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Modelling Gas-Water Flow at Oberbauenstock

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SUMMARY

Site characterization activities at NAGRA's potential low- and intermediate-level waste repository at Oberbauenstock have indicated the presence of an anomalous pressure zone within the potential host rock (Valanginian Marl). Two conceptual models have been proposed to relate the observed pressure anomaly to the presence of natural gas within the marl. Model A assumes that the underpressured conditions have originated due to the transient discharge of gas from a relatively localized gas "bubble" into the adjacent Seelisberg tunnel. Model B assumes that the observed low pressures are caused by regional (quasi) steady-state upward gas migration from some deeper source.

This report presents a set of quantitative analyses, using analytical and numerical models, to evaluate the two conceptual models. Material balance calculations with simple analytical equations suggest that gas depletion from a localized region into the tunnel can result in pressure profiles similar to those observed during testing. Detailed site-scale modelling with the multiphase Simulator TOUGH, using a 2-D vertical cross section of the Oberbauenstock region, also suggests that the scenario presented in Conceptual Model A is more likely than the Model B scenario. Thus, both local- and regional-scale modelling studies indicate that the underpressuring is most likely the effect of gas discharges into the Seelisberg tunnel via some high-conductive flow paths. The presence of gas alone does not appear to be a sufficient explanation for the observed anomalous pressure conditions.
ZUSAMMENFASSUNG

Im Rahmen der Standortuntersuchungen am Oberbauenstock, einem der vier potentiellen Standorte für schwach- und mittelaktive radioaktive Abfälle, konnte im potentiellen Wirtgestein (Valanginien-Mergel) die Existenz einer Zone mit anomal tiefem hydraulischem Druck nachgewiesen werden. Zwei konzeptionelle Modelle wurden vorgeschlagen, die die beobachtete Druckanomalie in Zusammenhang mit einem natürlichen Gasvorkommen im Mergel bringen. Modell A nimmt an, dass der Unterdruckzustand durch eine vorübergehende Entgasung eines relativ begrenzten, lokalen Gasvorkommens via den benachbarten Seelisbertunnel während dessen Bauphase verursacht wurde. Modell B führt die beobachteten tiefen Drücke auf eine regionale, aufwärtsgerichtete Gasmigration aus einer tieferliegenden Gasquelle zurück, die unter (quasi) stationären Bedingungen abläuft.

RESUME

Les activités de la Cedra liées à la caractérisation du site potentiel de l'Oberbauenstock pour déchets de faible et moyenne activité ont montré la présence d'une zone de pression anormale à l'intérieur de la roche d'accueil (marnes valanginiennes). Deux modèles conceptuels ont été proposés pour relier l'anomalie de pressions à la présence de gaz naturel dans les marnes. Le modèle A postule que les conditions de sous-pression sont dues à une décharge instationnaire de gaz à partir d'une bulle de gaz relativement localisée vers le tunnel adjacent du Seelisberg. Le modèle B prévoit que les basses pressions observées sont causées par une migration (quasi) stationnaire de gaz à partir d'une source profonde vers la surface.

Le présent rapport présente un ensemble d'analyses quantitatives, utilisant des modèles analytiques et numériques, afin d'évaluer ces deux modèles conceptuels.

Des calculs de bilan de masse avec des équations analytiques simples suggèrent que la décharge de gaz à partir d'une région définie vers le tunnel peuvent produire des profils de pression similaires à ceux observés durant la phase de tests.

Une modélisation à l'échelle du site avec le simulateur multiphase TOUGH, basé sur une profil vertical (2 D) de la région de l'Oberbauenstock, suggère également que le scénario présenté dans le modèle conceptuel A est plus probable que le modèle B. Ainsi, tant le modèle local que regional indiquent que la sous-pression est le plus probablement l'effet de gaz s'écoulant dans le tunnel du Seelisberg via quelque voie hautement perméable. La présence de gaz à elle seule n'est pas une explication suffisante pour les conditions de pression anormales observées.
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INTRODUCTION

1.1 Background, Location, Geology

NAGRA’s potential repository site for low- and intermediate-level wastes at Oberbauenstock (OBS) is located in the Canton of Uri, close to the west shore of Urnersee (Lake Uri) in the vicinity of the Seelisberg Tunnel (Figure 1.1). The basic concept of the OBS repository project is to store the radioactive waste in a horizontally accessed cavern system located at depth in geologic units of low permeability. The OBS area has a rugged relief which is typical of an alpine setting (Figure 1.2). Urnersee is the deepest main drainage in the system with an elevation of about 433 masl. The nearby peaks of Oberbauenstock and Niederbauen are at elevations of 2217 m and 1923 m, respectively. The host rock consists of marls of Valanginian age with variable clay and carbonate content, laminated, overprinted by alpine tectonics and with very low grade metamorphosis. The underlying rock is Valanginian limestone along with Tertiary sandstones and shales. Local discontinuities occur in the entire series of rocks. Fault lineaments and scraps are visible in both plan and cross-sectional landscape perspectives. The original flow system concept was that the Valanginian marls were made up of extensive thicknesses of matrix rock with rare but significant discontinuities in which most of the fluid movement was expected to occur. A system consisting of two shear zones and one bedding plane system was believed to be associated with the region. Investigations from the Phase 1 testing program (OBS-1) have indicated that this generalization is true. Detailed study of the geology of the project cores as well as geophysical work have indicated that the folding and faulting in the vicinity of the site are rather complex. Flow pathways are believed to occur definitely outside the rock matrix.

1.2 Gas at OBS - Historical Evidence

During the excavation of the Seelisberg Tunnel (1971-1978), it was apparent that methane gas was ubiquitous in the Valanginian marl to varying degrees. In some places only gas bubbles were observed, while more or less continuous gas blowers (Bläsers) were encountered at other locations. These observations are described in detail in SCHNEIDER & KAPPELER (1984). Given our present interest in gas at OBS, it is unfortunate that very limited data exist on the in-situ pressures of the free gas encountered in exploratory borings in advance of the tunneling operations. Also, there is no definite information on the gas volumes vented to the outside. The most significant gas shows encountered during the excavation of the Seelisberg Tunnel and related underground openings occurred in the vicinity of the exploratory borings drilled later during OBS-1. These data are summarized in ANDREWS (1988). Of particular interest is the pressure of about 5 bars observed in one borehole, and the reported gas flux of 2 to 3 l/s produced over 10 years from another
borehole. In addition, during times when the tunnel ventilation system was turned off, the observed methane concentration buildup indicated an average gas flux between 0.12 and 0.46 l/s per kilometer of tunnel. Methane gas shows at the surface have been observed at several localities around the Vierwaldstättersee (BüCHI 1971; PFISTER 1972). Gas shows were also observed along several transects performed near Bauen and Seelisberg during the construction of the tunnel (SCHNEIDER & KAPPELER 1984). The source rocks for methane gas are believed to include both the marl itself, as well as underlying Tertiary sediments or possibly even Permo-Carboniferous sediments with gas seepage occurring along discontinuities in the Valanginian marl and other overlying strata (SCHNEIDER & KAPPELER 1984).

