

GASTON

Evaluation of Modelling Approaches of Gas Transport in Clay Formations

Auswertung von Modellierungsansätzen zum Gastransport in Ton- formationen

H. Alkan
W. Müller

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SUMMARY

Considerable amount of experimental as well as numerical data has been published in the last years on modelling the fluid transport in clay formations based on physical and numerical considerations. The basic objective of the present study is the evaluation of the results of this data in terms of their applicability in numerical modelling. A compilation of the physical interpretation of the characteristics of the fluid transport in clay formations and their mathematical implementations in existing or new computer codes simulating the hydrodynamic and related process in geological media is another intention of this study.

In basic, the transport of gases is modelled by diffusion and dispersion supported advection. Gas moves either dissolved in liquid phase or together with liquid phase. In natural clay systems single-phase gas flow is not expected. There is no significant lack of knowledge regarding on phase behaviour of gas-liquid phase properties, except supporting the empirical parameters of equation of states such as solubility of gases in water with various ionic activities. The main problems arise from two specific issues. The first one is the physico-chemical interactions at gas-water-clay interfaces. The second one is the geometrical coupling of the flow pathways with mechanics. Both are key features for the formulation of the gas retention in transport models.

For a comprehensive introduction to the study on the modelling approaches, the properties related to transport phenomena and the processes contributing in the one/two phase flow and diffusion in clay formations are recapitulated with a literature survey. The transport properties such as permeability, diffusion, fracture networks and basic formulations for advection and diffusion are reviewed. The internal and external disturbances are also summarized with special emphasize on excavation damaged zones and self-sealing in clay formations. The mechanical properties of clay formations are examined both for plastic and indurated clays. The swelling and compaction of bentonite buffers are also briefly reviewed. The interactions between clay minerals and fluids are determined within chemical aspects.

The conventional numerical formulations for describing the advection-dispersion, diffusion and retardation as well as the well-known equations for modelling the thermal and chemical effects on transport phenomena are listed as a table. The conceptual models for modelling gas transport in clay formations are searched from the literature and described with their numerical formulations. The validation and/or application of these conceptual modelling efforts are also given briefly.

Empirical correlations describe the gas breakthrough pressure and gas flow rate as function of gas saturation, vertical stress and temperature. The attempts of defining gas entry pressure in terms of permeability can also be cited among the empirical, semi-empirical formulations. Definition of the transient flow in saturated linear elastic porous medium based on Biot's Theory of consolidation and Terzaghi effective stress concept are developed basically for one-phase flow of liquid phase in clay medium. A simplified conceptual model with a fracture as pathway with stress dependency width (as function of effective stress) is affirmed to be an effective model applicable for gas, two-phase flow in plastic as well as indurated clays

neglecting TC coupling. In one approach, the clay formations are assumed to consist from series of non-intersecting capillaries. Two-phase flow formulations in this structural model are used to define the gas entry pressure and saturation distribution. In an improved form, the stress dependency of the capillaries is introduced. Validation efforts by matching the core experiment are published. In a model called “Multiple Front Propagation” fluids (wetting and non-wetting) are assumed to advance through the clay of the tip of the propagating gas flow channel. The gas-filled pathways are assumed to dilate elastically for small displacements. The number of paths is set by an input channel density. Some other approaches conceptualize the clay formations as a crack-fracture network where the opening of the cracks is governed by deformation. The success of dual continua in fracture-matrix network is based on the well known transfer functions between matrix and fractures. The “brush model” emphasizes also the formulation of flow through the fractures whereas the matrix is defined as the medium for diffusion. The models to describe the flow and the effect of the internal and external factors in bentonite buffers are also briefly examined in this part of the study.

The implementation of the conceptual models and the use of conventional and non-conventional numerical modelling tools are surveyed in an individual chapter. A total of 15 codes which are used for modelling the transport phenomena in clay formations have been identified from the literature. The codes are listed principally after their properties and capacity on modelling the transport and related phenomena in clay formations. Two features are found especially important in evaluating the compared codes. These are, firstly, available fluid phases and secondly, available coupled processes. Some codes permit computations only for saturated media, in other terms they make the calculations for one-phase flow (FRAC3DVS, HYTEC). Some others describe the presence of a second phase only as air or vapour (Code_BRIGTH, PORFLOW). More developed codes in this regard, such as TOUGH2, TOUGHREACT offer more gas components like CO₂, H₂, CH₄. If the presence and generation of other gases than air has to be taken into considerations, neglecting the effect of these components may be an oversimplification.

