOLUTION, used to plot the evolution of a scalar at a point in the model;
- PLOT VECTORS, used to plot a vector field;

can be used to plot the following variables:

- The DISPLACEMENT VECTOR or a component;
- The STRESS TENSOR or a component / a principal component / a stress invariant (e.g. the Von Mises stress);
- The EFFECTIVE STRESS TENSOR or a component / a principal component / a stress invariant;
- The POROSITY;
- The LIQUID DENSITY;
- The LIQUID SATURATION;
- The FILTRATION VELOCITY or a component / a principal component;
- The LIQUID MASS FLUX or a component / a principal component;
- The LIQUID PRESSURE;
- The GAS PROPAGATION CRITERION;
- The GAS SATURATION;
- The GAS PERMEABILITY TENSOR or a component / a principal component;
- The GAS MASS FLUX or a component / a principal component;
- The GAS PRESSURE.
3.4 Application to the Modelling of Experimental Data

The GAMBIT-GWS model requires a number of parameters (see Table 3.2) to describe the behaviour of the bentonite, which is assumed to have homogeneous and isotropic properties. Some of these parameters can be related to measured material properties of either the clay (see subsection 3.4.1) or the fluids. For others there are no data available, and these parameters can be adjusted to optimise the fit between calculated and observed behaviour.

The GAMBIT-GWS model has fitting parameters that include $\tilde{R}_1$, $\tilde{R}_2$, and $k_o$, $S_{g_{c}}$, $S_{g_{r}}$. Note that:

a) $\tilde{R}_1$ determines how quickly gas-phase saturation is first created (Equation 3.38). The process involves compression of the pore water by the gas, and occurs quickly compared to the rate at which the pore water can drain from the clay. It therefore seems plausible to take $\tilde{R}_1 \approx \frac{1}{\phi \beta_w}$.

b) $\tilde{R}_2$ determines after breakthrough how quickly the gas-phase saturation responds to a change in matric suction (Equation 3.38). Its value has to be determined experimentally.

c) For Experiment Mx80-4A, at breakthrough the permeability to the gas phase is $\sim 10^{-20}$ m$^2$ [Nash et al., 1998], and the corresponding gas-phase saturation is $S_g \sim 10^{-20} k_0$ (see Equation 3.40). This gas-phase saturation has to be able to produce changes in the pressure of the pore water of order megapascals, which, assuming that the gas-phase saturation is created by compressing the pore water, implies $S_g \beta_w > 1$ MPa. These observations suggest that the gas-phase saturation at breakthrough should be $S_g > 5 \times 10^{-4}$, and therefore the gas permeability parameter should be $k_o < 4 \times 10^{-14}$ m$^2$.

d) The critical gas saturation at which flow ceases was chosen to be more than an order of magnitude less than the peak gas saturation, i.e. $S_{g_{c}} = 10^{-5}$.

e) The irreducible gas saturation was chosen to be an order of magnitude less than the critical gas saturation, i.e. $S_{g_{r}} = 10^{-6}$.

Guided by these thoughts, the data for Experiment Mx80-4A are used to determine values for the parameters $\tilde{R}_1$, $\tilde{R}_2$ and $k_o$ (subsection 3.4.2). These parameters are then used in simulations of Experiment Mx80-8 (subsection 3.4.3) and of a canister-scale system (subsection 4).
Table 3.2 Parameters in the GAMBIT-GWS model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value / Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Void ratio</td>
<td>$e$</td>
<td>See subsection 3.4.1</td>
</tr>
<tr>
<td>Young’s modulus</td>
<td>$E$</td>
<td>See subsection 3.4.1</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>$\nu$</td>
<td>See subsection 3.4.1</td>
</tr>
<tr>
<td>Clay modulus to suction</td>
<td>$\tilde{H}_m$</td>
<td>0 Pa</td>
</tr>
<tr>
<td>Gas modulus to suction</td>
<td>$\tilde{R}_g$</td>
<td>A model fitting parameter</td>
</tr>
<tr>
<td>Liquid reference density</td>
<td>$\rho_0$</td>
<td>$10^3$ kg m$^{-3}$</td>
</tr>
<tr>
<td>Liquid reference pressure</td>
<td>$p_0$</td>
<td>$1.01325 \times 10^5$ Pa</td>
</tr>
<tr>
<td>Liquid compressibility</td>
<td>$\beta_w$</td>
<td>$5 \times 10^{-10}$ Pa$^{-1}$</td>
</tr>
<tr>
<td>Liquid viscosity</td>
<td>$\mu_w$</td>
<td>$10^{-3}$ Pa s</td>
</tr>
<tr>
<td>Initial porosity</td>
<td>$\phi_0$</td>
<td>$e/(1 + e)$</td>
</tr>
<tr>
<td>Liquid permeability</td>
<td>$k_w$</td>
<td>See subsection 3.4.1</td>
</tr>
<tr>
<td>Acceleration of gravity</td>
<td>$g$</td>
<td>0 m s$^{-2}$ or 9.81 m s$^{-2}$</td>
</tr>
<tr>
<td>Gas molar mass</td>
<td>$M_g$</td>
<td>$4 \times 10^{-3}$ kg mol$^{-1}$</td>
</tr>
<tr>
<td>Ideal gas constant</td>
<td>$R_g$</td>
<td>8.31434 J K$^{-1}$ mol$^{-1}$</td>
</tr>
<tr>
<td>Temperature</td>
<td>$T$</td>
<td>293.15 K</td>
</tr>
<tr>
<td>Gas viscosity</td>
<td>$\mu_g$</td>
<td>$2 \times 10^{-5}$ Pa s</td>
</tr>
<tr>
<td>Henry’s constant</td>
<td>$H_g$</td>
<td>$1 / 3.5 \times 10^{-6}$ Pa mol$^{-1}$ m$^3$</td>
</tr>
<tr>
<td>Gas molecular diffusion</td>
<td>$d_m$</td>
<td>$10^{-9}$ m$^2$ s$^{-1}$</td>
</tr>
<tr>
<td>Tortuosity</td>
<td>$\tau$</td>
<td>10</td>
</tr>
<tr>
<td>Gas permeability parameter</td>
<td>$k_0$</td>
<td>A model fitting parameter (see Equation 3.40)</td>
</tr>
<tr>
<td>Critical gas saturation</td>
<td>$S_{g,c}$</td>
<td>$10^{-5}$</td>
</tr>
<tr>
<td>Irreducible gas saturation</td>
<td>$S_{g,i}$</td>
<td>$10^{-6}$</td>
</tr>
<tr>
<td>Smooth log$_e(S_g)$</td>
<td>$\epsilon_{S_g}$</td>
<td>$2 \times 10^{-1}$ (see Equation 3.70)</td>
</tr>
<tr>
<td>Gas modulus for fracture</td>
<td>$\tilde{R}_f$</td>
<td>A model fitting parameter</td>
</tr>
<tr>
<td>Clay tensile strength</td>
<td>$\tau_c$</td>
<td>0 Pa</td>
</tr>
<tr>
<td>‘Surface tension’</td>
<td>$\Sigma$</td>
<td>0 Pa m</td>
</tr>
<tr>
<td>Smooth $p_g$</td>
<td>$\epsilon_{p_g}$</td>
<td>$10^{-4}$ Pa (see Equation 3.70)</td>
</tr>
<tr>
<td>Applied load</td>
<td>–</td>
<td>See subsection 3.4.1</td>
</tr>
<tr>
<td>Applied fluid pressure</td>
<td>–</td>
<td>A model dependent parameter</td>
</tr>
</tbody>
</table>
3.4.1 Measured properties of bentonite

Material properties of bentonite that have been studied experimentally include swelling pressure, Young’s modulus and Poisson’s ratio, and permeability to liquid.

Swelling pressure

Börgesson et al. [1995, 1996] measured the relationship between swelling pressure, \( \Pi_s \), and void ratio, \( e \), for saturated bentonite, and fitted their experimental data with the function:

\[
\Pi_s = \frac{\alpha_s}{e^\gamma_s}.
\]  

(3.74)

The fitted values of \( \alpha_s \) and \( \gamma_s \) were 2 MPa and 5.35 respectively.

Horsemann and Harrington [1997] also fitted the experimental data\(^{12}\), and suggest values of \( \alpha_s = 1.963 \) MPa and \( \gamma_s = 4.85 \) for \( 0.6 < e < 2 \).

These fits imply a swelling pressure for the bentonite used in:

a) Experiment Mx80-4A (see subsection 3.4.2) of about 15 MPa (corresponding to a void ratio of 0.659), and

b) Experiment Mx80-8 (see subsection 3.4.3) of about 9 MPa (corresponding to a void ratio of 0.74).

Young’s modulus and Poisson’s ratio

The elastic deformation of the clay matrix in response to a change in effective stress is determined by values of Young’s modulus and Poisson’s ratio. The values for changes under drained conditions are required.

(i) Poisson’s ratio

Börgesson et al. [1995, 1996] give the value of Poisson’s ratio for saturated bentonite as \( \nu = 0.4 \). Daeman and Ran [1996] suggest the value should be at least 0.4, but do not relate the value to the compaction or other properties of the clay. A value of 0.4 has been used here.

\(^{12}\) This latter fit was used in the GAMBIT-GW model.
(ii) **Young’s modulus**

Equation (3.74) effectively defines the drained compressibility of the clay:

\[
-\frac{1}{V} \frac{dV}{d\Pi_s} = \frac{1}{V} \frac{dV}{d\Pi_s}.
\]  

(3.75)

Since:

\[
\frac{e}{e+1} = \frac{V_p}{V},
\]  

(3.76)

and assuming the solid grains are incompressible, so \( \Delta V = \Delta V_p \), it follows that:

\[
-\frac{1}{V} \frac{dV}{d\Pi_s} = -\frac{1}{\gamma_s \Pi_s} \frac{de}{d\Pi_s}.
\]  

(3.77)

where, from Equation (3.74):

\[
\frac{de}{d\Pi_s} = -\frac{e}{\gamma_s \Pi_s}.
\]  

(3.78)

The compressibility is related to Young’s modulus, \( E \), by [e.g. *Jaeger and Cook, 1979*]:

\[
-\frac{1}{V} \frac{dV}{d\Pi_s} = \frac{3(1-2\nu)}{E}.
\]  

(3.79)

Hence:

\[
E = \frac{3(1-2\nu)}{\left(\frac{e}{(e+1)\gamma_s \Pi_s}\right)}.
\]  

(3.80)

This equation, together with the values of \( \alpha_s \) and \( \gamma_s \) given above, implies a Young’s modulus for the bentonite used in:

a) Experiment Mx80-4A of about 100 MPa, and

b) Experiment Mx80-8 of about 60 MPa.

The analysis shows that Young’s modulus for the bentonite is not constant, but decreases with the void ratio (or, equivalently, increases with the swelling pressure). This variation is not insignificant, but since gas migration involves only a small change in void ratio, a constant value was assumed in the GAMBIT-GWS calculations reported here.
Permeability to liquid

Börgesson et al. [1995, 1996] also measured the relationship between permeability to the pore water, \( k_w \), and void ratio, \( e \), for saturated bentonite, and fitted their experimental data with the function:

\[
k_w = \alpha_k e^{\gamma_k} .
\]  

(3.81)

The fitted values of \( \alpha_k \) and \( \gamma_k \) were \( 3 \times 10^{-13} \left( \frac{\rho_w g}{\mu_w} \right) \) m\(^2\) and 4.64 respectively.

Horseman and Harrington [1997] also fitted the experimental data, and suggest values of \( \alpha_k = 3.45 \times 10^{-20} \) m\(^2\) and \( \gamma_k = 4.28 \). This latter fit has been used in the GAMBIT-GWS calculations reported here.

3.4.2 Simulation of Experiment Mx80-4a

Introduction

Horseman and Harrington [e.g. Horseman et al., 1997; Harrington and Horseman, 1997] have carried out a series of experiments on gas migration through compacted bentonite using a tri-axial apparatus (Figure 3.5).

An experiment is performed on a sheathed cylindrical bentonite sample, which is held at constant isotropic stress by containment in a vessel filled with pressurised fluid. Helium is injected at one end of the clay from a syringe whose volume is reduced by water displacing gas at a prescribed pumping rate. A constant pore water pressure (‘back pressure’) is applied at the other end of the clay.
Readings of the injection (upstream) gas pressure, and gas inflow and outflow rates are logged automatically at regular intervals throughout an experiment. These measurements are shown in Figure 3.6 for Experiment Mx80-4A.

The experiment initiates with an upstream pressure that is less than the total stress applied to the sample. As the syringe volume is reduced the pressure rises. When the pressure reaches a critical value, flow through the clay is observed.

After gas has broken through at the downstream end of the sample, the upstream pressure peaks and then reduces towards a steady-state value. (This is the first peak in Figure 3.6, and it just precedes the first appearance of flow from the downstream end of the sample.) The pumping rate is altered subsequently a number of times, producing
further pressure transients. A secondary peak in the upstream pressure occurs when the pumping rate is increased part way through the experiment. The experiment concludes with a zero pumping rate (‘shut-in’ period).