1.3 Results of OBS-1 Testing

In the course of a first phase of site investigations named OBS-1, NAGRA carried out a drilling and testing program in 1987. The general objective was to determine the geological, petrophysical and hydrogeological characteristics of the Valanginian marl. The OBS-1 testing program was performed from three boreholes drilled from the existing gallery (ca. 493 masl) which is an auxiliary structure of the Seelisberg Road Tunnel. Two shallow boreholes, HVB (vertical) and HGB (inclined at 42 degrees) were drilled to a total depth of 100 m, and the third borehole, SA (vertical), was drilled to a total depth of 350 m. The locations of these boreholes with respect to the Seelisberg Tunnel are shown in Figure 1.3.

1.3.1 Observations of Methane during OBS-1

Many direct and indirect observations of the occurrence of methane gas in the Valanginian marl were made during the OBS-1 testing program. These include: (i) methane and ethane concentrations of the drilling fluid during drilling, (ii) gas pressure buildup in the short vertical borehole (HVB) following its completion and capping, (iii) chemical and isotopic analysis of gas which accumulated in HVB, (iv) whole core and crushed core gas analysis, and (v) underpressured conditions observed during hydraulic testing.

1.3.2 Hydraulic Testing

Hydraulic testing involved isolating selected intervals using inflatable packers in either a single- or double-packer configuration and performing various transient tests including slug, pulse and constant rate/pressure tests. Interpretation of these tests were performed by three groups, and include a provisional interpretation based on initial field data reported in ANDREWS & HUFSCHMIED (1988), the final field interpretation reported in DAVIDSON & KENNEDY (1989), and detailed analysis of selected intervals reported in
ANDREWS et al. (1988). Estimates of hydraulic conductivities and static interval pressures obtained from this testing program are summarized below.

1.3.2.1 Hydraulic Conductivity Distribution

Figure 1.4 shows a simplified representation of the hydraulic conductivity profile, where the estimates of conductivity from ANDREWS & HUFSCHMIED (1988) are shown at the mid-point of the tested intervals. Hydraulic conductivities determined using packer tests ranged from about $10^{-7}$ m/s to less than $10^{-12}$ m/s. Most of the conductive features encountered during testing appear to be of limited lateral extent (ca. 10-100 m). These features may be divided into two classes, a more transmissive group with a transmissivity of about $4 \times 10^{-7}$ m$^2$/s comprising about 20% of the total, and a less transmissive group with an average transmissivity of about $10^{-8}$ m$^2$/s comprising the remainder. The matrix permeability of the marl is less than $10^{-11}$ m/s, while the bulk permeability of the marl is believed to be best represented by the geometric mean value of $10^{-10}$ m/s (ANDREWS 1988).

1.3.2.2 Static Pressure Distribution

Interval static pressures obtained from the three different sources mentioned above are generally consistent, especially in the conductive zones. Figure 1.5 shows a graph of the average estimated interval pressure (obtained by taking the mean of the estimates from the three sources described above) reported at the transducer depth. The general trend of pressure increases with depth upto about 125 m, followed by a zone of anomalously low pressures down to about 200 m. Pressure again appears to increase with depth below the 200 m zone. The pressure increase with depth is significantly less than what would be expected for hydrostatic conditions, which suggests the existence of a downward hydraulic gradient for water and/or an upward gradient for gas.

1.4 Scope of Present Study

Conceptual models which seek to qualitatively explain the pressure anomalies observed at OBS have been presented previously (ANDREWS 1988). The focus of this study is on providing a quantitative explanation of observed underpressuring in the marl body. Chapter 2 summarizes the key features of the conceptual models detailed by ANDREWS (1988). Simple analytical and numerical models of the near-tunnel region are used in Chapter 3 to relate the degree of underpressuring to the amount of gas reportedly vented into the Seelisberg Tunnel. Chapter 4 describes the development and application of a regional-scale model of gas-water flow. Finally, Chapter 5 presents a summary of the work related to hydrogeologic modelling of OBS. Appendix A briefly describe some basic concepts related to two-phase flow and the TOUGH code.
(1) regional model boundary, (2) Seelisberg Tunnel, (3) potential repository, (4) potential access gallery, (5) location of boreholes for phase-1 test activities.

Fig. 1.1: Plan view of the Oberbauenstock site and associated underground features (after HUFSCHEIMID et al. 1989).
Fig. 1.2: Geologic cross-section through the Oberbauenstock site (after HUFSCHEIM et al. 1989).
Fig. 1.3: Location of test boreholes at Oberbauenstock (after KENNEDY & DAVIDSON 1989).
Fig. 1.4: Estimated hydraulic conductivity profile at OBS.
Fig. 1.5: Estimated static pressure profile at OBS.
2 CONCEPTUALIZATION OF THE HYDROGEOLOGY AT OBS

During the first phase of testing at OBS, it was apparent that the estimated interval static pressures were much lower than what could be expected for hydrostatic as well as for reasonably conjectured dynamic conditions. Attention was therefore focussed on formulating some conceptual models for the hydrogeologic conditions for the Oberbauenstock site which would be consistent with observations. These are summarized below.

Figure 2.1 depicts the equivalent freshwater head profile estimated from the original pressure data. Also shown for comparative purposes are two head profiles predicted by hydrogeologic modelling prior to OBS-1 (HüRLIMANN 1987). These profiles assume that the strata underlying the marl is either a high permeability limestone aquifer, or a low-permeability shale aquitard. The observed heads clearly indicate underpressuring with respect to a reasonable groundwater flow regime, particularly in the zone between ca. 125-200 m.

Several causes can be envisioned to explain the observed underpressures at OBS, which include: (a) low regional head, (b) transient response following last ice age, (c) transient response following uplift and subsequent erosion, (d) transient tectonic response, (e) transient thermal response, (f) transient osmotic response, (g) transient diagenetic response, etc. However, the current consensus is that the low pressures have been caused by the degassing of marl over time, and two basic conceptual models have been postulated to explain the observed hydrogeologic conditions at OBS (ANDREWS 1988). These models are based on the idea that free gas in the Valanginian marl is responsible for the anomalous pressures, but they differ in the extent and cause of underpressurization. The basic elements of the two models are described in the following sections.

2.1 Conceptual Model A

Model A (Figure 2.2) consists of a relatively limited low pressure gas 'bubble' around the Seelisberg Tunnel. In this model, the observed low pressures are attributed to a degassing of gas filled (or partially filled) permeable features which intersect the tunnel. The degassing would have occurred rapidly following the intersection of the features by borings drilled in advance of the tunnel (which was observed) or by a slow degassing over time (which was also observed). The depressurization then represents a response of the groundwater flow regime to transients imposed by gas discharging into the Seelisberg Tunnel. As evidence supporting this model, we may cite:

- The permeable zones in the marl appear to be of limited extent.
- Gas discharges into the tunnel have been reported.
• The low conductivity of the marl implies that it would take a long time to refill the degassed zone.