The coupling of thermal, mechanical and chemical processes to the transport phenomena has been another important factor in code evaluation. Almost all codes provide the coupling of thermal processes and parameters for the hydraulic computations. FRAC3DVS or TOUGH2-FLAC have strong coupling with mechanics whereas some codes like TOUGHREACT and HYTEC provide well qualified chemical components without any mechanical coupling. It is concluded that although a great number of similar codes are available, a complete comprehensive modelling tool applicable for clay formations does not yet exist. A comparative list of the available codes is presented at the end of the study.

Modelling of transport phenomena in clay formations is more complex than that of the other host rocks. The obvious insufficiency of Darcy’s approach, the local and global heterogeneity, lack of experimental data on EDZ, the interactions of present fluids with clay minerals are some of the features creating the complexity. More experimental and theoretical studies should address the following issues for clay formations:

- Capillary forces and their relation to other petrophysical properties
- The configuration of the natural and induced fracture network

- Effect of surface forces on the transport potential and mechanisms
- Effect of the physical and chemical mechanisms (swelling, osmosis, etc) on the retention and diffusion of gas
- Scaling and up-scaling of the anisotropy and heterogeneity
- The EDZ properties and effect of self sealing on the long-term-behaviour

To simulate the transport phenomena in a performance analysis for clay repositories at full scale additional difficulties should be expected by numerical coupling of the mechanical and chemical disturbances. The difficulties on up-scaling of the geological and petrophysical features exhibit another complexity in the simulation. As the case in other host rocks, the EDZ should be taken in modelling efforts into consideration. The most important feature is the coupling of the hydraulic properties with mechanical changes. In clay formations the chemical coupling in EDZ is also important. The fracture mechanics considered in modelling the gas transport in near and far field of the indurated clay formations can also be used for this purpose. A validated hydraulic-mechanical coupling does not exist for clay formations.

ZUSAMMENFASSUNG

In den letzten Jahren wurde eine Vielzahl von experimentellen und numerischen Arbeiten zur Beschreibung des Fluidtransports in Tonformationen publiziert. Den Ergebnissen dieser Arbeiten und ihrer Interpretation liegt dabei eine Reihe von physikalischen und mathematischen Modellvorstellungen zu Grunde. Die vorliegende Studie hat sich zum Ziel gesetzt, die zu diesem Thema veröffentlichten Informationen auszuwerten im Hinblick auf ihre Anwendbarkeit zur numerischen Simulation von Fluidtransportvorgängen in Ton für die Praxis. Im Speziellen bestand das Ziel in einer Zusammenstellung der physikalischen Interpretation der charakteristischen Merkmale der Transportvorgänge und ihre numerische Umsetzung in vorhandenen oder in Entwicklung befindlichen Computerprogrammen zur Simulation von hydrodynamischen und damit in Verbindung stehenden Prozessen in geologischen Medien.

Vereinfacht ausgedrückt wird der Transport von Gasen in geologischen Formationen modelliert als Diffusion sowie als dispersionsunterstützte Advektion. Das Gas bewegt sich entweder gelöst in der flüssigen Phase oder zusammen mit der flüssigen Phase. Die Ausbildung einer eigenständig strömenden Gasphase wird in natürlichen Tonsystemen nicht erwartet. Die grundlegenden Kenntnisse zur Beschreibung des Phasenverhaltens von Flüssigkeit-/Gasgemischen und ihrer thermodynamischen Eigenschaften sind vorhanden mit Ausnahme der daraus abgeleiteten empirischen Parameter der Zustandsgleichungen wie z.B. die Löslichkeit von Gasen in Wasser unterschiedlicher Ionenstärke. Die wesentlichen Probleme ergeben sich allerdings durch zwei spezifische Punkte. Der erste ist die physikalisch-chemische Wechselwirkung an den Grenzflächen des Gas-Wasser-Ton-Systems. Der zweite Punkt betrifft die Kopplung der Strömungsgeometrie mit der Gebirgsmechanik. Beide Punkte sind Schlüsselmerkmale insbesondere für die Beschreibung der Gasrückhaltung/-verzögerung in Transportmodellen.