![Flow rate and Excess Gas Pressure](image)

*Figure 3.6 Results from Experiment Mx80-4A [Horseman et al., 1996; Harrington and Horseman, 1997].*
Model

A mathematical model for gas migration through compacted bentonite has been presented in Section 3.1.2, and parameterisation of the model has been discussed at the beginning of Section 3.4.

In order to complete specification of a model for Experiment Mx80-4A, it is necessary to choose a finite-element mesh and to set boundary and initial conditions.

(i) Finite-element mesh

A two-dimensional mesh with a cylindrical geometry was used to represent the bentonite sample in Experiment Mx80-4A. The mesh was divided into 5 equally sized elements in the radial direction, and 20 elements refined towards the outlet in the axial direction (Figure 3.7).

![Figure 3.7 Finite-element mesh used in the simulation of Experiment Mx80-4A.](image-url)
In addition, meshes having either 40 or 80 elements in the axial direction were used to show that the results were independent of the finite-element discretisation.

(ii) Boundary conditions

The boundary conditions applied to the surface of the bentonite sample were:

a) On the symmetry axis, \( r = 0 \), the radial displacement is zero and there is no flux of fluids (\( \frac{\partial p_w}{\partial r} = \frac{\partial p_g}{\partial r} = 0 \)).

b) On the outer cylindrical surface the applied load is constant (the confining pressure) and there is no flux of fluids (\( \frac{\partial p_w}{\partial r} = \frac{\partial p_g}{\partial r} = 0 \)).

c) On the inlet surface there is no radial or axial displacement (in the experiment the sheath confining the clay is held in place by a rigid metal band, and the sample is hung vertically in the confining vessel). There also is no flux of pore water (\( \frac{\partial p_w}{\partial r} = 0 \)), and the gas pressure is fixed by the reservoir boundary condition (see Equation 3.72).

d) On the outlet surface there is no radial displacement (in the experiment the sheath confining the clay is held in place by a rigid metal band), but there can be a vertical displacement (against the confining pressure). The pore water and gas pressures are equal to the applied back pressure.

Most of these boundary conditions are obvious. The choice of boundary conditions that is questionable is setting the pore water and gas pressures on the outlet surface equal to the applied back pressure. In the course of this study, some variations on this boundary condition were considered. In particular, the boundary condition at the outlet surface was changed so that:

a) Pore water was able to flow out of, but not into the clay, reflecting a gravitational segregation that might occur at the outlet surface [see Swift et al., 2001] as in the GAMBIT-GW model. In the GAMBIT-GWS model, this boundary condition lowers the second peak in the Experiment Mx80-4A. This is in contradistinction to the GAMBIT-GW model. The difference between the two models is due to the fact that the clay goes into suction, and the GAMBIT-GWS model uses effective stress but the GAMBIT-GW model uses total stress to determine gas entry.

b) The permeability of the gas phase was set to be small or large. Note that because both the pore water and gas pressures are fixed, the volumetric saturation, and hence permeability, of the gas phase at the outlet is constant.
Changing the value of the permeability of the gas phase at the outlet does not appear to affect the conclusions of the model. It is worth noting that in the GAMBIT-GWS model, as in previous models [Nash et al., 1998; Swift et al., 2001], much of the resistance to gas flow is due to a thin layer at the outlet, which must be properly resolved.

(iii) Initial conditions

The initial conditions set:

a) The stress tensor, \(-\sigma_{ij},\ i = j\), equal to the sum of the clay swelling pressure and the back pressure, and \(-\sigma_{ij},\ i \neq j\), equal to zero;

b) The porosity, \(\phi = \frac{e}{1+e} = 0.397\);

c) The pore water pressure, \(p_w\), equal to the back pressure;

d) The saturation of the gas phase, \(S_g\), equal to a small value, i.e. \(10^{-8}\), throughout most of the clay sample;

e) The permeability tensor of the gas phase, \(k_{g,ij}\), equal to the values calculated from the value of \(S_g\) using Equation (3.40);

f) The gas pressure, \(p_g\), equal to the back pressure.

Results

The objective of the simulations was to validate the model of gas migration in bentonite against the results obtained by Horseman and Harrington [e.g. Horseman et al., 1996; Harrington and Horseman, 1997].

Preliminary simulations of Experiment Mx80-4A showed that the compressibility of the clay, i.e. \(\frac{1}{K} = \frac{3(1-2\nu)}{E}\), which is discussed in Section 3.4.1, was too large, so the results did not match the experimental data.

The GAMBIT-GWS model can explain the behaviour of the upstream gas pressure after breakthrough (see Figure 3.6) only if there is a flow of pore water. If there were no flow of pore water the gas saturation would increase sufficiently (Equations 3.19 and 3.38) to accommodate the gas flow, and then would not change. Correspondingly, the upstream gas pressure after breakthrough would level off, and not decrease.
Now, the gas, as it propagates through the sample, compresses both the bulk clay and the pore water. If the bulk clay were much more compressible than the pore water, then it, rather than the pore water, would be compressed, with the result that there would be little change in the pressure of the pore water and no consequent flow. This fact, together with the observation that the permeability of the clay is very small, suggests it may be more appropriate to use the undrained than the drained compressibility for the bulk clay (see subsection 3.4.1). Assuming the solid grains are incompressible, this compressibility can be estimated from the compressibility of the pore water in the clay:

\[ \frac{1}{K_u} = \frac{3(1-2\nu_w)}{E_u} \approx \phi \beta_w \].

(3.82)

The shear strength of the clay should not change depending on whether conditions are drained or undrained. That implies for undrained conditions Young’s modulus should be virtually unchanged from its drained value and Poisson’s ratio should be close to its limiting value of 0.5. However, this choice of parameters can lead to inaccuracies in the stress calculation, and so Poisson’s ratio has been kept at 0.4 and Young’s modulus adjusted accordingly.

Some of the preliminary simulations showed instability in the formation of the gas pathway through the clay sample. One cause of instability is due to the first term in Equation (3.38) becoming too large, with the result that gas is drawn in from adjacent points instead of from the reservoir.

Figure 3.8 is a plot from a simulation in which the gas pathway collapsed showing the evolution of \( \frac{\partial p_g}{\partial t} \), \( \frac{\partial p_w}{\partial t} \) and \( \frac{\partial p_g}{\partial t} - \frac{\partial p_w}{\partial t} \) at a node in the interior of the model. Note that:

a) There is a large increase in \( \frac{\partial p_g}{\partial t} \), and hence \( \frac{\partial p_g}{\partial t} - \frac{\partial p_w}{\partial t} \), between 4.8 \( \times \) 10^5 s and 4.9 \( \times \) 10^5 s. This corresponds to the creation of gas saturation at the point.

b) Subsequently, there are small oscillations in \( \frac{\partial p_g}{\partial t} - \frac{\partial p_w}{\partial t} \), which are caused by the abrupt creation of gas saturation at nodes downstream of the point.

c) After 5.0 \( \times \) 10^5 s, \( \frac{\partial p_g}{\partial t} - \frac{\partial p_w}{\partial t} \) is mostly slightly negative. The negativity of this term causes the gas saturation at the point to decrease towards zero, i.e. the gas pathway collapses, and as a result the numerical simulation fails.

On the basis of observations like this, Equation (3.38) was modified so that the first term acts only when gas saturation is created. In particular, Equation (3.38) was replaced by:
\[ \frac{1}{R_m} = \frac{1}{R_i} \sum_{i=1}^{3} \theta \left[ p_g - (\sigma_i - p_w + \tau_s) - \Sigma_k \left[ \frac{\partial p_g}{\partial t} - \frac{\partial p_w}{\partial t} \right] \right] + \frac{1}{R_2} \theta \left( S_g - S_{g_i} \right) S_g . \] (3.83)

**Figure 3.8** Graphs showing the evolution of \( \frac{\partial p_g}{\partial t} \), \( \frac{\partial p_w}{\partial t} \) and \( \frac{\partial p_g}{\partial t} - \frac{\partial p_w}{\partial t} \) at a node in the simulation of Experiment Mx80-4A.

The GAMBIT-GWS model was then used to simulate Experiment Mx80-4A. The parameters that can be altered to fit the data are:
a) The gas modulus for fracture, $\tilde{R}_1$. As discussed at the beginning of Section 3.4, we set $\tilde{R}_1 = \frac{1}{\phi \beta_w}$.

b) The gas modulus to suction, $\tilde{R}_2$. This parameter was chosen to give a reasonable fit to the data post gas breakthrough.

c) The gas permeability parameter, $k_0$. As discussed at the beginning of Section 3.4, initially we set $k_0 = 3 \times 10^{-14}$ m². However, it was found that a better fit to the data post gas breakthrough could be obtained by increasing $k_0$ slightly to $10^{-13}$ m².

The resulting fit to the data, corresponding to the parameter value:

$$\tilde{R}_2 = 2.4 \times 10^6 \text{ Pa},$$

is shown in Figure 3.9.

![Figure 3.9 Fit to Experiment Mx80-4A obtained with the GAMBIT-GWS model.](image)

It should be emphasised that this is a crude fit to Experiment Mx80-4A in which only a couple of parameters in the GAMBIT-GWS model have been varied. However, apart from the first peak in the gas pressure, the GAMBIT-GWS model clearly is reproducing the behaviour of much of the data.
The GAMBIT-GWS model with these parameters was then used to simulate another experiment: Experiment Mx80-8 [Harrington and Horseman, 2003].

### 3.4.3 Simulation of Experiment Mx80-8

**Introduction**

Two gas migration tests have been performed on cylinders of pre-compacted Mx80 bentonite using a Constant Volume and Radial Flow (CVRF) apparatus [Harrington and Horseman, 2003].

In this geometry the sample volume is constrained (i.e. clay dilation is prevented). After hydration, gas is injected at a central porous filter and then flows to any of three arrays of sink filters mounted around the sample.

Figure 3.10 is a cut-away diagram showing:

a) The two end closures, with their embedded drainage filters and axial total stress sensors;
b) The central fluid injection filter;
c) The twelve radial sink filters;
d) The three radial total stress sensors; and
e) The pore fluid pressure sensor.

The central filter is embedded at the end of a 6.4 $10^3$ m diameter stainless steel tube and is used to inject fluid, either distilled water or helium. Figure 3.11 shows the approximate dimensions of the central filter.

Readings at the various sensors for Experiment Mx80-8 are shown in Figure 3.12. Although the two CVRF experiments give slightly different results, the following general conclusions can be drawn.

An experiment begins with the upstream syringe volume being reduced at a constant rate, causing the gas pressure to rise. The pressure reaches a peak just before a gas pathway intersects one of the sink filters, and gas is seen to flow. After the peak, the gas pressure reduces towards a steady-state value. When subsequently the pumping rate is set to zero, there is another transient in the gas pressure, which then falls towards a ‘shut-in’ value.
Figure 3.10 Cut-away diagram of the Constant Volume and Radial Flow apparatus. The sensors are as follows:

- **PT1**: Axial total stress on the back pressure end closure,
- **PT2**: Axial total stress on the injection end closure,
- **PT3**: Radial total stress close to the injection end closure,
- **PT4**: Pore fluid pressure close to the injection end closure,
- **PT5**: Radial total stress at the mid-plane, and
- **PT6**: Radial total stress close to the back pressure end closure.

Figure 3.11 Diagram showing the dimensions of the central filter in the CVRF apparatus.
Figure 3.12 Results from Experiment Mx80-8 [Harrington and Horseman, 2003].
Model

While a mathematical model for gas migration through compacted bentonite has been derived, in order to carry out a simulation of Experiment Mx80-8 it is necessary to choose a finite-element mesh and to set boundary and initial conditions.

(i) Finite-element mesh

A two-dimensional mesh with a cylindrical geometry was used to represent the bentonite sample in Experiment Mx80-8 (Figure 3.13).

The mesh explicitly represents the central filter, as well as the radial sink filters. In particular, the steel tube used to inject fluid is taken to enter the clay at the bottom left of Figure 3.13, and the central filter, modelled as a hemisphere of diameter $6.4 \times 10^{-3}$ m, is at the end of this tube. Because of the cylindrical geometry of the model, three hoop-shaped sinks approximate the three arrays of sink filters; one is located on the mid-plane, and the other two are located at a distance a third of the sample length from the end closures.

*Figure 3.13 Finite element mesh used in the simulation of Experiment Mx80-8.*
(ii) **Boundary conditions**

The boundary conditions applied to the surface of the bentonite sample were:

a) On the symmetry axis, $r = 0$, the radial displacement is zero and there is no flux of fluids ($\frac{\partial p_w}{\partial r} = \frac{\partial p_g}{\partial r} = 0$).

b) On the outer cylindrical surface and on the end closures the displacement is zero, and there is no flux of fluids ($\frac{\partial p_w}{\partial r} = \frac{\partial p_g}{\partial r} = 0$) except at the sink filters.

c) On the inlet surface the gas pressure is fixed by the reservoir boundary condition (see Equation 3.72). The gas pressure applies a load to the clay surface. Finally, there is no flux of pore water ($\frac{\partial p_w}{\partial r} = 0$).

d) At the sink filters, the pore water and gas pressures are set equal to the applied back pressure.