• There exists a downward pressure gradient between the 100 m zone and the zone at about 160 m depth in the SA borehole.

• The head in the underlying units appears unaffected by the local depressurization.

On the negative side, we may list the following:

• The volume of the gas reported to have been released by the tunnel would occupy a significantly larger volume than could be explained by local degassing.

• Because the pressure drop has spread significantly throughout the rock, it is difficult to assume that the fracture zones are of limited extent.

2.2 Conceptual Model B

Model B (Figure 2.3) consists of a relatively large region of subnormal hydraulic pressures caused by more or less continual flow of gas from depth to the surface. Because free gas can flow at a much lower pressure gradient with depth than water, the pressure (and thus head) at any particular depth would be much smaller than under normal hydrostatic conditions. In this model, the flow regime may be more or less at steady state. The gas source in this model is presumably a reservoir of large areal extent located at some depth beneath the marl. In support of this model, we note:

• The volume of gas reported to have been discharged from one of the boreholes seems to require a much larger source area.

• The continual flow of gas seems to require an extensive feature connected to a larger source area.

• Gas shows have been reported at the surface over a wide area.

Facts which tend to refute the concepts of this model are:

• The gas flow is reported to have stopped after 10 years.

• There is a pressure reversal in the ca. 125-200 m zone.

• The formations below the underpressured zone appear to be unaffected by regional gas flow.
2.3 **Conceptual Model C**

As presented above, Models A and B represent two end-member scenarios of groundwater flow conditions at OBS, with reality perhaps falling somewhere in between. One might postulate an alternative conceptual model which combines the basic elements of both Models A and B. To recapitulate, there is a general flow of gas towards the surface from some source at depths beneath the marl. There is also an underpressured zone within the marl, created by degassing into the Seelisberg Tunnel. This zone was created because the rate of upward gas flux into the marl was smaller than the rate at which gas flowed into the tunnel. Since flow into the tunnel ceased after a period of approximately ten years, this would suggest that the original volume of the degassed zone has grown smaller with time by refilling due to the upward gas flux. The measurements from OBS-1 are indicative of only one instant in time, hence it is difficult to validate speculations about conditions at other times. Nonetheless, the alternative conceptual model presented above is an attempt to combine the advantages of Model A (i.e., an underpressured zone of limited extent within the marl, pressure reversals in the 125-200 m zone) with those of Model B (i.e., large volume of gas flow into the tunnel, surface gas shows over a wide area).
Fig. 2.1: Comparison of observed and predicted hydraulic head profiles at OBS (after HUFSCHEMIED et al 1989).
MODEL A: Local Potential Sink due to Outgassing

Fig. 2.2: Schematic cross-section of Conceptual Model A (after ANDREWS 1988).
MODEL B:
Regional Potential Sink due to Outgassing

Fig. 2.3: Schematic cross-section of Conceptual Model B (after ANDREWS 1988).
3 LOCAL-SCALE MODELLING

3.1 Scope and Objectives

As mentioned in the previous section, the results of Phase-1 testing at OBS (i.e., permeability and pressure measurements) have only been used in the past as a basis for proposing qualitative conceptual models of gas-water flow at OBS. Here we present a preliminary quantitative analysis using simple analytical and numerical models of the near-tunnel region with the objective of: (i) explaining the observed underpressures, and (ii) relating the degree of underpressuring to the amount of gas reportedly produced into the Seelisberg Tunnel. The basic premise of these calculations is similar to those postulated in Model A. We assume that the Valanginian marl contains a two-phase mixture of gas and water, with the gas being relatively more mobile than water. It is also assumed that the ca. 125-200 m interval is somehow connected to the tunnel, perhaps via a high conductive feature. This zone contributed essentially all the gas that was vented during the construction of the Seelisberg Tunnel, which has resulted in the observed underpressured conditions. Note that in the simplified analyses presented below, we have not included the effects of tunneling or the presence of the lake on regional gas-water flow.

3.2 Analytical Calculations

Figure 3.1 shows pressure as a function of depth from the floor of the Seelisberg Tunnel up to a depth of 200 m as measured in the HVB, HGB and SA boreholes. As in Figure 1.5, the pressure shown is the mean of the estimated pressures at the transducer depth. Although there is significant scatter in the data, a distinct trend of pressure increasing with depth at a rate of ca. 4 kPa/m can be observed. By extrapolating this apparent gradient line to the 125-200 m zone, it is possible to estimate apparent static pressures for this zone. These estimated static pressures are tabulated in Table 1 along with the pressures actually measured. As a first approximation one might assume that the difference between the estimated and measured values is due to gas production into the Seelisberg Tunnel from these intervals. Although it is unlikely that initial (pre-tunnel) static conditions in the marl were similar to current observations in the 0-100 m zone (or extrapolations thereof), our current objectives preclude considerations of more complex scenarios.

<table>
<thead>
<tr>
<th>Interval</th>
<th>Thickness (m)</th>
<th>Meas. Pr. (kPa)</th>
<th>Est. Initial Pr. (kPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>137.0 D</td>
<td>127 - 147</td>
<td>325</td>
<td>605</td>
</tr>
<tr>
<td>160.6 S</td>
<td>157 - 166</td>
<td>285</td>
<td>725</td>
</tr>
<tr>
<td>196.5 D</td>
<td>187 - 206</td>
<td>615</td>
<td>845</td>
</tr>
</tbody>
</table>
To further simplify the analysis, the ca. 125-200 m zone is taken to be a single interval with an initial pressure of 725 kPa and a current average pressure of 408 kPa. These values are the averages of the corresponding quantities as given in Table 3.1. For material balance calculations, the first scenario we consider is based on the reported gas production rate of 2-3 l/s for 10 years into the tunnel. In addition to this production history, we also consider the case of exponential decline starting from an initial rate of 2.5 l/s, because transient rate decline typically results when flowing against a constant back-pressure (i.e., 1 bar or 100 kPa at the tunnel).

### 3.2.1 Constant Production

For a gas reservoir producing from gas expansion due to pressure decline, a simple material balance yields: 

\[ \text{[Gas produced]} = \text{[Initial Gas]} - \text{[Gas currently in place]}, \]

or symbolically

\[ \frac{G_p}{T_{sc}} = \frac{p_i V_i / T_i}{p V / T_i} \]  \hspace{1cm} (3.1)

where \( G_p \) is the cumulative volume of gas produced at surface conditions (pressure \( p_{sc} \) and temperature \( T_{sc} \)), \( V_i \) is the initial gas in place at \( p_i \) and \( T_i \) and \( p \) is the current average reservoir pressure (CRAFT & HAWKINS 1959). Assuming a cylindrical reservoir with external radius \( r_e = 400 \) m, thickness \( z \approx 80 \) m (ca. 127-206 m interval), effective porosity \( \phi = 0.03 \) and average gas saturation \( S_g = 0.20 \) (FINSTERLE et al. 1990), initial gas in place is estimated to be \( V_i = 240 \times 10^3 \) m\(^3\). Further, assuming \( p_i = 725 \) kPa, \( p = 408 \) kPa, \( T_i = 293 \)°K (20°C), \( T_{sc} = 283°K \) (10 °C), and \( p_{sc} = 100 \) kPa, the cumulative gas production calculated from Eq. 3.1 is \( G_p = 735 \times 10^3 \) m\(^3\). If this is taken to be the total production over 10 years, the corresponding average rate is 2.3 l/s which agrees well with the reported range of 2-3 l/s. Note that these calculations are dependent on the assumed geometry as well as the initial conditions. Notwithstanding these uncertainties, we have demonstrated that this simple model of gas production and pressure decline from a \( \sim 400 \) m radius cylindrical reservoir of \( \sim 80 \) m thickness is consistent with actual observations.