Für eine umfassende Einführung in die Modellierungsansätze werden in der vorliegenden Studie die für die Transportphänomene relevanten Eigenschaften sowie die Prozesse rekapituliert, die für den Ein-/Zwei-Phasen-Fluss und die Diffusion in Tonformationen entscheidend sind. Die für den Transport relevanten Eigenschaften wie Permeabilität, Diffusion, Rissnetzwerke und die grundlegenden Gleichungen für Advektion und Diffusion werden erläutert. Die internen und externen Einflussfaktoren werden zusammenfassend dargestellt mit besonderer Betonung der EDZ und der Selbstheilungsvorgänge in Ton. Die mechanischen Eigenschaften der Tonformation werden sowohl für (plastischen) Ton als auch für Tonstein diskutiert. Das Schwellungs- und Kompaktionsverhalten von Bentonit als Puffer-/ Versatzmaterial wird betrachtet. Die Wechselwirkung zwischen Tonmineralen und Fluiden wird unter den chemischen Aspekten mit abgehandelt.

Die konventionellen numerischen Formulierungen zur Beschreibung von Advektion-Dispersion, Diffusion und Rückhaltung/Verzögerung sowie die bekannten Gleichungen zur Modellierung der thermischen und chemischen Effekte auf Transportphänomene werden in Form einer Tabelle aufgelistet. Die konzeptionellen Modelle zur Simulation des Gastransports in Tonformationen werden aus der Literatur entnommen und beschrieben. Die Validierung und/oder Anwendung der konzeptionellen Ansätze werden ebenfalls zusammengestellt.

Der Gasdurchbruchsdruck und die Gasströmungsrate als Funktion der Gassättigung, der vertikalen Spannung und der Temperatur werden durch empirische Korrelationen charakterisiert. Zu diesen Korrelationen zählen auch die Versuche, den Gasschwellendruck in Abhängigkeit von der Permeabilität darzustellen. Die Beschreibung der transienten Strömung in einem gesättigten, linear-elastischen, porösen Medium wird abgeleitet auf der Grundlage der Biot-Theorie der Konsolidierung und des Konzepts der effektiven Spannung nach Terzaghi für einphasige Strömung der flüssigen Phase in Ton. Für ein vereinfachtes konzeptionelles Modell mit einem Riss als Strömungspfad mit spannungsabhängiger Rissweite (als Funktion der effektiven Spannung) wird die Anwendbarkeit für Gas- oder Zwei-Phasenströmung in Ton und Tonstein bei Vernachlässigung thermischer und chemischer Effekte bestätigt. In einem Modellierungsansatz wird angenommen, dass die Tonformationen aus einer Serie von sich nicht schneidenden Kapillaren bestehen. Die Beschreibung der Zwei-Phasen-Strömung in diesem strukturellen Modell wird herangezogen zur Definition des Gasschwellendruckes und der Sättigungsverteilung. In einer verbesserten Version wird die Spannungsabhängigkeit der Kapillargeometrie eingeführt. Über Arbeiten zur Validierung dieses Modells durch Anpassung an die Ergebnisse an Bohrkernen wird in der Literatur berichtet.

In einem so genannten „Multiple Front Propagation“ – Modell (Mehrfronten-Ausbreitungsmodell) wird angenommen, dass Fluide (benetzend und nicht benetzend) an der Spitze eines sich ausbreitenden Gasströmungskanals durch den Ton fortschreiten. Die mit Gas gefüllten Strömungspfade werden im Modell bei kleinen Verschiebungen elastisch aufgeweitet. Die Anzahl der Strömungspfade wird in Form einer Eingangskanaldichte festgelegt. Einige andere Ansätze setzen die Tonformation konzeptionell um in ein Netzwerk aus Rissen und Klüften, wobei die Öffnung der Risse und Klüfte durch die Deformation bestimmt wird. Der Erfolg des Doppelkontinuums in Kluft-Matrix-Netzwerken basiert auf den bekannten Transferfunktionen zwischen Kluft und Matrix. Das „Bürsten-Modell“ betont ebenfalls die Formulierung der Kluftströmung, während die Matrix als Medium für die Diffusion definiert wird. Die Modelle zur Beschreibung der Strömung und des Effekts externer und interner Einflussgrößen in Bentonit werden ebenfalls in diesem Teil der Studie erörtert.