(iii) **Initial conditions**

The initial conditions set:

a) The stress tensor, $-\sigma_{ij}$, $i = j$, equal to the sum of the clay swelling pressure and the back pressure, and $-\sigma_{ij}$, $i \neq j$, equal to zero;

b) The porosity, $\phi = \frac{e}{1+e} = 0.425$;

c) The pore water pressure, $p_w$, equal to the back pressure;

d) The saturation of the gas phase, $S_g$, equal to a small value, i.e. $10^{-8}$, throughout most of the clay sample;

e) The permeability tensor of the gas phase, $k_{g,ij}$, equal to the values calculated from the value of $S_g$ using Equation (3.40);

f) The gas pressure, $p_g$, equal to the back pressure.

**Results**

The simulation was carried out in two stages:
a) First, a standard poroelastic calculation was used to determine when the minor principal component of the effective stress tensor becomes tensile. It has been postulated that this criterion for failure determines when gas first is able to enter the clay as a ‘free’ phase [Swift et al., 2001; Harrington and Horseman, 2003].

b) Secondly, the full GAMBIT-GWS model was used to simulate the formation of a gas pathway through the clay, and the flow of gas post breakthrough.

The first simulation showed that the minor principal component of the effective stress tensor first becomes tensile at the tip of the injection filter after $3.17 \times 10^6$ s (Figure 3.14).

![Figure 3.14](image)

*Figure 3.14 Minor principal component of effective stress at the tip of the injection filter in the simulation of Experiment Mx80-8.*

Note that the kink in the curve shown in Figure 3.14 is due to replenishment of the gas reservoir at $2.42 \times 10^6$ s.
Figures 3.15, 3.16, 3.17 and 3.18 show respectively: the gas pressure in the reservoir; the deformation of the clay; the effective stresses in the clay; and the pore water and incipient gas pressures in the clay just prior to gas entry.

**Figure 3.15** Pressure in the gas reservoir in the simulation of Experiment Mx80-8. (The kink in the curve is due to replenishment of the gas reservoir.)
Figure 3.16 (a) Radial and (b) axial displacements just prior to gas entry in the simulation of Experiment Mx80-8.
Figure 3.18  (a) Pore water and (b) gas pressures just prior to gas entry in the simulation of Experiment Mx80-8.

It is worth noting that although there is a small inflow of pore water at the Sink Array closest to the injection end closure, and small outflows at the other two Sink Arrays, the flows are small (i.e. less than $10^{-2}$ $\mu$L h$^{-1}$). These flows are much less than the precursor flows (i.e. about 1 $\mu$L h$^{-1}$) that have been seen in the experimental data.

Finally, an attempt was made to use the GAMBIT-GWS model to simulate the formation of a gas pathway through the clay, and the flow of gas post breakthrough. However, as of now it has not been possible to simulate the full experimental history of Experiment Mx80-8 with the GAMBIT-GWS model, because:

a) The simulation appears to require very many small time steps after breakthrough. (Gas breakthrough is predicted to occur at about $3.20 \times 10^6$ s,
compared to an experimentally observed breakthrough time of $3.22 \times 10^6$ s.) A possible explanation for the small time steps is that after breakthrough the simulation has to track the evolution of the two-dimensional gas pathway in response to rapid, large changes in gas pressure.

b) Some simulations failed. Whether the failure is due to numerical instability or to the physical intractability of the problem is not known.

It follows that even if resources were available to solve the current problem, the difficult nature of the problem is likely to make the computations costly to carry out.

The conclusion that may be drawn is that the GAMBIT-GWS model can be used to simulate (pseudo) one-dimensional problems (e.g. Experiment Mx80-4A), but at present not two-dimensional problems (e.g. Experiment Mx80-8). The GAMBIT-GW model provides an alternative approach for one-dimensional problems.
4 APPLICATION OF THE ENTWIFE MODEL TO A CANISTER-SCALE SYSTEM

The Swedish KBS 3 repository concept is typical of designs for the deep disposal of long-lived waste.

Copper/steel canisters containing spent nuclear fuel will be placed in disposal boreholes drilled into the floor of a repository tunnel at a depth of about 500 m in a crystalline host rock (Figure 4.1). The space around each canister will be filled with bentonite blocks. Over time the bentonite will hydrate and swell, closing up any gaps between the blocks.

*Figure 4.1 KBS 3 concept for storage of spent nuclear fuel [SR 97, 1999].*

Figure 4.2 shows the design of the engineered barrier.

If the copper outer canister were to fail, corrosion of the steel inner canister would lead to the formation of hydrogen. Radiolysis of water will produce additional gas. Depending on the rate of gas production and the rate of diffusion of gas in the pores of the bentonite, it is possible that gas might accumulate in the void-space of a canister. This gas will enter the buffer when the gas pressure exceeds a critical value.

This section presents a simulation for the formation of gas in the void space of a canister, and its subsequent migration through the bentonite buffer.
4.1 Model

It was assumed that:

a) Gas is generated at a rate corresponding to the steel inner canister being corroded at a rate of 1 μm per year; and

b) This gas is injected into a void space between the canister and the bentonite, taken to be a uniform gap of 100 μm all around the canister.

The model represents the bentonite buffer around the canister.

4.1.1 Finite-element mesh

A two-dimensional mesh with a cylindrical geometry was used to represent the bentonite buffer (Figure 4.3).
Figure 4.3 Finite element mesh used in a simulation of gas migrating from a canister through bentonite buffer in a deposition hole.

The corners on the inner surface of the mesh, where the bentonite contacts the canister, have been rounded to avoid possible numerical problems due to stress concentrations.

4.1.2 Boundary conditions

The boundary conditions applied to the surface of the bentonite were:

a) On the symmetry axis, \( r = 0 \), the radial displacement is zero and there is no flux of fluids (\( \frac{\partial p_w}{\partial r} = \frac{\partial p_x}{\partial r} = 0 \)).

b) On the outer cylindrical surface and on the bottom surface the displacement is zero and there is no flux of fluids (\( \frac{\partial p_w}{\partial r} = \frac{\partial p_x}{\partial r} = 0 \)). The latter condition arises because it is assumed that the surrounding host rock is impermeable.
c) On the inner surface the gas pressure is fixed by a reservoir boundary condition (see Equation 3.72). The gas pressure applies a load to the clay surface. Finally, there is no flux of pore water \( \left( \frac{\partial p_w}{\partial r} = 0 \right) \).

d) At the top surface, the pore water pressure is set equal to the hydrostatic pressure at a depth of 500 m. The gas pressure is set to zero.

### 4.1.3 Initial conditions

The initial conditions set:

a) The stress tensor, \( -\sigma_{ij}, \ i = j \), equal to the sum of the clay swelling pressure and the hydrostatic pressure, with a correction for the weight of the canister, and \( -\sigma_{ij}, \ i \neq j \), equal to zero;

b) The porosity, \( \phi = \frac{e}{1+e} = 0.425 \);

c) The pore water pressure, \( p_w \), equal to the hydrostatic pressure;

d) The saturation of the gas phase, \( S_g \), equal to a small value, i.e. \( 10^{-8} \), throughout most of the clay;

e) The permeability tensor of the gas phase, \( k_{g,ij} \), equal to the values calculated from the value of \( S_g \) using Equation (3.40);

f) The gas pressure, \( p_g \), equal to zero.

### 4.2 Results

The build-up of gas pressure in the void space between the canister and the bentonite is shown in Figure 4.4.
As for Experiment Mx80-8, the simulation was carried out in two stages:

a) First, a standard poroelastic calculation was used to determine when the minor principal component of the effective stress tensor becomes tensile.

b) Secondly, the full GAMBIT-GWS model was used to simulate the formation of a gas pathway through the clay, and the flow of gas post breakthrough.

The first simulation showed that the minor principal component of the effective stress tensor first becomes tensile at the top corner of the canister after $2.83 \times 10^8$ s (i.e. about 9 years; see Figure 4.5). This is taken to be the time at which gas first is able to enter the clay as a ‘free’ phase.

*Figure 4.4 Build-up of gas pressure in the void space between the canister and the bentonite.*
Figures 4.5, 4.6, 4.7 and 4.8 show respectively: the deformation of the clay; the effective stresses in the clay; and the pore water and incipient gas pressures in the clay just prior to gas entry.

The results are as expected:

a) The radial displacements are small, but the axial displacements have a maximum of almost $10^{-2}$ m on the axis above the canister.

b) The minor principal component of the effective stress tensor first becomes tensile at the corners of the canister.

c) The pore water pressure has both a hydrostatic component, and a component due to the load exerted on the clay by the canister and the gas in the void space. After $2.83 \times 10^8$ s the gas has diffused sufficiently far through the bentonite to
reach the vertical wall of the deposition hole, but not to cross the layer of bentonite above the canister.

**Figure 4.6** (a) Radial and (b) axial displacements just prior to gas entry in the simulation of the canister.
Figure 4.7 (a) Major principal component and (b) minor principal component of the effective stress tensor just prior to gas entry in the simulation of the canister.
Figure 4.8 (a) Pore water and (b) gas pressures just prior to gas entry in the simulation of the canister.

Finally, an attempt was made to use the GAMBIT-GWS model to simulate the formation of a gas pathway through the clay, and the flow of the gas post breakthrough. However, for the reasons discussed at the end of Section 3.4.3, it has not been possible to extend the simulation into the future.
5 INVESTIGATION AND IMPLEMENTATION OF A DUAL-POROSITY MODEL

As discussed in the Introduction (Section 1), in addition to exploring the extension, discussed in Sections 3 and 4, of the Phase 2 GAMBIT-GW model of gas migration to incorporate a proper treatment of the stress field in the bentonite, it was also planned, in the Phase 3 work, to examine other possible extensions to the Phase 2 model. Specifically, it was intended to investigate whether the model could be improved by taking some account of the effect of the clay fabric on gas migration in bentonite and of some hysteresis in the response to gas pressure changes. These latter attempts are described in this section.

The essence of the GAMBIT-GW model [Swift et al., 2001] is that gas cannot enter the clay until pathways have been created by a combination of squeezing water from and compressing water in the clay matrix. All the water resides in the clay matrix, which can change volume as indicated, in accordance with the swelling behaviour of the clay, thereby leaving voids that can be occupied by gas, but the gas cannot enter and displace water from the clay matrix itself. This model is summarised briefly in subsection 5.1.

As discussed in the introduction, other models of gas migration have been proposed on the basis of the assumption that both the water and gas permeability of compacted clays arise primarily from the presence of “interstack” voids in the clay where, in the saturated clay, there is loosely bound water which can flow more readily than the tightly bound “intrastack” water [e.g. Pusch et al., 1990]. Gas migration can then occur by displacing water from the “interstack” channels. The situation may be complicated by the presence of clay gels in the interstack voids, and the behaviour of these might influence both water and gas flows.

The purpose of the first development to the GAMBIT-GW model considered in this section is to try to reconcile these two approaches. This was to be attempted by adding a dual porosity feature to the model to represent two elements of the clay fabric: the clay stacks and the interstack voids. This means defining two porosities: the porosity associated with the bound water in the clay stacks and that associated with the gas and water in the interstack voids.

The second enhancement, the introduction of a time delay in the response to gas pressure changes, was a simple attempt to represent the experimentally observed “overshoots” in the behaviour of the upstream gas pressure.

These enhancements were added to the original GAMBIT-GW model, not the model incorporating the full stress treatment described in Section 3.
5.1 Summary of the Phase 2 GAMBIT-GW Model

In the Phase 2 GAMBIT-GW model [Swift et al., 2001], when both gas and water are present the state of the system is defined by specification of the gas and water pressures at all points, where the water pressure is the externally measurable equilibrium water pressure corresponding to the particular position. Equations for the evolution of these pressures can be constructed from the conservation equations for gas and water by assuming the flows obey Darcy’s law. The equations for water and gas are respectively:

\[
\frac{\partial}{\partial t} \left((1 - \phi_g) \phi_w \rho_w\right) = \frac{\partial}{\partial x} \left(\rho_w \frac{k_w}{\mu_w} \frac{\partial p_w}{\partial x}\right) \tag{5.1}
\]

\[
\frac{\partial}{\partial t} (\phi_g \rho_g) = \frac{\partial}{\partial x} \left(\rho_g \frac{k_g}{\mu_g} \frac{\partial p_g}{\partial x}\right) \tag{5.2}
\]

where
- \(p_w\) is the water pressure [Pa],
- \(p_g\) is the gas pressure [Pa],
- \(\phi_w\) is the water porosity in the water-clay system considered separately,
- \(\phi_g\) is the gas porosity,
- \(\rho_w\) is the water density [kg m\(^{-3}\)],
- \(\rho_g\) is the gas density [kg m\(^{-3}\)],
- \(k_w\) is the water permeability [m\(^2\)],
- \(k_g\) is the gas permeability [m\(^2\)],
- \(\mu_w\) is the water viscosity [Pa s],
- \(\mu_g\) is the gas viscosity [Pa s].