### 3.2.2 Exponential Decline

As mentioned previously, exponential decline in the production rate typically results when flowing against a fixed back-pressure, i.e., atmospheric conditions in the tunnel. Although the sparse production data only indicates an apparent constant rate between 2-3 l/s for 10 years, we present here for completeness material balance calculations assuming exponentially declining production from a initial rate of 2.5 l/s. FETKOVICH (1980) has provided an expression to calculate gas in place for such conditions from a knowledge of the initial rate \( q_i \), the initial pressure \( p_i \) and the average reservoir pressure \( p \) at time \( t \), viz.
\[ V_i = \{p_{sc}T_j\}/\{T_{scp}\} \{q(t)\}/ln(p/p) \quad (3.2) \]

For \( q_i = 2.5 \text{ l/s}, t = 10 \text{ years}, p_i = 725 \text{ kPa}, p = 408 \text{ kPa} \), initial gas in place can be calculated from Eq. 3.2 to be \( V_i = 200 \cdot 10^3 \text{ m}^3 \). For the same cylindrical geometry considered previously, this volume translates to an equivalent external radius \( r_e = 365 \text{ m} \).

### 3.3 Numerical Modelling

In order to verify the analysis presented in Section 3.2, simulations of gas-water flow were conducted using the multiphase simulator TOUGH (PRUSS 1987). TOUGH is a numerical code for modelling the transport of gas, water and heat in porous and fractured media. It uses the Integrated Finite Difference formulation which allows a flexible specification of element geometries, volumes and connections. A previous application of TOUGH in the NAGRA program, for design calculations related to gas tests at the Grimsel Rock Laboratory, has been reported by FINSTERLE (1989). Some basic concepts related to the modelling of two-phase flow, and a brief description of TOUGH, are presented in Appendix A. The simulations reported in this section were intended to of an investigative nature, with the objectives of determining: (i) the degree of pressure depletion following gas flow into a permeable feature maintained at a constant pressure of 1 bar, and (ii) the corresponding gas flow rate history.

#### 3.3.1 Model Geometry and Assumptions

A 2-D cross-sectional geometry measuring 500 m across and 300 m deep was selected for the simulations, with the third dimension taken to be 500 m. The system was discretized into 8 rows (layers) and 8 columns using rectangular elements. The system was divided into three hydraulic zones, with the top three layers forming the first zone, the next two layers forming the second zone, and the final three layers forming the third zone. The second zone was selected so as to coincide with the permeable interval between 127-206 m. The first and the third zones were taken to be relatively impermeable.

Gas production was assumed to occur via a permeable feature (fracture?), represented by column 5, which was maintained at a constant pressure of 1 bar (100 kPa). The bottom layer (288-300 m) was kept at a constant pressure of 25 bars (2500 kPa). The top, left and right boundaries were taken to be no flow boundaries. Assumed initial conditions were a static gradient of 4 kPa/m with \( S_g = 0.6 \), from the tunnel floor downwards. Gas and water phase pressures were assumed to be the same, i.e., capillary effects were neglected. In the absence of any information concerning gas-water relative permeability curves for marl, Corey's functions were chosen with a residual gas saturation of 5% and a residual liquid saturation of 30%.
3.3.2 Results of Simulations

Two preliminary simulations were conducted in this initial modelling exercise. In the first simulation (Run 1), the fracture was assumed to be connected to all three hydraulic zones (i.e., all the eight layers). In the second simulation (Run 2), the fracture was assumed to be in connection only with the second zone (i.e., the two middle layers). A schematic of the discretizations used in Runs 1 and 2 are shown in Figure 3.2. The results from these two simulations are discussed below.

3.3.2.1 Pressure History

Figure 3.3 shows the pressure history at the centroid of the elements in column 4 which are connected to (or closest to) the producing fracture. Note that the depth of 166 m is the point at which the centroid of the most permeable zone (127-206 m interval) is located. In Run 1, the effect of gas production and the associated pressure decline appears to increase with depth. This is not surprising in view of the fact that: (a) all layers are connected to the fracture, and (b) the driving potential for gas flow into the fracture (maintained at a constant pressure of 1 bar) increases with depth - since the initial static pressure increases with depth. However, note the enhanced pressure drop in the most permeable layer (166 m depth) due to its higher permeability.

The pressure history in Run 2, when only the 127-206 m interval is connected to the fracture, is quite different from that of Run 1. The top layers do not contribute to flow and the pressure there is essentially unchanged. There is some flow from the bottom layers to the most permeable zone to replace the produced gas and hence there is some pressure drop, particularly in layer 6 (227 m) which is just below the second zone (layers 4 and 5). As expected, almost all the gas flowing into the tunnel is drawn from the middle zone which also exhibits a significant pressure drop. It is interesting to note that the pressure at 166 m is approximately 4.5 bars (450 kPa), which is remarkably close to the average pressure of 408 kPa estimated for the 127-206 m interval.

3.3.2.2 Gas Flow Rate History

The total gas flow rate into the fracture for Runs 1 and 2 is shown in Figure 3.4 as a function of time. These rates represent the average flow rates over successive 2 year intervals. In both cases, the rate drops from approximately 2 l/s at 1 year to about 1 l/s at 9 years. While these trends substantiate the arguments for performing material balance calculations using the exponential decline case, they are at variance with reported gas flow rates of 2-3 l/s remaining approximately constant for 10 years. However, the simulated flow rates are at least in the same range as the observed values. Note also that the total amount of gas produced over the 10 year period is approximately...
400·10$^3$ m$^3$ for both Run 1 and Run2. This is somewhat less than the estimated total of 790·10$^3$ m$^3$, assuming an average rate of 2.5 l/s for 10 years.