Die Implementierung der konzeptionellen Modelle und die Anwendung konventioneller und nicht konventioneller numerischer Modellierungsansätze werden in einem eigenen Kapitel ausgewertet. Insgesamt 15 Codes, die für die Modellierung der Transportphänomene in Tonformationen eingesetzt werden, wurden aus der Literatur zusammengetragen. Die Codes sind grundsätzlich aufgelistet nach ihren Eigenschaften und Fähigkeiten in Bezug auf die Modellierung von Transportvorgängen und damit verknüpfter Prozesse in Tonformationen. Zwei Merkmale stellten sich als besonders wichtig heraus bei der Auswertung der verglichenen Codes. Zum ersten, die verfügbaren Fluidphasen, und zum zweiten, verfügbare Kopplungen zwischen den berücksichtigten Prozessen. Einige Codes erlauben nur Berechnungen für gesättigte Medien, anders ausgedrückt, es werden nur einphasige Rechnungen durchgeführt (FRAC3DVS, HYTEC). Einige andere beschreiben die Anwesenheit einer zweiten Phase nur unter der Annahme, dass es sich um Luft oder Dampf handelt. (Code_BRIGHT, PORFLOW). In diese Hinsicht weiter entwickelte Codes wie TOUGH2 oder TOUGHREACT bieten die Berücksichtigung mehrerer Gaskomponenten wie CO_2 , H_2 , CH_4 . Falls das Vorhandensein oder die Bildung von anderen Gasen als Luft betrachtet werden müssen, kann

die Vernachlässigung der verschiedenen Gaskomponenten eine zu starke Vereinfachung darstellen.

Die Kopplung thermischer, mechanischer, and chemischer Prozesse mit den Transportphänomenen bildet eine weitere wichtige Bewertungsgröße für die untersuchten Codes. Nahezu alle Codes verknüpfen thermische Prozesse mit den Parametern der hydraulischen Berechnungen. FRAC3DVS oder TOUGH2-FLAC weisen eine enge Kopplung mit mechanischen Prozessen auf, während einige Codes wie TOUGHREACT und HYTEC über qualifizierte chemische Komponenten verfügen ohne irgend eine Verknüpfung mit mechanischen Prozessen. Als Schlussfolgerung aus diesem Kapitel lässt sich ableiten, dass es zwar eine große Zahl ähnlicher Codes gibt, Ein umfassendes vollständiges Werkzeug für die Anwendung auf Tonformationen liegt allerdings noch nicht vor. Eine vergleichende tabellarische Zusammenstellung der verfügbaren Codes findet sich am Ende dieser Studie.

Die Modellierung von Transportvorgängen in Tonformationen gestaltet sich komplexer als in anderen Wirtsgesteinen. Die offensichtlichen Unzulänglichkeiten des Darcy-Ansatzes, die lokalen und globalen Heterogenitäten, das Fehlen experimenteller Daten über die EDZ und die Wechselwirkung der vorhandenen Fluide mit der Tonformation sind einige der Merkmale, die für diese Komplexität verantwortlich sind. Weiterführende experimentelle und theoretische Studien sollten daher insbesondere die folgenden Punkte klären:

- Kapillarkräfte und ihre Beziehung zu anderen petrophysikalischen Eigenschaften
- Struktur der natürlichen und induzierten Rissnetzwerke
- Auswirkung der Oberflächenkräfte auf den Fluidtransport und die damit verknüpften Mechanismen
- Auswirkung der physikalischen und chemischen Mechanismen (Schwellen, Osmose u.a.) auf die Rückhaltung und Diffusion von Gasen
- Skalierung der Anisotropie und Heterogenität
- EDZ-Eigenschaften und der Einfluss von Selbstheilungsprozessen auf das Langzeitverhalten

Für die komplette Simulation von Transportprozessen in Sicherheitsanalysen (Performance Assessment) für Endlager in Tonformationen ergeben sich zusätzliche Schwierigkeiten aus der numerischen Kopplung von mechanischen und chemischen Prozessen. Hinzu kommen die Schwierigkeiten mit der Skalierung der geologischen und petrophysikalischen Parameter, die die Komplexität der Simulation noch steigern. Wie für andere Wirtsgesteine auch, sollte die EDZ bei der Modellierung berücksichtigt werden. Das wichtigste Merkmal der Modellierung ist die Kopplung der hydraulischen Eigenschaften mit den Änderungen der geomechanischen Belastung. Für Tonformationen kann ferner die chemische Wechselwirkung in der EDZ von Bedeutung sein. Für die Modellierung des Gastransports im Nah- und Fernfeld eines Endlagers in Tonstein können auch Methoden und Ergebnisse der Bruchmechanik herangezogen werden. Eine validierte hydraulisch-mechanische Kopplung bleibt eine Aufgabe für die Zukunft.