Note that the water-filled porosity, \(\phi_{wc}\), is the volume fraction of water in the water and clay alone, therefore the overall water-filled porosity is \(\phi_w = (1 - \phi_g)\phi_{wc}\). Equations (5.1) and (5.2) are written in terms of the gas and water density, permeability and occupied porosity (fractional volume), so that equations relating these quantities, directly or indirectly, to the phase pressures are also required.

Relating the densities to the pressures is straightforward. The gas density is obtained from the Ideal Gas law

\[
\rho_g = \frac{M_g}{RT} p_g \tag{5.3}
\]

where
- \(M_g\) is the molar mass of the gas [kg mol\(^{-1}\)],
- \(R\) is the gas constant [J mol\(^{-1}\)K\(^{-1}\)],
- \(T\) is the temperature [K].
For the water density, a standard compressibility model is used.

\[ \rho_w = \rho_{w0} e^{\beta(p_w - p_{w0})} \]  

where

- \( p_{w0} \) is the reference water pressure (Pa),
- \( \rho_{w0} \) is the water density at the reference pressure (kg m\(^{-3}\)),
- \( \beta \) is the water compressibility (Pa\(^{-1}\)).

To construct an equation relating the water-filled porosity to the pressures, the additional assumption that (where gas exists) the gas pressure is equal to the stress, \( \sigma \), on the water-clay system \( (p_g = \sigma) \) is invoked. Then the swelling pressure is

\[ \Pi_s = \sigma - p_w = p_g - p_w \]  

According to the fit to the experimental data of \( \text{Börgresson et al. [1996]} \), quoted by \( \text{Horsemam and Harrington [1997]} \), the swelling pressure of Mx80 bentonite can be represented empirically to a good approximation by

\[ \Pi_s = \frac{\alpha}{e^\gamma} \]  

where

- \( \alpha, \gamma \) are fitting parameters,
- \( e \) is the void ratio, defined as

\[ e = \frac{\phi_{wc}}{1 - \phi_{wc}} \]  

The particular form of the empirical relationship of Equation (5.6) is not essential to the model; it could be replaced by any improved representation that becomes available, or by relationships appropriate to different types of bentonite if required.

Combining Equations (5.5) to (5.7)

\[ \phi_{wc} = \frac{\frac{1}{\alpha^\gamma}}{\left(\sigma - p_w\right)^{\frac{1}{\gamma}} + \frac{1}{\alpha^\gamma}} = \frac{\frac{1}{\alpha^\gamma}}{\left(p_g - p_w\right)^{\frac{1}{\gamma}} + \frac{1}{\alpha^\gamma}} \]  

Since the sum of the volume fractions of each of the components, solid, water, and clay, must be unity, then the gas porosity can be related to the pressures via the water porosity.
where 
\[ \phi_s \] is the solid volume fraction.

Provision has been made in the model to allow the volume of the clay to vary, particularly, for example, to dilate in response to gas invasion, as might occur in a gas migration experiment under constant stress confinement. This is described by Swift et al. [2001]. A constant volume constraint is imposed by specifying a zero volume change.

The gas is only expected to take up a small fraction of the volume of the system \( (\phi_g < 0.01) \), so the fraction of water will be approximately constant. It is therefore reasonable to make the approximation that the water permeability is constant.

\[ k_w = k_{w0} \quad (5.10) \]

This assumption could be replaced by a constitutive relationship relating water permeability to other system variables if required.

Finally, the gas permeability is assumed to be a function of the gas porosity depending on the geometry of the gas flow paths. For example, the following gas permeability is derived from the permeability obtained assuming flow along capillaries.

\[ k_g = \frac{(\phi_g - \phi_{gc})^2}{8n_c} \quad , \quad \phi_g > \phi_{gc} \quad (5.11) \]

where
\[ \phi_{gc} \] is the critical gas porosity below which the gas permeability is zero,
\[ n_c \] is the number density of capillaries \( (\text{m}^{-2}) \).

Alternatives to Equation (5.11) for prescribing the gas permeability were also tried; one of these is the exponential form

\[ k_g = k_{g0} \left( e^{\lambda \phi_g} - e^{\lambda \phi_{gc}} \right) \quad , \quad \phi_g > \phi_{gc} \quad (5.12) \]

where
\[ k_{g0} \] is a constant \( (\text{m}^{-2}) \),
\[ \lambda \] is a constant.

Where no gas is present, the system can be defined by the water pressure alone using Equation (5.1) with \( \phi_g = 0 \). However, it is convenient to define the stress to replace the
gas pressure. In this case Equation (5.2) is replaced with the first relationship in Equation (5.5), but the void ratio (given by Equation (5.7)) defining the swelling pressure is now defined in terms of the solid volume fraction as

\[ e = \frac{1}{\phi_s} - 1 \]  

(5.13)

5.2 Description of the Phase 3 GAMBIT-GW Model Enhancements

The additional elements introduced in the enhanced model compared with the original Phase 2 GAMBIT-GW model are:

a) the assignment of an initial porosity to the interstack voids and a model for the overall permeability of the channels these voids form (changes in the channel volume require changes in the clay matrix volume in the same way as in the Phase 2 model);

b) a model for the transfer of water between the water in the interstack spaces and in the clay matrix (intrastack water);

c) a model for the entry of gas into the interstack channels and displacement of water from them;

d) a prescription for the relationship between the change in interstack channel volume and changes in the gas and water pressures in the channel.

Although the modified model has the same facility for allowing overall volume expansion as in the Phase 2 version, this is ignored for the present reporting purposes; that is, only the constant volume case is discussed.

As in the Phase 2 model, water pressures in the clay matrix are defined as the pressure of external water in equilibrium with the water in the matrix. Data from the work by Pusch et al. [1990] has been used to provide initial estimates of channel properties.

At present, the additional features listed above are modelled as described below. Since the available experimental data is not sufficient to characterise the mechanistic details of the two-phase flow behaviour involved, model details have been chosen to provide generally plausible behaviour and to mirror known (or expected) limiting behaviours (e.g. the swelling behaviour of saturated bentonite). However, there is arbitrariness and uncertainty in the choices made.

The overall permeability, \( k_c \), of the channels is given by:

\[ k_c = k_{c0} \left( \frac{\phi_c}{\phi_{c0}} \right)^{n_c} \]  

(5.14)
where

- \( k_{c0} \) is the permeability due to the channels at the initial equilibrium \([m^2]\),
- \( \phi_c \) is the current channel volume fraction (i.e. the part of the overall porosity associated with the channels),
- \( \phi_{c0} \) is the channel volume fraction at the initial equilibrium,
- \( n_c \) is a fitting parameter.

It is assumed that the flow rate (per unit sample length), \( q_x \), of water between matrix and channels is proportional to the pressure difference between water in the two situations; that is the flow is Darcy like. Specifically

\[
q_x = \begin{cases} 
\chi \rho_m \frac{k_m}{\mu_w} (p_m - p_w) & , \quad p_w \leq p_m \\
\chi \rho_m \frac{k_m}{\mu_w} (S_w - S_{wc1})(p_m - p_w) & , \quad p_w > p_m, \quad S_w > S_{wc1} \\
0 & , \quad \text{otherwise}
\end{cases}
\]

(5.15)

where

- \( \chi \) is a constant depending on the geometric arrangement of the channels,
- \( S_w \) is the water saturation of the channels,
- \( S_{wc1} \) is a critical water saturation in the channels (the minimum saturation required for channel to matrix flow),
- \( p_w \) is the water pressure in the channels [Pa],
- \( p_m \) is the pressure of water in equilibrium with water in the matrix [Pa],
- \( \rho_m \) is the water density in the matrix [kg m\(^{-3}\)],
- \( k_m \) is the matrix permeability [m\(^2\)],
- \( \mu_w \) is the water viscosity [Pa s],

The term in the channel water saturation is introduced to prevent water flowing from the channels when flushing by gas has lowered the water saturation to the point \( S_{wc1} \) when it becomes immobile.

Treatment of gas flow and displacement of water in the channels proved difficult to describe in a way that mirrors the behaviour seen in general in the experiments carried out by BGS of a threshold pressure below which gas does not flow and above which gas breakthrough is rapid and usually the immediate flow is substantial. If the model is not to reduce to simply the original Phase 2 GAMBIT-GW model or to the simple displacement of water from pre-existing channels, a model also implemented in the Phase 2 programme, it appears necessary to make the threshold pressure and gas permeability for flow in the channels depend on the gas content of the channels (i.e. the channel gas saturation). This produces a model of two-phase flow in the channels which is formally similar to the use of capillary pressure and saturation functions in
conventional porous medium flow theory, although the form of these functions may be different from those conventionally adopted (for example they may be determined by the compression of clay gels in the channels).

At present it is assumed that the relationship between the gas and water pressures is given by the capillary-pressure-like function

\[ p_g = p_w + p_d \left[ \theta + (1 - \theta)S_w \right]^{-n_p} \left( \frac{\phi_c \theta}{\phi_c} \right)^{1/2} \]  

(5.16)

where

- \( p_d \) is the gas entry capillary pressure when \( \phi = \phi_0 \) [Pa],
- \( \theta, n_p \) are fitting parameters (with \( \theta \ll 1 \)).

The gas and water relative permeabilities in the channels, \( k_{rg} \) and \( k_{rw} \) respectively, are given by

\[
k_{rg} = \begin{cases} 
\left( \frac{1 - S_w - S_{gc}}{1 - S_{gc}} \right)^{n_g} , & 1 - S_w > S_{gc} \\
0 , & 1 - S_w \leq S_{gc} 
\end{cases} \]  

(5.17)

and

\[
k_{rw} = \begin{cases} 
\left( \frac{S_w - S_{wc2}}{1 - S_{wc}} \right)^{n_w} , & S_w > S_{wc2} \\
0 , & S_w \leq S_{wc2} 
\end{cases} \]  

(5.18)

where

- \( n_g, n_w \) are fitting parameters.
- \( S_{gc} \) is the critical gas saturation of the channels (the minimum saturation required for gas flow).
- \( S_{wc} \) is a critical water saturation for the channels (the minimum saturation at which water can flow along the channels).

In fact, in the numerical implementation, some smoothing to the functional form in Equation (5.17) is applied.

The final element of the model extension is the specification of how the channel volume fraction varies with the pressures of gas and water in the channels. The model used is
\[ \phi_c = \phi_{c0} \left( \xi + \eta e^{e \left[ S_w p_w + (1 - S_w) p_g - \sigma \right]} \right) \] (5.19)

where

\( \xi, \eta, \varepsilon \) are constant fitting parameters,
\( \sigma \) is the stress in the clay matrix.

The parameters \( \xi, \eta, \varepsilon \) cannot be chosen independently since they are constrained by the initial conditions of the sample. Normally the water saturation would initially be \( S_w = 1 \). If the initial water pressure is \( p_{w0} \) and the initial stress is \( \sigma_0 \), the relationship between the three parameters is:

\[ \xi = 1 - \eta e^{e (p_{w0} - \sigma_0)} \] (5.20)

It is assumed that the stress in the clay matrix is still determined by the swelling behaviour of the clay matrix following Equations (5.5) and (5.6)

\[ \sigma = \frac{\alpha}{e^\gamma} + p_m \] (5.21)

where

\( \varepsilon \) is the void ratio of the clay matrix.

In the new dual porosity formulation

\[ e = \frac{1 - \phi_c - \phi_s}{\phi_s} \] (5.22)

To illustrate how the model of the variation of channel volume fraction behaves, consider the case in which the water in the channels and matrix are in equilibrium; that is, \( p_w = p_m \). Assuming there is no change in \( \phi_c \) until gas enters the bentonite, the gas cannot enter the bentonite until (Equation (5.16))

\[ p_g > p_w + p_d \] (5.23)

When this condition is not satisfied, \( S_w = 1 \), and, using Equations (5.21) and (5.22), Equation (5.19) becomes:

\[ \phi_c = \phi_{c0} \left( \xi + \eta e^{e \left[ \frac{\phi_g}{1-\phi_g-\phi_s} \right]^\gamma} \right) \] (5.24)

When gas does enter the clay, Equation (5.16), with \( \theta = 0 \), can be used to eliminate \( S_w \) from Equation (5.19), which then becomes:
Figure 5.1 shows the variation of $\phi_c$ with gas pressure from Equations (5.20) and (5.25), assuming the water pressure is constant. The total stress and the gas saturation of the channels are also shown. The parameters used in creating these graphs are shown in Table 5.1. The graph illustrates how once the gas pressure reaches the entry pressure, not only can it enter the interstack channels, displacing water, but it can also dilate those channels by “squeezing” water from the clay matrix, causing the overall stress to rise. This is the qualitative behaviour that Equation (5.19) was intended to represent, although its selection is otherwise arbitrary.
The final feature that has been examined in the Phase 3 extensions to the GAMBIT-GW model is the inclusion of a time lag in the response of the channel permeability to changes that drive adjustment to the channel permeability. This is exactly analogous to the similar feature introduced in the Phase 1 fracture propagation model [Nash et al., 1998], except that in that case the parameter to which it was applied was the fracture aperture. It has been introduced here to try to address the difficulty found in the Phase 2 programme in modelling cases in which there was an “overshoot” in the response of the upstream gas pressure to various changes. This time dependence is introduced by replacing the value, $k_c$, of the channel permeability given by Equation (5.14) in calculations of gas and water flows in the channels by the value $k_{ct}$ given by

$$\frac{d}{dt}(k_{ct} - k_c) = -\lambda (k_{ct} - k_c)$$

where $\lambda$ is a parameter [s$^{-1}$] controlling the time lag in the change of channel permeability.