3.4 Summary

In this chapter, we have presented a reanalysis of the pressure data obtained from OBS-1 using simplified analytical and numerical models. Material balance computations show that a cylindrical reservoir with a radius of ca. 400 m can account for the observed gas production into the tunnel. Numerical computations using a 2-D cross-sectional geometry were performed with the multiphase simulator TOUGH. Preliminary simulations showed that realistic pressure profiles could be obtained when only the zone between ca. 125-200 m was allowed to be in communication with the conductive feature (representing the Seelisberg Tunnel). Computed gas flow rates generally declined with time, although the overall range was similar to observed flow rates.
Fig. 3.1: Estimated static pressure profile showing gradient.
Discretizations used for local-scale modelling.
Computed pressure history at the centroids of elements adjacent to the 'fracture'.
Fig. 3.4: Computed history of total gas flow into 'fracture'.
4 REGIONAL-SCALE MODELLING

4.1 Scope and Objectives

The analytical and numerical modelling work described in the previous chapter was confined to a small area extending downwards from the floor of the Seelisberg Tunnel so as to consider primarily local-scale effects. In this section, we develop a more comprehensive numerical model of gas-water flow at OBS which includes flow in a larger section of the geologic profile and also considers the effects of major topographic features such as Lake Uri. The numerical simulations are carried out in two stages. The objective of the first stage is to obtain a steady (or at least a quasi-steady) distribution of the pressure and saturation fields prior to the excavation/construction of the Seelisberg Tunnel. These distributions are then used as initial conditions for the second stage of the simulations in which gas discharges from the marl into the tunnel are investigated. Sensitivity analysis is carried out to evaluate the effects of uncertainty in assumed relative permeability and capillary pressure functions, boundary conditions, and model configuration.

The data available from OBS-1 testing are restricted to a small spatial domain near the tunnel openings. Therefore it is difficult to properly calibrate a model for the site with a much larger spatial scale, particularly in regions away from the test boreholes. Furthermore, there is considerable uncertainty regarding: (i) two-phase flow parameters appropriate for the marl, (ii) initial pressure and gas saturation distributions prior to tunnelling operations, (iii) nature of boundary conditions, etc. Such considerations have motivated the choice of a simplified hydrogeologic configuration for numerical modelling studies, as well as the use of measured pressure profiles for qualitative calibration purposes only. Our primary objective is thus to develop a model which can explain the observed underpressuring in the Valanginian marl while providing a numerical test for the hypotheses advanced in Conceptual Models A and B (cf. Section 2).

4.2 Model Description

The basic concepts used in the regional-scale modelling are similar to those used earlier for the local-scale studies. Gas is assumed to be present everywhere in the marl at a saturation higher than the residual saturation. There exists a gas 'reservoir' covering the depths of ca. 125-200 m below the tunnel where underpressuring was observed, which is assumed to have a lateral extent of ~500 m, a higher permeability than the marl, and also a higher gas saturation. This reservoir is linked to the tunnel via a connection which is activated only during the transient simulation phase (i.e., degassing of the marl into the tunnel). These concepts are similar to those outlined in Conceptual Model A. Furthermore, as provided in Conceptual Model B, we introduce a gas source at depth by assuming that the bottom boundary is a source of gas.
4.2.1 Model Domain

Figure 4.1 shows a WNW-ESE vertical stratigraphic section through Oberbauenstock. Note the presence of Lake Uri to the East, and the location of permeable limestone formations above and below the thick Valanginian marl. The model domain, depicted in Figure 4.2, is chosen to include primarily the marl and the underlying limestone, and is bounded from above by the contact with the limestone on the western flank, and by the steeply dipping ground surface to the east. The eastern boundary is taken to be the contact with Lake Uri, while the western boundary is arbitrarily located at a distance of approximately 2 km from the lake. A similar section was previously used by NAGRA (1985) in NGB 85-08 for modelling single-phase groundwater flow. Note that in Figure 4.2 the elevation of Lake Uri is taken as the reference depth so that the tunnel is now located at a vertical position of 60 m, with the underpressured zone located between -65 and -140 m.

4.2.2 Computational Grid

In order to utilize the suite of pre- and post-processing utilities developed in-house for the single-phase groundwater model FEM301, several interface programs were written to generate input files in TOUGH format as well as to process TOUGH output files for graphical display. Rectangular volume elements were used to discretize the flow domain in the x-z plane, with the thickness along the y-direction taken to be 1 m for convenience. The FEM301 utilities HSHRINK and VSHRINK were used to preserve a fine discretization near the tunnel and thus reduce the total number of elements. The sloping boundaries to the east and the west were represented via a stair-stepping sequence of elements. Special considerations in grid generation included: (a) representing the Seelisberg Tunnel as two 10 m x 10 m square elements approximately 50 m apart, and (b) providing special elements to link the 'reservoir' with the tunnel for the transient simulations. The final grid, shown in Figure 4.3, consisted of 374 elements with 687 connections between elements.

4.2.3 Boundary and Initial Conditions

Boundary conditions imposed on the model domain are similar to those used previously for 2-D single-phase modelling studies (NAGRA 1985). The sloping eastern flank boundary represents the ground surface in contact with the atmosphere and was also maintained at a 1 bar constant pressure. The sloping western flank was also assumed to be at atmospheric conditions, i.e., the hydraulic influence of the overlying limestone formations was assumed to be negligible. The section of the eastern boundary in contact with Lake Uri was kept at constant fluid potential. The underlying limestone formation was assumed to be in hydraulic connection with the lake and hence at the same potential as the lake. The western boundary was assumed to be impermeable.
The initial pressure field was estimated from the quasi-steady simulations subject to the given boundary conditions. The initial gas saturation was taken to be 40% in the 'reservoir', 25% in the marl, 15% in the boundary elements, and 16% in the underlying limestone - which was slightly above the residual value of 15% (see Table 2).

### 4.2.4 Formation Parameters

Although it is likely that the Valanginian marl is a complex fractured rock mass, the paucity of data necessitated the adoption of a homogeneous porous medium approach for modelling purposes. Formation parameters were taken from the results of well test interpretation using a single-phase approach (ANDREWS 1988), as well as a two-phase approach (FINSTERLE et al. 1990). The porosity of the rock body was taken to be 1% throughout the model domain. Three permeability classes were used to distinguish the marl, the underlying permeable limestone formation, and the gas 'reservoir' taken to be coincident with the observed underpressured zone. The elements comprising the western boundary, the eastern boundary, and the tunnels were assigned the same permeability as the marl. These parameters are also presented below in Table 2.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Permeability:</td>
<td>V.G. Marl: (10^{-17}) m²</td>
</tr>
<tr>
<td></td>
<td>Reservoir: (5 \times 10^{-16}) m²</td>
</tr>
<tr>
<td></td>
<td>Limestone: (10^{-15}) m²</td>
</tr>
<tr>
<td>Porosity:</td>
<td>1% (uniform value)</td>
</tr>
<tr>
<td>Model Thickness:</td>
<td>1 m (in y-direction)</td>
</tr>
<tr>
<td>Gas saturation:</td>
<td>V.G. Marl: 25%</td>
</tr>
<tr>
<td></td>
<td>Reservoir: 40%</td>
</tr>
<tr>
<td></td>
<td>Limestone: 16%</td>
</tr>
<tr>
<td></td>
<td>Boundary: 15%</td>
</tr>
<tr>
<td>Relative Perm.:</td>
<td>Corey (1954) function (Base Case)</td>
</tr>
<tr>
<td></td>
<td>(S_{wr} = 0.30, S_{gr} = 0.15)</td>
</tr>
<tr>
<td></td>
<td>Grant (1977) function (Sensitivity)</td>
</tr>
<tr>
<td></td>
<td>(S_{wr} = 0.30, S_{gr} = 0.15)</td>
</tr>
<tr>
<td>Capillary Pr.:</td>
<td>Narasimhan (1975) form (Sensitivity)</td>
</tr>
<tr>
<td></td>
<td>(P_e = \alpha = 1) bar, (\beta = 1)</td>
</tr>
</tbody>
</table>
No laboratory data regarding relative permeability ($k_r$) and capillary pressure ($P_c$) functions for the Valanginian marl are available. Previous attempts at estimating parameters of assumed functional forms for $k_r$-$S_g$ and $P_c$-$S_g$ relationships from the analysis of hydraulic test data (FINSTERLE et al. 1990) indicate considerable uncertainty in the results. Our approach therefore was to use the commonly used functional forms of COREY (1954) and GRANT (1977) as two end-members of a suite of likely relative permeability functions. The functional form suggested by NARASIMHAN (1975) was chosen as the default capillary pressure relationship for sensitivity analysis. Table 2 lists the parameters for the reference case and sensitivity simulations.