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1 INTRODUCTION

Clay rich (argillaceous) formations are strong candidates for underground storage of radioactive wastes. The sealing properties of especially deep clay rich formations seem promising for the isolation prerequisites of underground storage and therefore a great number of studies have been conducted and are conducted on the related subjects. HADES, MONT TERRI, CORALUS, SELFRAC, FEBEX can be cited among these projects. One of the critical issues of these projects is the determination of the hydraulic properties and the sensitivity of these properties to thermal, mechanical and chemical perturbations in and around the storage locations. An enormous volume of literature from various fields such as hydrogeology, petroleum geology, geochemistry, thermodynamics, soil and rock mechanics, engineering geology accompanies these research activities. The elaboration and commenting of existing literature is supported also with experimental works conducted on clay formations with various levels of sophistication. The conventional way of studying an underground repository continues with the physical interpretation of these experiments. Numerical studies follow this step with the aim of modelling the hydraulic behaviour of the system under various internal and external disturbances.

Experimental work deals especially with measuring the hydraulic properties such as permeability and capillary characteristics under in-situ and repository conditions. Main objective is to forecast the capacity of clay formations to seal the radioactive or other toxic waste. Disturbances are created in laboratory by some artificial ways to increase the representation of the results. Nevertheless the ultimate problem of the experimental works especially in underground sciences is herewith present, too; a one-to-one analogy of geologic and repository conditions is not possible to simulate in the laboratory. Therefore some assumptions have to be made by performing the experimental work. Another important issue of the experimental works is that the experiments could only represent a very limited part of the overall system, only the location where the applied materials originate from. This means that experiments conducted under various representative conditions should be interpreted based on complementary information acquired from the underground mainly.

Despite of the complexity of the experiments, modelling efforts of the transport of fluids throughout clay formations reveals problems in many levels. The transport of fluids in clay formations does not always obey the classical rules of flow dynamics in porous media; entry pressure, intermittent or episodic flow. Swelling induced hydro-mechanics are some typical concepts applied to overcome the difficulties on the physical basis. On the numerical level, modelling efforts try to formulate these new concepts for describing the flowing behaviour through clay formations. The use of numerical simulators applied for modelling transport and related phenomena such as retention in sedimentary and crystalline rocks with success are doubtful for their direct applications in clay formations. Many of the numerical codes that are applied for modelling the transport of fluids in geologic media originate from similar studies for other host rocks than clay. Some of them are even originally for modelling the production of geologic energy resources such as oil and geothermal but not for simulating the behaviour of underground repositories.

Problems on modelling the transport of fluids in clay formations physically and numerically necessitate the elaboration of the present models for their validity and applicability within numerical codes. Investigations on the validation of the physical as well as numerical models are limited by extent and quality. A comparison of the existing numerical codes for modelling the fluid transport in clay formations is required for qualifying the success capacity of the efforts.

The safety requirements for an underground waste repository will take for granted the investigation and forecasting of the transport of fluids in corresponding geologic media. This is not a priori true and necessitates physical as well as numerical attempts. Taken into consideration of the above indicated problems of experimenting, evaluating, interpreting and mathematical modelling of these attempts, this step should be very carefully conducted. The selection of the numerical tools should take the physical modelling considerations into account. This is especially important for the design and management of the repositories in clay where the interaction between various disciplines for determining the transport laws is of the highest level.

In this study the physical and numerical attempts to model the gas transport in clay formations are investigated, compared and ranked according to their modelling capacity. "Gas transport" is accepted here as the term covering the movement of the gas in all ways, as one phase or two-phase flow in liquid taking the retention and/or retardation mechanisms into consideration. Instead of fluid, the term "gas transport" is selected intentionally for this study as the gas is interpreted as the main released source from the waste in the repository. The geologic media, on the other hand, is in most of the cases not homogeneously distributed and can be examined under the two main mechanisms: porous media and fractured network. To make all these concepts a comprehensive part of the study they are investigated from the related available literature and summarised emphasizing their relation and contribution to the transport of gas in clay formations. The gas generation mechanisms and rates are also searched within this context and evaluated as possible source terms. The evaluation of the codes using various numerical formulations for the description of the transport phenomena are performed mainly based on testing and numerical validation if possible. If the numerical validation is not possible, it is contented with the information and expertise reports from the literature. The results are presented as tables listing the evaluation comments for each code. A comparative listing of all codes is also given in terms of primary and secondary numerical aspects of modelling the gas transport in clay formations. A comparison of the available know-how on gas transport in clay formations with other host rocks is also included.