$k_{ct}$ tends to $k_c$ at a rate controlled by the value of $\lambda$.

The modified Phase 2 gas migration model has been successfully implemented and tested in a computer program. The evaluation of the computer model is described in subsection 5.3 below.

### 5.3 Evaluation of the Dual-porosity Model Extension

The evaluation of the enhancements to the Phase 2 GAMBIT-GW model described in the above subsection with respect to their ability to simulate experimentally observed gas migration behaviour in bentonite has been concentrated mainly on the BGS Mx80-9
gas injection experiment. A suite of test cases to simulate this experiment have been run. This experiment was chosen for the main focus of the evaluation as it involves one-dimensional flow and it is perhaps more appropriate to approximate its radially constrained geometry as a constant volume system than is the case for earlier experiments which were confined under a constant isotropic stress. It was preferred to restrict the modelling to a constant volume system because of lack of information about the overall dilation of other systems with changes in gas pressure; this would require the selection of even more parameters than are already required. Experiment Mx80-9 had also proved particularly difficult to simulate in previous work [Swift et al., 2001], because of the very sharp drop in upstream gas pressure after initial breakthrough, and the minima in its value that followed this.

A less extensive range of calculations was also undertaken to model the earlier Mx80-4A experiment carried out by BGS [Horseman and Harrington, 1997].

Some example results from the range of calculations undertaken to try to simulate the Mx80-9 experiment are shown in Figures 5.2 and 5.3. The calculated evolutions of the upstream gas injection pressures are compared with the experimental results. Figure 5.3 shows the result of introducing a time delay in the response of the change in channel permeability to change in gas pressure.

![Figure 5.2](image-url)

**Figure 5.2** Representative Calculations with the “Dual Porosity” Model for BGS Experiment Mx80-9.
The subset of parameters that differ between the runs shown in Figure 5.2 include the exponent \( n_p \) from Equation (5.16) for the capillary pressure in the channels, the parameter \( \eta \) in Equation (5.19) for the change in channel porosity, the contribution to the permeability from channels at equilibrium, \( k_{c0} \), and the exponent \( n_g \) in the expression for the gas relative permeability in the channels (Equation (5.17)). The values for these parameters are shown in Table 5.2. Other parameters are unchanged between these runs with the following values \( p_d = 7.8 \) MPa (Equation (5.16)), \( n_w = 2 \) (Equation (5.18)), \( \varepsilon = 1 \times 10^{-7} \) Pa\(^{-1} \) (Equation (5.19)), \( S_w = 0.01 \) (Equation (5.18)), \( S_{wc} = 0.01 \) (Equation (5.17)).

<table>
<thead>
<tr>
<th>Run</th>
<th>( n_p ) Eqn (5.16)</th>
<th>( \eta ) Eqn (5.19)*</th>
<th>( k_{c0} ) (m(^2)) Eqn (5.14)</th>
<th>( n_g ) Eqn (5.17)</th>
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</tr>
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</tr>
<tr>
<td>x939</td>
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<td>1.0</td>
<td>( 1.5 \times 10^{-19} )</td>
<td>6.0</td>
</tr>
</tbody>
</table>

* Note that the parameters in Equation (4.6) are not all independent as it is necessary that the term in curved parentheses be equal to 1 at the initial conditions.

The variation of capillary pressure with channel porosity in Equation (5.16), the last set of parentheses in the equation, was omitted in runs x933 and x939.
Figure 5.3 Illustration of the Effect of Time Delay in the Change in Channel Permeability.

Figure 5.3 shows the effect of adding some time delay in the response of the channel permeability to changes in channel properties. In run x972 the value of the time dependence parameter, \( l \), was \( 3 \times 10^{-5} \text{s}^{-1} \); in run x973 it was \( 1 \times 10^{-5} \text{s}^{-1} \). In these and other trial runs, it was not possible to improve the fits to the experimental data in a significant way by adjusting this parameter. This was probably because of the small changes that occur in the channel porosity during the runs.

Figure 5.4 shows some attempts to simulate the BGS Experiment Mx80-4a [Horseman and Harrington, 1997]. This was the subject of simulation efforts in both the Phase 1 and Phase 2 programmes. The parameters that were varied between the runs are shown in Table 5.3. Those that were unchanged were \( n_p = 0; S_{wc} = 0.01; \eta = .1; n_w = 3.0; S_{gc} = 0.1; n_g = 6. \)
Simulations of BGS Experiment Mx80-4a [Horseman and Harrington, 1997].

Table 5.3 Parameters Varied in the Simulations of BGS Experiment Mx80-4a.

<table>
<thead>
<tr>
<th>Run</th>
<th>$p_d$</th>
<th>$\varepsilon$ (Pa$^{-1}$)</th>
<th>$k_{e\theta}$ (m$^2$)</th>
<th>$\lambda$ (s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>x4A32</td>
<td>13.1</td>
<td>$1 \times 10^{-6}$</td>
<td>$8 \times 10^{-20}$</td>
<td>$5 \times 10^{-6}$</td>
</tr>
<tr>
<td>x4A33</td>
<td>12.6</td>
<td>$1 \times 10^{-7}$</td>
<td>$3 \times 10^{-20}$</td>
<td>$2 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

It has proved more difficult with the dual porosity model than with some of the previous models to reproduce the key features of the experimental results. It has, for example, proved difficult to reproduce the sharp fall in the upstream gas pressure after initial gas breakthrough. This is particularly pronounced in the Mx80-9 experiment, and attempts to improve this aspect of the fit for this experiment have tended to make other aspects less good, for example, the shape and limiting values of the pressure behaviour after the two shut ins.
The difficult with the dual-porosity model appears to be that the presence of the pre-existing channels provided by the interstack pore space tends to dominate the gas migration behaviour and in fact produce a gas migration model that is more akin to a conventional porous-medium flow model than to the other types of model that have been proposed in the GAMBIT Club programme. It appears difficult to represent aspects of the observed behaviour using a model with similarities to a conventional two-phase porous-medium flow models. For example, the sharp fall in gas pressure after breakthrough, is suggestive of a mechanism involving a sudden opening of the gas pathways, which is difficult to represent with this type of model. Similarly, the shape of the pressure response with changes in upstream gas injection rate after breakthrough is quite well represented by a model in which pathways substantially occupied by gas are established, but whose permeability shows some variation with pressure [Nash et al, 1998]. It may be that the difficulties experienced in improving the fit to the data by using the dual-porosity model suggest that the mechanisms represented by this model are not a good description of the physical processes that govern gas migration in bentonite. Alternatively, it could be that the correct functional relationships from which to build such a model have not been found.
6 CONCLUSIONS

The work described in this report has explored ways in which the macroscopic model, GAMBIT-GW, developed in Phase 2 of the GAMBIT Club programme to model gas migration in compacted bentonite, might be improved. Basically, two conceptually significant improvements were separately considered:

a) Inclusion of the effects of the full stress field in the bentonite on the gas migration;

b) The representation of clay fabric effects in the form of a distinction between inter- and intra-stack pore space.

Both the development of the original GAMBIT-GW model and the exploration of these extensions to the model faced the same difficulty of uncertainty about the precise mechanism of gas migration in compacted bentonite, and indeed about whether different mechanisms might operate under different circumstances. The report provides a summary of the available experimental data on gas migration in bentonite and comments on the extent to which the data is suggestive of a particular gas transport mechanism.

Three possible basic mechanisms have been proposed for gas invasion of water-saturated compacted bentonite:

a) Behaviour of the bentonite as a conventional porous medium, with the gas flow governed by conventional concepts of capillary pressure and relative permeability.

b) Microfissuring of the clay, in which small fissures are created or opened by the invading gas to provide the pathways for the gas to enter the clay.

c) Macroscopic fracturing of the clay to provide fracture pathways for gas flow. This differs from (b) by the scale of the fracturing; it is assumed that in the laboratory macroscopic fracturing would involve fracture lengths comparable to the sample size (e.g. typically cutting right across the sample), whereas microscopic fissuring would involve fissures that have lengths small compared to the sample size (and that the sample remains intact when removed from the experiment).

It is possible that there is a spectrum of behaviour involving more than one of the above mechanisms simultaneously.

Examination of the experimental data has not produced a unique explanation of the experimental results in terms of these mechanisms, and in relation to this the following observations can be made:
In a few experiments, the “radial” flow experiments at constant volume [Harrington and Horseman, 2003], there is compelling evidence that fracturing or fissuring is involved in the establishment of gas pathways.

In these “radial” flow experiments, explanations can be found of the high gas entry pressures (e.g. much higher than the swelling pressure) in terms of the development of the radial stresses around the source leading to tensile failure of the clay. However, it is not clear how such arguments relate to the threshold pressures (where they exist) required for gas entry into the end face of bentonite samples in a linear flow geometry; for example, are different modes of failure involved in the different geometries.

The high gas entry pressure in some constant volume experiments may be suggestive that the threshold pressure is sensitive to the boundary conditions, although theoretical studies [Swift et al., 2001] suggest that the amount of deformation of the clay required for the formation of gas pathways may be too small for gas flow to be strongly influenced by boundary conditions. This may particularly be the case for field-scale system, in which the gas at the entry point to the clay may not “see” the more distant boundary condition.

Where stresses and porewater pressures have been measured, couplings between gas flow events and these parameters have been observed, but the physics which controls these couplings has not been satisfactorily established.

In the cases in which a threshold pressure for gas entry into the clay is observed experimentally, which is most cases, once gas flow is established it is found that the flow will continue until the gas pressure is reduced substantially below the threshold pressure. Precisely why the gas flow continues at pressures considerably below the entry pressure and what controls the upstream pressure at which gas flow finally stops has not been established.

Modelling suggests that if gas flow occurs by capillary displacement, then this must occur in a large number of very small capillaries in order to reproduce the gas entry pressures and provide the observed gas permeability after breakthrough. A fissure propagation mechanism for creating gas pathways is thought likely to involve a very much smaller number of pathways. This implies a distinct difference in the nature of the gas pathways that are formed by these two mechanisms, although experimental data on the dimensions and numbers of gas pathways that might discriminate between the two would be difficult to obtain.

Some experiments have shown intermittency and instability in the flow of gas from the downstream end of the sample; this suggest that closing and reopening of pathways occurs. What controls this is not clear. For example, does it arise from mechanical closure of pathways or from capillary pressure effects. This
produces ambiguity in the way the downstream boundary condition should be defined. For models in which the gas permeability is dependent on gas pressure it is found that, for the gas pressure change with distance, most of the pressure drop occurs close to the downstream boundary. There is no data to determine whether this is a modelling artefact or a feature of real systems.

These uncertainties constitute considerable difficulties in the development of models of gas migration in bentonite, because of the ambiguity that results in the constitutive relationships needed for such models. However, it should be noted that the experimental data that has been collected does give a substantial degree of confidence that saturated compacted bentonite will function satisfactorily as a buffer material:

a) It has been shown that gas can pass through saturated bentonite buffers (although whether the rather high entry pressures that have been observed in recent “radial” flow experiments would actually be observed or be acceptable in full-scale systems is a matter for further consideration).

b) Very little water is expelled from the buffer by migrating gas.

c) When resaturated, the buffer seems to reseal, with restoration of the hydraulic and transport properties that it possessed prior to the passage of gas.

These features are seen to be key conditions for the performance of a buffer as far as gas migration is concerned. Note that if the buffer water saturation is not close to one, gas migration through the buffer is expected to occur easily.

To extend the model developed in Phase 2 of the GAMBIT Club project (the GAMBIT-GW model) to include a proper treatment of the stress field in the bentonite, the original plan was to use a sophisticated pre-existing finite element modelling code, FEAT. This has a macro language facility, which allows the definition of specific elasto-plastic models and the coupling, in the case of porous materials, of the stress-strain behaviour with fluid flow through the medium. This had the potential to make use of constitutive models of deformation behaviour that had already been developed for bentonite. However, it was found that the FEAT model would not handle the propagation of gas through the bentonite. Analysis of the problem pointed to the fact that the quadratic finite elements used in FEAT, which are well suited to stress analysis, were not appropriate for simulating the sharp front that was formed at the leading edge of a gas pathway propagating through the bentonite. Essentially the front developed oscillations which made the scheme unstable.