4.3 Simulation Scenarios

As mentioned previously, TOUGH simulations of gas-water flow were carried out in two stages. In the first stage, conditions prior to the excavation and construction of the Seelisberg Tunnel were investigated. Simulations of regional gas-water flow were conducted for a time period of 200 years to obtain quasi-steady distributions of pressure and gas saturation. The tunnel was introduced as a local sink (maintained at a constant pressure of 1 bar) at the onset of the second stage of simulations. This stage involved transient simulations for a 10 year period to account for gas flow into the tunnel directly from the adjacent marl, as well as indirectly from the gas reservoir via preferential connection elements also maintained at atmospheric (1 bar) pressure. Pressure and saturations were computed over the entire model domain as a function of time. Other quantities monitored include the vertical pressure profile adjacent to the tunnel, gas flow rate into the tunnel, and gas flow between different material types.

4.4 Simulation Results

Figure 4.4 shows the computed quasi-steady state pressure distribution (after 200 years) for the base case. Pressure contours indicate a spatial pattern that is closely related to the topography and the specification of constant pressure boundaries along the top western flank, the steeply dipping eastern flank, and the bottom. The pressure field also suggests an upward flow of gas and a downward flow of water.

Transient pressure distributions obtained after a further simulation period of 10 years are shown in Figure 4.5. The nature of the tunnels as local sinks is clearly visible. Note that flow from the reservoir to the tunnel is not seen because the connecting element between the two is not in the plane of the cross-section shown in the figure. Thus, the reservoir is indicated as a local sink to signify the amount of gas flowing in to replenish the volume flowing out to the tunnel.
The temporal evolution of vertical pressure profiles computed at the approximate mean location of the OBS-1 test boreholes are depicted in Figure 4.6. Also shown for comparative purposes are the estimated static pressures from hydraulic testing. It is worth noting here that the measured pressures are averaged over some (unknown) volume of rock, whereas the computed pressures only represent an average value over the appropriate element in the numerical model. Notwithstanding these differences, the simulated pressures appear to match the measured values reasonably well. Note in particular the agreement at the zone of maximum underpressuring. There is some overprediction for pressures just below the tunnel. This can be attributed to the fact that the permeability to gas in the near-tunnel region is insufficient to allow a greater volumetric depletion. No attempts were made to fine-tune the permeability of this region to obtain a better pressure match.

The total gas flow rate into the tunnel is shown in Figure 4.7. Recall that the observed gas influx in one borehole was in the range of 2-3 l/s (i.e., $2-3\times10^{-3}$ m$^3$/s). Assuming a formation thickness of 500 m, the average influx per meter thickness would be $5\times10^{-6}$ m$^3$/s. Our simulation results indicate an exponential decline in gas flow rates from 25 to $2\times10^{-6}$ m$^3$/s over a 10 year period. The nature of rate decline is consistent with the concepts of flow against a fixed back pressure (i.e., 1 bar at the tunnel), and the predicted range in flow rates compares well with the observed values.

Figure 4.8 is a bar graph showing relative gas flux between different material types. The amount of upward gas flow from the bottom limestone (gas source) into the marl is taken as the reference value. The order of magnitude by which gas flow between material type pairs (e.g., reservoir-tunnel, marl-tunnel, marl-reservoir, and marl-out_of_system) differs from the reference value is shown at three time slices. Note the relative importance of the flow from the reservoir into the tunnel at early times, and how it is balanced by the inflow from the marl into the reservoir at $t=10$ years - thus causing a relative stabilization in the reservoir pressure (Figure 4.6). Also note the reduction in the flow from the marl into the tunnel with time.

4.5 Sensitivity Analysis

Because of the inherent uncertainty in two-phase flow parameters as well as in model assumptions, a few simulations were carried out for sensitivity analysis purposes. The first simulation involved evaluating the concepts outlined in Conceptual Model B, viz., the existence of a gas source at depth without preferential flow of gas from the 'reservoir' into the tunnel. The objective of the second simulation was to use GRANT's (1977) function for relative permeability instead of the COREY (1954) model. Capillary effects, as represented by NARASIMHAN's (1975) parameterization, were added to the base case conditions for the final sensitivity simulation. The results of these calculations are described below.
4.5.1 Conceptual Model B

For this simulation, the grid was modified for the transient simulation so that the connections between the gas reservoir and the tunnel elements could be deactivated. The resulting vertical pressure profile is shown in Figure 4.9. Although there is some temporal movement in the profile immediately beneath the tunnel, the predicted pressures in the actual underpressured zone are much too high. This is obviously due to a lack of depletion of gas from the gas reservoir, leading to the stabilization of pressures at a much higher level. An examination of the gas flow rate history (Figure 4.10) indicates that the flow into the tunnel is also smaller than the base case, since the flow is restricted to the near-tunnel region only. These results suggest that the concepts of Conceptual Model B alone are unable to explain the underpressuring and the pressure reversal observed in the ca. 65-125 m vertical position. Elements of Conceptual Model A, viz. preferential connection between the tunnel and the 'reservoir', have to be incorporated into the overall model to provide a better explanation of the observed pressure anomalies.

4.5.2 Grant Relative Permeability Functions

The primary difference between the Grant and the Corey functions is that the Grant model predicts a much larger relative permeability to gas than the Corey model (see also Appendix A, Figure A.1). The relative permeability functions were changed from Corey's form to Grant's form but with the same values for the end-point saturations (Table 4.1). Figure 4.11 shows the vertical pressure profile predicted when using the Grant relative permeability functions. The higher pressure drop in the near tunnel region, compared to the base case (Figure 4.7), is consistent with the higher gas relative permeabilities induced by the Grant model. The gas flow rate history, depicted in Figure 4.12, exhibits the same declining trend as obtained for the base case simulations.