By consideration of an idealised version of the gas migration problem, an alternative numerical scheme was developed based on linear elements and a particular integration method which was guaranteed to be oscillation free in the idealised problem. This numerical approach has been used in the ENTWIFE package to implement a gas migration model that takes account of the stresses in the clay that develop as a consequence of the gas invasion. The ENTWIFE code provides the facility for
automatically generating finite element computer code from a model specification in the form of the model equations. This allows different models to be easily explored.

The model constructed using ENTWIFE contains the following features:

a) A generalised strain-stress relationship in which changes in strain depend not only on changes in stress but also on gas and water pore fluid pressures (equivalently the water pressure and the matric suction).

b) A condition for gas entry into the clay, which determines whether the gas pressure is high enough for gas to exist in the clay. This condition includes a term that keeps the gas pathways open even once the gas pressure has dropped below the entry pressure.

c) A model of the dependence of gas permeability on system variables. Here this relationship is simplified to a dependence on gas saturation.

Note that the clay deformation relationships implied by point (a) are assumed to be purely elastic. It was considered that an elastic model should be adequate for the small deformations that are expected to be involved in gas migration.

The model does not explicitly simulate fissure propagation, so for those experiments in which this mechanism is indicated, the approach necessarily provides only a continuum representation of the presence of fissures.

The model is designed to be an extension of the GAMBIT-GW model, and the relationship between this and the new model is described. However, inclusion of the full stress field has necessitated recasting the GAMBIT-GW model in terms of a number of elastic moduli, which means that some of the features of the GAMBIT-GW are not represented as they were previously, but are implied by the selection of the form specified for the elastic moduli, which may be as functions of model variables.

As for previous GAMBIT Club models, the new one has been tested by trying to simulate the results of some laboratory experiments. Models of experiments have been set up which mimic the imposed stress-strain boundary conditions.

For a linear flow experiment under (mostly) constant isotropic stress, the model reproduces the experimental results reasonably satisfactorily. For this experiment, gas entry is assumed to occur when the gas pressure exceeds the minimum principal effective stress.

An experiment, in which gas was injected from a central source in a constant volume of bentonite, was also modelled. In this model, as the applied gas pressure is increased, the gas exerts a boundary stress on the bentonite, causing both the stresses and the porewater pressure in the clay to evolve (a small amount of water may also be expelled from the clay). When the minimum principal effective stress becomes tensile, it is
assumed that gas can enter the clay. This condition is different from that used in the linear flow geometry because of the experimental evidence that gas migration in this system involves some degree of fracturing of the bentonite. The model successfully simulates the development of the stress field in the clay as the applied gas pressure is increased up to the point at which gas entry occurs. However, it subsequently fails during the propagation of the gas through the sample. The cause of this computational difficulty has not been established. It is not clear whether it is due to the inherent difficulty of modelling the propagation of a physically realistic sharp, unstable front, or whether there is something unphysical about the conceptual model being represented. Similar behaviour was found with the modelling of the migration of gas from a waste canister through buffer-bentonite at the field scale.

In addition to the work to model the effects of the stress field on gas migration in bentonite, two other separate extensions to the GAMBIT-GW model were investigated to see if they improved the capability to model experiments. The two factors to be investigated were:

a) the effect of the clay fabric on gas migration in bentonite; and

b) the introduction of additional hysteresis in the deformation response of the clay to gas pressure changes.

These improvements were investigated by introducing a dual porosity element into the GAMBIT-GW model, based on a distinction between interstack and intrastack porosity. These were assumed both to be initially water filled. Gas invasion would occur through the larger interstack voids. The extensions implemented in the GAMBIT-GW model to achieve this were:

a) characterisation of the porosity and permeability of the interstack channels;

b) a model for the transfer of water between the two types of porosity;

c) a model for gas entry into and displacement of water from the interstack channels;

d) a prescription of the relationship between interstack channel volume and water and gas pressures in the channels.

In the absence of experimental data that could be used to characterise the above features and relationships, modelling assumptions that were considered generally plausible but had no other justification had to be made.

Additional hysteresis in the model was introduced by providing for a time lag in the way that channel permeability responded to changes that affected the permeability.
It was found that the dual porosity version of GAMBIT-GW was no improvement over the original version in trying to reproduce the experimental results examined; indeed, it was more difficult to reproduce key features of the experimental results with the revised model that with the original one. The difficulty with the dual-porosity model appears to be that the presence of the pre-existing channels provided by the interstack pore space tends to dominate the gas migration behaviour and in fact produce a gas migration model that is more akin to a conventional porous-medium flow model than to the other types of model that have been proposed in the GAMBIT Club programme. The difficulties experienced in improving the fit to the data by using the dual-porosity model suggest that the mechanisms represented by this model are not a good description of the physical processes that govern gas migration in bentonite. Alternatively, it could be that the correct functional relationships from which to build such a model have not been found.

In summary, the results of the attempts described here to extend the GAMBIT-GW model introduced in Phase 2 of the GAMBIT Club project are as follows:

a) Careful analysis of the numerical requirements for modelling a sharp gas front advancing through bentonite clay indicates that finite-element schemes based on quadratic elements are not suitable and an alternative more robust numerical approach has been devised.

b) Using this approach, a model of gas migration in which the full (elastic) stress-strain behaviour of the clay is incorporated into the model, with gas entry being determined by the relationship between gas pressure and the local effective stress. This model has been implemented using the ENTWIFE program to construct finite element computer code directly from the model equations, which gives the flexibility easily to explore different modelling options.

c) At present the constitutive relationships governing gas entry into saturated bentonite and the relationships between gas pressure, water pressure, gas filled porosity, and the stresses and strains in the clay are not established, but the creation of the ENTWIFE model provides a tool through which different possibilities can be readily explored in future work. This could be particularly valuable as more experimental data become available.

d) The model incorporating the full stress field has been used successfully to model a BGS experiment on gas migration through a highly compacted water-saturated bentonite sample constrained under isotropic stress. For this linear flow configuration, the new model gives agreement with experiment that is comparable with that obtained with the original GAMBIT-GW model. For this experiment, under isotropic stress conditions, it is perhaps to be expected that detailed representation of the full stress field in a model is not required to simulate the experimental results.
e) Difficulties have been experienced in applying the model to radially symmetric models of gas flow in cylindrical coordinates, both in the case of flow from a “central” source in a constant volume experiment, and the case of gas migration from a canister in a field-scale application.

f) Simulations of the radially symmetric models proceed successfully to model the evolution of the stresses within the bentonite as the applied gas pressure builds up to the point at which gas entry would occur. The stress distribution shows where gas entry would occur in the model.

g) However, the model fails at present in modelling the propagation of gas across the bentonite once it has started to enter the clay in the radially symmetric models. Despite the investment of considerable effort, it has not been possible to resolve the outstanding computational difficulties satisfactorily, and this has limited the investigation of the effects of varying the details of the conceptual model of gas migration in bentonite.

h) Incorporation of representations of the clay fabric into a derivative of the GAMBIT-GW model by distinguishing between interstack and intrastack porosity did not provide any improvement in the ability to model experiments compared with the original GAMBIT-GW. The reason for this is that the connected interstack porosity added to the model dominates the gas migration behaviour, with the result that the model behaves more like a conventional two-phase porous medium flow model than one in which the porosity occupied by the gas is created by deformation and squeezing of water from the clay.

i) It is considered that further development of models of gas migration in bentonite is likely to depend on obtaining better characterisation of gas pathways in bentonite and of the couplings that exist in the clay between stress and strain, gas and water fluid pressures, and gas-filled porosity.
7 REFERENCES


ACKNOWLEDGEMENTS

The work reported here was funded by members of the GAMBIT Club: SKB, ANDRA, Enresa, JNC, Nagra, and Posiva Oy. The authors are grateful to these organisations for their support and encouragement of the work.

The authors also are grateful to Drs Steve Horseman and Jon Harrington for providing access to the unpublished results of experiments carried out at BGS, and for giving permission to reproduce their pictures of their experimental apparatuses.
APPENDIX A: THE DERIVATION OF THE GENERALISED HOOKE’S LAW

A.1 Single-phase Flow

Hooke’s Law:

\[ \varepsilon_{ij} = C_{ijkl} \sigma_{kl} , \]  

(A.1)

for an isotropic elastic material:

\[ C_{ijkl} = \frac{1 + \nu}{2E} \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) - \frac{\nu}{E} \delta_{ij} \delta_{kl} , \]  

(A.2)

can be generalised to the case in which a pore fluid is present [Biot, 1941; Rice and Cleary, 1976; Palciauskas and Domenico, 1989].

Here:

- \( \varepsilon_{ij} \) is the strain tensor [-];
- \( \sigma_{ij} \) is the stress tensor [Pa];
- \( C_{ijkl} \) is a 4th-order constant tensor of elastic moduli;
- \( \nu \) is Poisson’s ratio [-];
- \( E \) is Young’s modulus [Pa].

The generalisation assumes that:

a) There is a linear relation between the components of strain (including the change in the volume of the pore fluid, \( \Delta V_p \), per unit volume, \( V \)) and the components of stress (including the pressure of the pore fluid, \( p_w \)):

\[ \varepsilon_{ij} = C_{ijkl} \sigma_{kl} + \frac{1}{3H} p_w \delta_{ij} , \]  

\[ \frac{\Delta V_p}{V} = \frac{1}{H'} \frac{\sigma_{ij}}{3} + \left( \frac{1}{R} - \phi \beta_w \right) p_w . \]  

(A.3)

Here:

- \( H, H', R \) are material properties\(^1\) [Pa];
- \( \phi \) is the volume of the pore space per unit volume of the porous material (i.e. \( \phi = V_p / V \) [-]);
- \( \beta_w \) is the compressibility of the pore fluid [Pa\(^{-1}\)].

---

\(^1\)Biot [1941] considered the case of an incompressible pore fluid, and therefore neglected the term \( \phi \beta_w \) in Equation (A.3).
b) It is possible to define the strain energy per unit volume, or elastic potential:

\[ W = \frac{1}{2} \left[ \varepsilon_{ij} \sigma_{ij} + \frac{\Delta V}{V} p_w \right] \]

\[ = \frac{1}{2} \left[ C_{ijkl} \sigma_{ij} \sigma_{kl} + \left( \frac{1}{H} + \frac{1}{H'} \right) \frac{\sigma_{ij}}{3} p_w + \left( \frac{1}{R} - \phi \beta_w \right) p_w^2 \right] . \tag{A.4} \]

From the existence of the elastic potential, it follows that:

\[ C_{ijkl} = C_{klij} , \]

\[ H = H' . \tag{A.5} \]

Combining Equations (A.2), (A.3) and (A.5) gives Equation (3.2).

Note that an assumption implicit in the above derivation is that the components of strain and the components of stress should be work conjugate pairs.

### A.2 Two-phase Flow

Next, Biot’s [1941] model can be extended to the case of two-phase flow through a deformable porous medium.

![Diagram of two-phase flow](image)

**Figure A.1** An element of unsaturated clay (after Fredlund and Rahardjo, 1993).

As above, the generalisation assumes that:

a) There is a linear relation between the components of strain and the components of stress:

\[ \varepsilon_{ij} = C_{ijkl} \sigma_{kl} + \frac{1}{3H} p_w \delta_{ij} + \frac{1}{3} \frac{R}{H_m} p_g \delta_{ij} \]

\[ \frac{\Delta(S)_w V_p}{V} = \frac{1}{H'} \frac{\sigma_{ij}}{3} + \frac{1}{R} p_w + \frac{1}{J} p_g . \tag{A.6} \]

\[ \frac{\Delta(S)_g V_p}{V} = \frac{1}{H_m'} \frac{\sigma_{ij}}{3} + \frac{1}{R_m} p_w + \frac{1}{J_m} p_g . \]
Here:  
$$H, H_\text{w}, H', R, J, H'_m, J', R_m$$  are material properties [Pa]; 
$$S_g$$ is the volumetric saturation of the gas phase, which is related to $$S_w$$,  
the volumetric saturation of the liquid phase, by $$S_g = 1 - S_w$$ [-].

b) It is possible to define the strain energy per unit volume, or elastic potential:

$$W = \frac{1}{2} \left[ \varepsilon_{ij} \sigma_{ij} + \frac{\Delta(S_w V_p)}{V} p_w + \frac{\Delta(S_g V_p)}{V} p_g \right].$$  \hspace{1cm} (A.7)

From the existence of the elastic potential, it follows that:

$$C_{ijkl} = C_{klij}$$  
$$H = H'$$,  
$$H_m = H'_m$$,  
$$J = J'$$.

(A.8)

c) In addition, it is assumed that the solid grains are incompressible. Consequently, the change in volume of a small element of the porous medium is equal to the change in pore volume of the element:

$$\varepsilon_{ij} = \frac{\Delta V_p}{V}.$$  \hspace{1cm} (A.9)

Using this constraint in Equation (A.6) implies that:

$$\frac{1}{H} = \frac{1}{K} - \frac{1}{H_m}$$  
$$\frac{1}{J} = \frac{1}{H_m} - \frac{1}{R_m}.$$  \hspace{1cm} (A.10)

Combining Equations (A.6), (A.8) and (A.10) gives Equations (3.14) and (3.15).

A.3 Incremental Stress-Strain Relation

The stress-strain relations derived in Sections (A.1) and (A.2) finally are written in incremental form to allow for the possibility that the material properties may depend on scalar invariants of the stress / strain state (e.g. see the discussion of Elastic Moduli in Section 3.1.2).
APPENDIX B: THE INSTABILITY OF A GAS-LIQUID INTERFACE

The behaviour observed when, for example, a gas flows in a Hele-Shaw cell\textsuperscript{13} filled with viscous fluid (assuming an initially plane interface) falls into one of three classes.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{schematic_diagram}
\caption{Schematic diagram of gas flow in a Hele-Shaw cell.}
\end{figure}

If $u$ [m s\textsuperscript{-1}] is the velocity of the interface due to an imposed pressure gradient, then:

(a) at small $u$, the interface between the two fluids is a straight boundary;

\textsuperscript{13} The geometry of a Hele-Shaw cell is shown schematically in Figure B.1. A volume of viscous fluid is trapped between two closely spaced plates. The spacing of the plates is $b$ and the half-width of the cell is $L$. 
(b) at intermediate \( u \), a perturbation to the interface grows to form a stable finger whose width is a calculable fraction of \( L \);

(c) at large \( u \), a chaotic behaviour is observed in which several fingers are formed that may branch or split.

The chaotic behaviour seen at large \( u \) is a classic example of the instability of a gas-liquid interface.

**B.1 Stability Analysis**

The first step towards understanding this behaviour [Chuoke et al., 1959] is to look at the stability of an almost plane interface. In particular, let the position of the interface, which moves with velocity \( u \) relative to the walls, be at \( x = ut \), and then suppose it is disturbed by a plane wave

\[
x = ut + A(t)\cos(qy)
\]

where the amplitude, \( A \) [m], is considered to be small and the wave vector is \( q \) [m\(^{-1}\)].

It is assumed, for the purpose of the mathematical analysis, that the gas and viscous fluid are separated by a sharp interface, across which the normal component of velocity is continuous and the pressure has a discontinuity determined by surface tension [Park and Homsy, 1984; Reinelt, 1987]. Thus,

\[
p_g - p_w = \frac{2\Sigma}{b} + \frac{\pi \Sigma}{4a}
\]

where:

- \( p_g \) is the pressure of the gas phase [Pa];
- \( p_w \) is the pressure of the viscous fluid [Pa];
- \( \Sigma \) is the surface tension [N m\(^{-1}\)];
- \( a \) is the local radius of curvature of the two-dimensional projection of the interface [m].

It follows from continuity of the normal velocity that the velocity potentials [Batchelor, 1967; Landau and Lifshitz, 1987] in the upper and lower fluid satisfy on the interface

\[
\frac{\partial \phi_w}{\partial \xi} = \frac{\partial \phi_g}{\partial \xi} = u + \dot{A}(t)\cos(qy).
\]

Hence, to first order in the amplitude \( A \),

\[
\phi_w = u(x - ut) - \frac{A(t)}{q}e^{-q(x-ut)} \cos(qy)
\]

and
\[ \phi_g = u(x-ut) + \frac{1}{q} e^{q(x-ut)} \cos(qy), \]  

(B.5)

de the being the appropriate solutions of \( \nabla^2 \phi_w = \nabla^2 \phi_g = 0 \) that satisfy Equation (B.3) and for which the disturbance vanishes at \( x \to \pm \infty \).

According to Darcy’s Law, the motion of a fluid in a homogeneous porous medium can be derived from a velocity potential

\[ -\frac{k}{\mu} (\rho + \rho g, x) \]  

(B.6)

where:

- \( k \) is the ‘permeability’ (in the case of a Hele-Shaw cell, \( k = b^2/12 \) [m²];
- \( \mu \) is the fluid viscosity [Pa s];
- \( \rho \) is the fluid density [kg m⁻³];
- \( g_i \) is the component of the acceleration due to gravity in the plane of the Hele-Shaw cell [m s⁻²].

It follows that, in the upper fluid (viscous fluid) the pressure is

\[ p_w = -\frac{\mu_w}{k} \phi_w + \rho_w g_i (x-ut), \]  

(B.7)

and in the lower fluid (gas) is

\[ p_g = -\frac{\mu_g}{k} \phi_g + \rho_g g_i (x-ut) + \frac{2\Sigma}{b}. \]  

(B.8)

A ‘free slip’ boundary condition on \( u \) at the side-wall requires the wave vector \( q \) to be

\[ q = \frac{\pi n}{L}, \quad \text{where } n \text{ is a positive integer}, \]  

(B.9)

and (from Equation B.2, where \( a \) has been approximated by \( d^2 y/dx^2 \)) the pressure drop through the interface is

\[ p_w \approx p_g - \frac{2\Sigma}{b} + \frac{\pi}{4} \Sigma \frac{d^2 x}{dy^2} \]

\[ = p_g - \frac{2\Sigma}{b} - \frac{\pi}{4} \Sigma q^2 (x-ut). \]  

(B.10)

Combining the above equations, by

(a) substituting in Equation (B.10) for \( p_w \) and \( p_g \) using Equations (B.7) and (B.8) respectively;
(b) substituting for $\phi_w$ and $\phi_g$ using Equations (B.4) and (B.5) respectively;

(c) substituting for $x$ using Equation (B.1);

and also neglecting terms of higher order in the amplitude $A$, gives

$$
\dot{A} = A \left[ \frac{u}{k/(\mu_w - \mu_g)} - \left( \rho_w - \rho_g \right) g_i - \pi \Sigma q^2 \right] \frac{k}{(\mu_w + \mu_g)q^2} . \quad (B.11)
$$

This result is easily interpreted. $A$ has an exponential dependence on time; when the quantity in parentheses is positive/negative the interface is unstable/stable against a disturbance of the given wave number. Since, according to Equation (B.9), the minimum value of $q$ is $\pi/L$, the initially flat interface will be unstable against some perturbation whenever the dimensionless parameter

$$
B = \pi^2 \frac{k}{L^2} \frac{1}{C_a} , \quad (B.12)
$$

where

$$
C_a = \frac{u(\mu_w - \mu_g) - k(\rho_w - \rho_g)g_i}{\frac{\pi \Sigma}{4}} . \quad (B.13)
$$

($C_a$ is a local capillary number, i.e. is of the form $u\mu/\Sigma$, where $u$ is the local velocity normal to the interface and $\mu$ is the viscosity of the viscous fluid.)

Taking account of the boundary conditions that apply at the edges of the cell, Bensimon et al. [1986] deduce from Equation (B.12) that the interface is unstable against perturbations of wavelength $l = 2\pi/q > 2L\sqrt{B}$. Surface tension tends to stabilise and smooth out the narrowest fingers, those with a radius of curvature less than $2L\sqrt{B}$. These narrow fingers have a large pressure drop across the interface at their tips; viscous fluid flows toward these low-pressure regions, pushing the fingers backward.
APPENDIX C: THE ATTEMPTED USE OF ‘FEAT’ TO INCLUDE THE STRESS TENSOR IN THE PHASE 2 GAS MIGRATION MODEL

At the outset of this project the intention was to implement the GAMBIT-GWS model using a pre-existing sophisticated finite-element program called FEAT (Finite Element Analysis Toolbox). FEAT has capabilities for analysing coupled problems in stress analysis, heat transfer and fluid flow, including flow in porous media. It has been used extensively in the British Nuclear industry by both British Energy and BNFL Magnox Generation, and has a long track record of successful application to engineering problems relevant to the reactor systems used in the UK.

FEAT is currently supported and maintained by Serco Assurance on behalf of British Energy and BNFL Magnox Generation. The FEAT web site (www.featsite.com) contains much useful information about FEAT, including case studies illustrating its application. The user documentation for the code can be viewed or downloaded.

One of the main attractions of FEAT from the point of view of this project, besides its reputation for quality, was that it has a wide range of capabilities for stress analysis. In particular, FEAT supports a number of different models for plastic deformation. The yield surface can be prescribed as a function of the mean stress and the Von Mises stress, and the flow law does not have to be of the associated type. These inputs to the plasticity model can be specified using FEAT’s powerful programmable command language. In particular, it is not necessary to write additional Fortran or C code in order to specify the plasticity model. The CLAYTECH [Borgesson et al., 1995] model for the elastic-plastic behaviour of certain clays has been implemented in FEAT using the command language interface.

The first task undertaken on the project was to implement Biot’s consolidation model in FEAT. Initially, this was done using FEAT’s command language. The coupling between the water flow and the stress model was treated explicitly, and although this worked well in some cases, in others convergence was slow. The model therefore was implemented in Fortran. The performance of FEAT for Biot’s consolidation model was very good. In particular, the program was applied to the test case described in Section 3.2.2, and the results are shown in Figures C.1 and C.2.
Comparison of FEAT results for the displacement of the top of the column (crosses ×) with the analytic solution (solid line) for one-dimensional consolidation.

**Figure C.1** Comparison of FEAT results for the displacement of the top of the column (crosses ×) with the analytic solution (solid line) for one-dimensional consolidation.

Next, the full GAMBIT-GWS model was implemented in FEAT in Fortran. It is a large and complicated model, and proved quite difficult to implement. Nevertheless, after careful checking and testing the model was implemented accurately. However, FEAT did not perform well even for the simple test cases that were tried. Typically the program would take a large number of time steps, and would show signs of numerical instability close to the region where the pressure first exceeds the threshold value for the transition from dissolved to free gas.

**Figure C.2** Comparison of FEAT results for the pressure at the bottom of the column (crosses ×) with the analytic solution (solid line) for one-dimensional consolidation.
After trying a number of ad hoc modifications to get FEAT to perform better, it became clear that a more radical approach was required. At that point the finite-element program ENTWIFE, with both its greater flexibility and its rapid prototyping capability based on a symbolic-algebra pre-processor, was used to study simplified versions of the GAMBIT-GWS model.

With hindsight, and the understanding developed from the work described in Section 3.2, it is clear that the reason for FEAT’s poor performance on this problem was that it is based on a standard implementation of the Galerkin finite-element method. This works well for the sort of problems to which FEAT normally is applied. However, a crucial feature of the GAMBIT-GWS model is that it generates very sharp fronts in the gas pressure, and under these circumstances the Galerkin finite-element method performs poorly.
APPENDIX D: MATHEMATICA FILE DEFINING THE GAMBIT-GWS MODEL FOR INPUT TO ENTWIFE’S PRE-PROCESSOR

(* PREAMBLE *)
(* PREAMBLE *)

(* fn[x] is an approximation to Heaviside's Function, i.e. 1 / ( 1 + Exp[-2x] ). *)

Derivative[1][ fn][x_] := dfn[x]
Derivative[1][dfn][x_] := d2fn[x]

(* gn[x] is Sinh[x] / x, which is indeterminate at x = 0. *)

Derivative[1][ gn][x_] := dgn[x]

(* Tiny is the Sqrt[ smallest positive double precision number ]. *)

Tiny = Sqrt[ 2^( -1021 - 1 ) ]

(* PARAMETERS *)
Young    = pvals[1]
Poisson   = pvals[2]
HMatric   = pvals[3]
RMatric   = pvals[4]
DenW0     = pvals[5]
FW0       = pvals[6]
BW        = pvals[7]
ViscW     = pvals[8]
Por0      = pvals[9]
PermPW    = pvals[10]
g         = pvals[11]
MolGas    = pvals[12]
RGas      = pvals[13]
T         = pvals[14]
ViscG     = pvals[15]
Henry     = pvals[16]
DiffG     = pvals[17]
Tortuosity= pvals[18]
PermPG    = pvals[19]
CritSatG  = pvals[20]
IrredSatG = pvals[21]
DLogSatG  = pvals[22]
RFRac     = pvals[23]
Tensile   = pvals[24]
SurfTens  = pvals[25]
DPG       = pvals[26]
Lagrange = pvals[27]
Scale = pvals[28]

(* COORDINATES *)

R = r[1]
Z = r[2]

(* VARIABLES *)

U = var[1]
dUdt = vart[1]
d2Udrt = dvdrt[1,1]
d2Udzt = dvdrt[1,2]

W = var[2]
d2Wdrt = dvdrt[2,1]
d2Wdzt = dvdrt[2,2]

Srr = var[3]
Syy = var[4]
Szz = var[5]
\[
\begin{align*}
Srz & = \text{var}[6] \\
Por & = \text{var}[?]
\end{align*}
\]
\[
\begin{align*}
PW & = \text{var}[8] \\
\text{dPWdt} & = \text{var}[8] \\
\text{dPWdr} & = \text{dvdr}[8,1] \\
\text{dPWdz} & = \text{dvdr}[8,2]
\end{align*}
\]
\[
\begin{align*}
G & = \text{var}[9] \\
\text{LKrr} & = \text{var}[10] \\
\text{LKzz} & = \text{var}[11] \\
\text{LKrz} & = \text{var}[12]
\end{align*}
\]
\[
\begin{align*}
\text{PG} & = \text{var}[13] \\
\text{dPGdt} & = \text{var}[13] \\
\text{dPGdr} & = \text{dvdr}[13,1] \\
\text{dPGdz} & = \text{dvdr}[13,2]
\end{align*}
\]
\[
\begin{align*}
\text{GR} & = \text{var}[14] \\
\text{dGRdr} & = \text{dvdr}[14,1] \\
\text{dGRdz} & = \text{dvdr}[14,2]
\end{align*}
\]
\[
\begin{align*}
GZ & = \text{var}[15]
\end{align*}
\]
dGZdr = dvdr[15,1]
dGZdz = dvdr[15,2]