Although the agreement between the simulations results and the observed pressures as shown in Figure 4.11 is extremely good, it should be emphasized that various combinations of parameters can lead to similar responses for a two-phase flow system. Therefore too much importance should not be placed on the actual values of the parameters used in generating these responses. Of greater fundamental significance is the conclusion that gas flow into the tunnel, both from adjacent areas and the 'reservoir', is a plausible cause of the observed underpressuring - as explained in Conceptual Model A.

4.5.3 Capillary Pressure Effects

The base case simulations, presented in Section 4.4, do not include capillary pressure effects. This simplification was necessitated by the absence of any laboratory measured data, and the questionable value of the capillary
displacement pressure deduced from a gas injection test. In this sensitivity simulation, we use a typical capillary pressure functional form suggested by NARASIMHAN (1975). Parameters for this empirical model, given in Table 4.1, are considered to be reasonable in the absence of any other information. Figure A.2 in Appendix A shows the capillary pressure curve based on the assumed parameters. Note the increase in capillary pressure from 1 bar to approximately 10 bars as gas saturation increases from the residual value to its maximum (and the water saturation decreases).

The temporal evolution of vertical pressure profiles as computed by adding capillary pressure effects to the base case is depicted in Figure 4.13, and the corresponding gas flow rate history in Figure 4.14. It is interesting to note that both of these curves appear very similar to the base case responses shown in Figures 4.6 and 4.7. This suggests that when capillary pressures are roughly comparable to the ambient pressure levels ($-10^6$ bars), dynamic effects (e.g., flowing against a fixed back-pressure of 1 bar) seem to be more dominant. However, significant uncertainties in the capillary pressure function parameters preclude any definitive conclusions regarding the general influence of capillary pressure effects. The uncertainty is further compounded by our representation of a highly fractured heterogeneous system as an equivalent continuum.

4.6 Summary

In this chapter, we have described the development and application of a numerical model to simulate gas-water flow in a 2-D vertical cross-section at OBS. The basic hydrogeologic assumptions in the model are occurrence of gas throughout the Valanginian marl and presence of a gas ‘reservoir’ with some preferential connection to the Seelisberg Road Tunnel. External boundaries are explicitly incorporated, with the bottom boundary modified to act as a gas source. Quasi-steady state simulations conducted for a 200 year period suggest that the resultant pressure profile in the model domain is strongly topography dependent. Transient simulations for a 10 year period indicate that it is possible to duplicate the observed vertical pressure profile adjacent to the tunnel when a preferential connection between the underpressured zone and the road tunnel is established. Sensitivity analyses show that the results are more affected by the choice of the relative permeability curve than by capillary pressure effects - at least for the range of parameters investigated.

An important finding from our simulations is that the observed underpressuring cannot be explained solely by upward migration of gas as suggested by Conceptual Model B. It is necessary to have some depletion of the zone between -65 and -140 m (below the level of Umersee) in order to generate the observed pressure reversal. While it is not necessary that reality should include a horizontal gas ‘reservoir’ with a vertical connection to the tunnel, this is perhaps the most simplistic representation of a limited extent gas bearing feature with some preferential connection to the tunnel.
It is also important to emphasize again that several combinations of two-phase flow parameters can result in the same overall system response. We have not investigated the entire range of parameters, and hence, the 'best-fit' parameters should be considered only as indicative values. Since the available information is restricted to a small zone of the total modelled domain, one can only attempt to extract some very general ideas about the flow system. Our conclusions from this simulation study - guided by these principles - is that the underpressuring observed at OBS is most likely caused by the depletion of localized gas-bearing units into the Seelisberg Road Tunnel via some permeable flow paths, as originally indicated by Conceptual Model A.
Fig. 4.1: Vertical stratigraphic section through OBS (after NAGRA NGB 85-08 1985).
Fig. 4.2: Schematic diagram of the flow domain for the 2-D gas-water flow model of OBS.
Fig. 4.3: Integrated finite difference mesh for the 2-D model showing rock types with different material properties and/or boundary conditions.
Fig. 4.4: Computed quasi-steady (pre-tunnel) pressure distribution at $t = 200$ yr for base case.
Fig. 4.5: Computed transient pressure distributions after 10 years of gas flow into tunnel - base case.
Fig. 4.6: Comparison of estimated and computed vertical pressure profiles adjacent to tunnel - base case.
Fig. 4.7: Computed history of gas flow rate into tunnel - base case.
Fig. 4.8: Bar graph showing computed gas flow between different material types - base case.
Fig. 4.9: Comparison of estimated and computed vertical pressure profiles adjacent to tunnel - sensitivity simulation with Conceptual Model B.
Fig. 4.10: Computed gas flow rate history into tunnel - sensitivity simulation with Conceptual Model B.
Fig. 4.11: Comparison of estimated and computed vertical pressure profiles adjacent to tunnel - sensitivity simulation with Grant relative permeability model.
Fig. 4.12: Computed gas flow rate history into tunnel - sensitivity analysis with Grant relative permeability model.
Fig. 4.13: Comparison of estimated and computed vertical pressure profiles adjacent to tunnel - sensitivity analysis with Narasimhan's capillary pressure function.
Fig. 4.14: Computed gas flow rate history into tunnel - sensitivity analysis with Narasimhan's capillary pressure functional relationship.
5 CONCLUSIONS

5.1 Summary of Observations

Data from the first phase of testing at OBS indicate that the potential repository host rock, Valanginian marl, is highly heterogeneous with hydraulic conductivities ranging from $10^{-7}$ m/s to less than $10^{-12}$ m/s. Estimates of interval static pressures suggest an increase in pressure with depth, but at a less rapid rate than would be anticipated for water saturated media. The intervals between ca. 125-200 m depths (from the floor of the Seelisberg Tunnel) exhibit anomalously low pressures with a pressure reversal occurring between the 137.0 D and the 160.6 S intervals. The presence of natural gas (methane) in the marl is indicated by drilling and coring data, as well as by historical evidence of gas discharges into the Seelisberg Tunnel during the period of its excavation and construction.

5.2 Conceptual Models

Two conceptual models have been proposed to relate the observed abnormal pressure profiles at OBS to the presence of natural gas in the Valanginian marl. Model A assumes that the underpressured conditions have originated due to the transient discharge of gas from a relatively localized gas 'bubble' into the Seelisberg Tunnel. On the other hand, Model B assumes that the low gradient is the driving force for regional steady-state (or quasi-steady-state) upward gas migration from some deeper source.

5.3 Local-Scale Modelling Results

Material balance calculations using simple analytical equations, as well as numerical modelling using TOUGH, suggest that a depletion of gas from the ca. 125-200 m zone can result in vertical pressure profiles similar to those observed during OBS-1. Computed gas flow rates, based on assumed cylindrical reservoirs of ca. 400 m radius, appear to be of the similar to the observed values of 2-3 l/s.