(* AUXILIARY VARIABLES *)

SatG = fn[ G ]
dSatGdt = dfn[ G ] vart[9]

(* PROPERTIES of the bulk phase *)

(* Definitions of some elastic constants *)

Mu = Young / 2 / ( 1 + Poisson )
Lambda = Young Poisson / ( 1 + Poisson ) / ( 1 - 2 Poisson )
K = Young / 3 / ( 1 - 2 Poisson )

(* Definition of the strain tensor *)

dErrdt = d2Udrt
dEyydt = dUdt / R
dEzzdt = d2Wdzt
\[ dE_{zdrt} = \frac{d^2U_{zdrt} + d^2W_{zdrt}}{2}; \]
\[ dE_{zrdt} = dE_{zdrt} \]
\[ dVolumedt = dErrdt + dEyydt + dEzzdt \]

(* Calculation of the principal stresses *)

\[
\text{PrincipalStress}[1] = \frac{(S_{rr} + S_{zz})}{2} - \sqrt{\left(\frac{\text{Sr}_z}{2} + \left(S_{rr} - S_{zz}\right)^2 / 4 + \text{Tiny}\right)}
\]
\[
\text{PrincipalStress}[2] = S_{yy}
\]
\[
\text{PrincipalStress}[3] = \frac{(S_{rr} + S_{zz})}{2} + \sqrt{\left(\frac{\text{Sr}_z}{2} + \left(S_{rr} - S_{zz}\right)^2 / 4 + \text{Tiny}\right)}
\]

(* Calculation of the octahedral normal stress *)

\[
SO_{Oct} = \frac{(S_{rr} + S_{yy} + S_{zz})}{3}
\]
\[
dSO_{Octdt} = \frac{(dS_{rr}dt + dS_{yy}dt + dS_{zz}dt)}{3}
\]

(* Evaluation of the clay fracture criterion *)

\[
\text{Derivative}[1,0,0,0,0,0][\text{Curv}][x_1_,x_2_,x_3_,x_4_,x_5_,x_6_] := d\text{Curv}1[x_1_,x_2_,x_3_,x_4_,x_5_,x_6_]
\]
\[
\text{Derivative}[0,1,0,0,0,0][\text{Curv}][x_1_,x_2_,x_3_,x_4_,x_5_,x_6_] := d\text{Curv}2[x_1_,x_2_,x_3_,x_4_,x_5_,x_6_]
\]
\[
\text{Derivative}[0,0,1,0,0,0][\text{Curv}][x_1_,x_2_,x_3_,x_4_,x_5_,x_6_] := d\text{Curv}3[x_1_,x_2_,x_3_,x_4_,x_5_,x_6_]
\]
\[
\text{Derivative}[0,0,0,1,0,0][\text{Curv}][x_1_,x_2_,x_3_,x_4_,x_5_,x_6_] := d\text{Curv}4[x_1_,x_2_,x_3_,x_4_,x_5_,x_6_]
\]
\[
\text{Derivative}[0,0,0,0,1,0][\text{Curv}][x_1_,x_2_,x_3_,x_4_,x_5_,x_6_] := d\text{Curv}5[x_1_,x_2_,x_3_,x_4_,x_5_,x_6_]
\]
Derivative[0,0,0,0,0,1][Curv] [x1_,x2_,x3_,x4_,x5_,x6_] := dCurv6[x1,x2,x3,x4,x5,x6]

Curvature = Curv[ GR, dGRdr, dGRdz, GZ, dGZdr, dGZdz ]

FracCriterion = fn[ ( ( PrincipalStress[1] + PW - Tensile ) - SurfTens Curvature + PG ) / DPG ] +
fn[ ( ( PrincipalStress[2] + PW - Tensile ) - SurfTens Curvature + PG ) / DPG ] +
fn[ ( ( PrincipalStress[3] + PW - Tensile ) - SurfTens Curvature + PG ) / DPG ]

(* Specification of the [functional dependencies of the] multiphase elastic moduli *)

InverseHMatric = 0 / HMatric
InverseRMatric = FracCriterion / RMatric +

(* PROPERTIES of the liquid phase *)

(* Specification of the density for the liquid phase *)

DenW = DenW0 Exp[ BW ( PW - PW0 ) ]

(* Specification of the saturation for the liquid phase *)
SatW = 1 - SatG
\( d\text{SatW}dt = - d\text{SatG}dt \)

(* Calculation of the filtration velocity *)

\[ Q_r = - \frac{\text{PermPW}}{\text{ViscW}} ( \frac{d\text{PW}dr}{d} ) \]
\[ Q_z = - \frac{\text{PermPW}}{\text{ViscW}} ( \frac{d\text{PW}dz + \text{DenW} g}{d} ) \]

(* PROPERTIES of the gas phase *)

(* Specification of the density for the gas phase *)

\[ \text{DenG} = \left( \frac{\text{MolGas}}{\text{RGas}} \div \text{T} \right) \text{PG} \]

(* Calculation of the permeability tensor for the gas phase *)

\[ \text{KInvariant} = \{ \left( \frac{\text{LKrr} + \text{LKzz}}{2}, \sqrt{\left( \text{LKrz} \right)^2 + \left( \text{LKrr} - \text{LKzz} \right)^2 / 4 } + \text{Tiny} \right) \} \]
\[ \text{Krr} = \text{Exp}[ \text{KInvariant[[1]]} ] \left( \cosh[ \text{KInvariant[[2]]} ] + \left( \frac{\text{LKrr} - \text{LKzz}}{2} \frac{\text{gn}[ \text{KInvariant[[2]]} ]}{\text{Krr}} \right) \right) \]
Kzz = Exp[ KInvariant[[1]] ] ( Cosh[ KInvariant[[2]] ] + 
- LKrr + LKzz ) / 2 gn[ KInvariant[[2]] ] )
Krz = Exp[ KInvariant[[1]] ] ( 0 + 
2 LKrz ) / 2 gn[ KInvariant[[2]] ] )

(* EQUATIONS for the bulk phase *)

(* Generalisation of Biot's Law, assuming incompressible solid grains *)

dSrrdt = Lambda dVolumedt + 2 Mu dErrdt - SatW dPWdt - SatG dPGdt - 
K InverseHMatric ( dPGdt - dPWdt )
dSyydt = Lambda dVolumedt + 2 Mu dEyydt - SatW dPWdt - SatG dPGdt - 
K InverseHMatric ( dPGdt - dPWdt )
dSzzdt = Lambda dVolumedt + 2 Mu dEzzdt - SatW dPWdt - SatG dPGdt - 
K InverseHMatric ( dPGdt - dPWdt )
dSrzdt = 2 Mu dErzdt; dSrdt = dSrdt

(* Force balance equations *)

StrainEnergy = R dN1dr dSrrdt + N1 dSyydt + R dN2dz dSzzdt + R ( dN2dr + dN1dz ) dSrdt

e[1] = Coefficient[StrainEnergy,N1]
er[1,1] = Coefficient[StrainEnergy,dN1dr]
er[1, 2] = Coefficient[StrainEnergy, dNldz]

er[2, 1] = Coefficient[StrainEnergy, dN2dr]
er[2, 2] = Coefficient[StrainEnergy, dN2dz]

(* [Total] stress equations *)

er[3, 1] = 0
er[3, 2] = 0

er[4, 1] = 0
er[4, 2] = 0

er[5, 1] = 0
er[5, 2] = 0

er[6, 1] = 0
er[6, 2] = 0

(* EQUATIONS for the liquid phase *)
(* Constitutive law for the porosity *)

er[7,1] = 0
er[7,2] = 0

(* Flow law for the liquid phase *)

PWRate[1] = DenW SatW Por BW
PWRate[2] = DenW Por
PWRate[3] = DenW SatW

PWFlux[1] = DenW Qr
PWFlux[2] = DenW Qz


e[8] = Coefficient[PWEquation, N8]
er[8,1] = Coefficient[PWEquation, dN8dr]
er[8,2] = Coefficient[PWEquation, dN8dz]
(* EQUATIONS for the gas phase *)

(* Constitutive law for the saturation of the gas phase *)

e[9] = Por dSatG \text{d}t - 
   (\text{InverseHMatric}) \left(dSO\text{ct} \text{d}t + dP\text{W} \text{d}t \right) - 
   (\text{InverseRMatric} - \text{InverseHMatric SatG}) \left(dP\text{Gd}t - dP\text{W} \text{d}t \right)

er[9,1] = 0 
er[9,2] = 0

(* Specification of the [log of the] permeability tensor for the gas phase *)

k[0] = 2 fn[ - \left( \text{var}[9] + \text{Log}\left(1 / \text{CritSatG} - 1 \right) \right) / 2 \right] / D\text{LogSatG} \right] \text{var}[9] / D\text{LogSatG} + 
      4 fn[ - \left( \text{var}[9] \right) \right] \text{var}[9]

k[1] = 0 
k[2] = 0

e[10] = \text{var}[10] - \left(k[0] + k[1] dSrrd\text{d}t + k[2] \left(dSrrd\text{d}t dSrrd\text{d}t + dSzrdt \text{d}S\text{z} \text{d}t \right) \right)

er[10,1] = 0 
er[10,2] = 0

e[11] = \text{var}[11] - \left(k[0] + k[1] dSzzd\text{d}t + k[2] \left(dSzrd\text{d}t dSzrd\text{d}t + dSzrd\text{d}t dSzrd\text{d}t \right) \right)

er[11,1] = 0 
er[11,2] = 0
er[12,1] = 0
er[12,2] = 0

(* Flow law for the gas phase *)

PGRate[1] = ( SatW MolGas / Henry + SatG MolGas / RGas / T ) Por
PGRate[2] = PG ( - MolGas / Henry + MolGas / RGas / T ) Por
PGRate[3] = PG ( SatW MolGas / Henry + SatG MolGas / RGas / T )

PGFlux[1] = - MolGas / Henry ( - PG Qr + SatW Por DiffG / Tortuosity dPGdr ) -
           ( DenG Krr / ViscG ( dPGdr ) + DenG Krz / ViscG ( dPGdz + DenG g ) )
PGFlux[2] = - MolGas / Henry ( - PG Qz + SatW Por DiffG / Tortuosity dPGdz ) -
           ( DenG Kzr / ViscG ( dPGdr ) + DenG Kzz / ViscG ( dPGdz + DenG g ) )


e[13] = Coefficient[PGEquation,N13]
er[13,1] = Coefficient[PGEquation,dN13dr]
er[13,2] = Coefficient[PGEquation,dN13dz]

(* Curvature for the pressure of the gas phase *)
\[ m = \text{Table}[\text{xhat}[l,k], \{l,2\}, \{k,2\}] \]

\[ dG = \text{Table}[m[[l]].\{GR - dPGdr, GZ - dPGdz\}, \{l,2\}] \]
\[ d2G = \text{Table}[m[[l]].\{m[[l,1]] dGRdr + m[[l,2]] dGRdz, m[[l,1]] dGZdr + m[[l,2]] dGZdz\}, \{l,2\}] \]

\[ F = (dG[[1]])^2 + \text{Lagrange} (dG[[1]] + dx[1] d2G[[1]])^2 + (dG[[2]])^2 + \text{Lagrange} (dG[[2]] + dx[2] d2G[[2]])^2 \]

\[ \text{ElementArea} = 4 \, dx[1] \, dx[2] \sqrt{\text{Det}[m]^2} \]

\[ e[14] = \text{Scale} (\text{D}[F, GR]) / \text{ElementArea} \]
\[ er[14,1] = \text{Scale} (\text{D}[F, dGRdr]) / \text{ElementArea} \]
\[ er[14,2] = \text{Scale} (\text{D}[F, dGRdz]) / \text{ElementArea} \]

\[ e[15] = \text{Scale} (\text{D}[F, GZ]) / \text{ElementArea} \]
\[ er[15,1] = \text{Scale} (\text{D}[F, dGZdr]) / \text{ElementArea} \]
\[ er[15,2] = \text{Scale} (\text{D}[F, dGZdz]) / \text{ElementArea} \]

POSIVA 2004-01 Reduction of Uranyl Carbonate and Hydroxyl Complexes and Neptunyl Carbonate Complexes Studied with Chemical-Electrochemical Methods and Rixs Spectroscopy
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April 2004
ISBN 951-652-127-4

POSIVA 2004-02 Modelling Gas Migration in Compacted Bentonite: GAMBIT Club Phase 3 Final Report
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Serco Assurance
April 2004