5.4 Regional-Scale Modelling Results

Detailed modelling of gas-water flow at the OBS site using TOUGH indicates that the scenario presented in Conceptual Model A is more likely than the Model B scenario. Pressure profiles predicted with reasonable estimates of formation parameters, boundary and initial conditions, and two-phase flow parameters agree well with those observed during hydraulic testing.
Thus, both local- and regional-scale modelling studies suggest that the underpressuring observed at OBS is most likely the effect of gas discharges into the Seelisberg Tunnel via some high-conductive flow path. The presence of gas alone does not appear to be a sufficient explanation for the existing low gradients and the pressure reversals.

5.5 Implications for Repository Siting

The presence of free gas in the Valanginian marl, either in a mobile or in an immobile condition, raises interesting questions regarding the siting of a waste repository. Simulations of gas generation and migration from repositories in tight rocks have shown that gas released from corrosion of waste packages will cause a pressure buildup in the repository until its saturation exceeds some critical value (PRUESS 1990). If there is gas already present in the host rock forming some continuous flow path, then gaseous corrosion products can flow out immediately. While this helps dissipate the excess pressure rise in the repository itself, the travel time of radioactive gases through the geosphere to the biosphere could be considerably reduced.

The existence of two-phase conditions in the host rock prior to repository construction thus presents both favourable and unfavourable prospects. Attention should therefore be given to a proper characterization of the host rock so as to ascertain the magnitude and the extent of gas bearing features.

6 ACKNOWLEDGEMENTS

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APPENDIX A

OVERVIEW ON TWO-PHASE FLOW

1 Basic Equations

Consider a system with two mobile phases (gas and liquid), and two components (air and water). A mass balance on each component, assuming the phases to be immiscible with each other, leads to the following phase continuity equations (HUYAKORN & PINDER 1983):

\[ \frac{\partial}{\partial t} \left\{ \phi S_i \rho_i \right\} = \nabla \cdot \left\{ \rho_i \mathbf{v}_i \right\} + q_i \quad [A-1] \]

where the phase index, \( i \), denotes either gas (g) or liquid water (l), \( S_i \) is the saturation of phase \( i \), \( \rho_i \) is the phase density, \( q_i \) is the source/sink term, and \( \mathbf{v}_i \) is the phase velocity vector given by Darcy’s Law:

\[ \mathbf{v}_i = -k \cdot \left\{ k_{ri} \left\{ \nabla P_i - \rho_i g \mathbf{D} \right\} \right\} \quad [A-2] \]

with \( k \) the absolute permeability tensor, \( k_{ri} \) the relative permeability for phase \( i \) (i.e., the ratio of the permeability at the given saturation to the absolute permeability), \( \mu_i \) the phase viscosity, \( P_i \) the phase pressure, \( g \) the gravitational acceleration, and \( D \) the depth. Substitution of [A-2] in [A-1] yields the equation of motion for the phase of interest. Note that the phase saturations must sum to unity because of volumetric balance:

\[ S_g + S_l = 1 \quad [A-3] \]

The phase pressures are related by the capillary pressure relationship:

\[ P_g = P_l + P_c(S_l) \quad [A-4] \]

where \( P_c \) is the capillary pressure. The relative permeabilities are also related to the saturation of the wetting (liquid water) phase, viz:

\[ k_{ri} = k_{r_l}(S_l) \quad [A-5] \]

2 Constitutive Relationships

The functional relationships between \( P_c \) and \( S_l \), and \( k_{ri} \) and \( S_l \), are referred to as the constitutive relationships for the problem at hand. These are either determined from laboratory experiments, or empirically expressed via one of several parametric models. A commonly used model for relative permeabilities is that of COREY (1954):

\[ S_e = \left( S_l - S_{f_l} \right) / \left( 1 - S_{f_l} - S_{e_f} \right) \quad [A-6] \]

\[ k_{rl} = S_e^4 \quad [A-7] \]

\[ k_{rg} = (1 - S_e)^2 \left( 1 - S^2 \right) \quad [A-8] \]
where $S_{ir}$ is the residual water saturation and $S_{gr}$ is the residual gas saturation. These values represent minimum saturations that must be achieved before the corresponding phase (i.e., liquid or gas) becomes mobile. An alternative expression for $k_{rg}$ is given by the GRANT (1977) model:

$$k_{rg} = 1 - k_{rl}$$  \[A-9\]

which uses the same expression for $k_{rl}$ as the Corey model, viz. [A-7]. In the absence of any experimental data, the Corey and Grant models may be regarded as end-members of a likely suite of gas relative permeability models. A typical set of Corey and Grant relative permeability curves with $S_{ir}=0.2$ and $S_{gr}=0.1$ is presented in Fig. A-1.

In a similar manner, the capillary pressure function may be represented by the empirical model of NARASIMHAN (1975):

$$S^* = \frac{(1 - S_l)}{(S_t - S_{ir})}$$  \[10\]

$$P_c = P_e + \alpha (S^*)^\beta$$  \[11\]

where $P_c$ is the air-entry (capillary displacement or threshold) pressure, and $\alpha$ and $\beta$ are other model parameters. The air-entry pressure is the minimum pressure difference that must exist between the gas and liquid phases before gas can begin to displace the liquid. It can also be considered as the capillary pressure corresponding to the largest continuous pore radius, because this is the first site where displacement by gas occurs. Note that $(P_c+\alpha)$ is just the capillary pressure when $S^*=1$ (i.e., when the mobile pore volume is equally distributed between gas and liquid), while the exponent $\beta$ determines the curvature of the capillary pressure function. A typical capillary pressure curve, generated utilizing the Narasimhan model with $P_e=\alpha=5$ bars and $\beta=1$, is also shown in Fig. A-1.

3 Brief Description of TOUGH

In order to solve Eq. [A-1] for modelling the migration of gas and liquid water, the multiphase simulator TOUGH (PRUESS 1987) is employed. This numerical code was developed for simulating the multi-dimensional transport of water, vapour, air and heat in porous and fractured media. TOUGH considers immiscible Darcy flow of liquid and gaseous phases with mutual interference between phases due to relative permeability and capillary effects. Thermophysical properties for water are represented by steam table equations, while the gaseous phase is treated as an ideal gas. Dissolution of air in water is modeled with Henry’s Law. The governing transport equations are discretized using first-order finite difference in time and integral finite differences in the space variables (NARASIMHAN 1975). All flux terms are evaluated implicitly at the new time level for numerical stability. Local thermodynamic equilibrium is assumed to exist so that each volume element of the integrated finite difference grid can be uniquely characterized by a set of thermodynamic state variables (e.g., pressure, temperature, gas saturation). The coupled set of nonlinear algebraic equations, resulting from the discretization procedure, is solved by Newton-Raphson iteration. A sparse Gaussian elimination routine is used to solve the linear equations arising at each iteration step.
Fig. A-1: Typical relative permeability relationships using the COREY (1954) and GRANT (1977) models, and capillary pressure relationships using the NARASIMHAN (1977) model.