The present study should not be considered as a benchmark of the software available for the numerical modelling of the gas transport in clay although this is one of the deficits of the know-how on modelling the fluid transport. It is rather aimed at a comprehensive overview of the know-how on gas transport in clay formations and it is thought to give the researchers, engineers and managers of the safety concepts in a geologic repository the possibility of evaluating the numerical approaches and available software on the subject.

2 OBJECTIVES AND BASIC DEFINITIONS

The wastes stored in geological repositories generate gases (CO₂, CH₄, H₂, others) depending on their compositions, the packing material and on the prevailing thermodynamical conditions in the emplacement chambers and surrounding geological volume. Thus the thermodynamics and the properties of the engineered or geological medium are two main external determinant of this basic feature. They determine the initial and boundary conditions of the physical and numerical modelling efforts, too. The fundamental phase and transport characteristics of the gas being generated are predefined by the dominating thermodynamics. The flow media where the transport phenomenon takes place on the other hand, assign the hydraulic conditions. The thermal, mechanical and chemical components of the transport phenomena are also structured by these main components.

Considerable amount of experimental as well as numerical data has been published on the last years on the modelling of the fluid transport in clay formations on a physical as well as on a numerical basis. The basic objective of this study is the elaboration of the results of this data in terms of their applicability in numerical modelling for practical applications. A compilation of the physical interpretation of the characteristics of the fluid transport in clay formations and their mathematical implementations on the existing or new computer codes simulating the hydrodynamic and related process in geological media is intended in addition. The effects of internal and external disturbances such as mechanical, thermal and geochemical effects define the initial and boundary conditions of the gas transport qualitatively and quantitatively. This study should not be classified as a benchmark of the existing software to model the gas transport in clay formations. This is an initial comprehensive attempt for evaluating the numerical codes and should give to the reader an overview of available modelling tools and developments in this context.

The terminology used in the literature related to waste repository in clay formations exhibits a high degree of variety. To be consistent in the framework of the objectives of the study a specific terminology is selected and used during the study. Beside of the classical terms of underground repositories published elsewhere /HOR 96/, the term “gas” is used for all components or mixture of gases unless the type of the gas is not pronounced. As usual fluid is used both for gas and liquid phases. A decision for the terminology that has to be used in the study for determining the flow media was not as easy as in the case of fluids. In general, in the literature related to geological repositories argillaceous media or rock is used to describe the clay-rich formations that can be used as repository volumes. From the geological perspective argillaceous describes rocks or sediments containing particles that are silt- or clay-sized, less than 0,625 mm in size /SCH 06/. Most have a high clay-mineral content, and many contain a sufficient percentage of organic material to be considered a source rock for hydrocarbon. The widely used synonym of argillaceous rock is mudrock. However, the term mudrock describes a variety of rocks encompassing a very wide range of lithotypes ranging from unlithified muds and clays, through moderately indurated mud stones and clay stones to fissile and often highly indurated shales and then, finally, to metamorphosed rocks such as argillites and slates. Across this wide spectrum, the characteristics and physical properties of argillaceous rocks can vary enormously. A standardized classification of these rocks is not available yet and the present terminology reveals a number of inconsistencies with the defini-

tions in /HOR 96/. Instead of mudrocks or argillaceous media the term “clay formation” is preferred in this study to describe the geological unit with a predominance of clay minerals which exhibit the mechanical attribute of plasticity. Other terms unless taken directly from literature are avoided in order to seek the simplicity. The basic classification of the clay formations as indurated and plastic clays is applied in the study to distinguish the main formation types and related applications. The bentonite used as backfill material in excavated caverns is a highly plastic clay containing large amounts of montmorillonite formed by the weathering or hydrothermal alteration of volcanic ash or rock. From a geologic point of view bentonite is a commercial term, applied to any of numerous variously coloured clay deposits containing montmorillonite as the essential mineral and representing a very large surface area, characterized either by the ability to swell in water or to be slaked and to be activated by acid, and is used chiefly to thicken oil-well drilling mud /BAT 87/. The definitions related to clay and clay formations as used in this study and related literature are given in Table 2-1.

Table 2-1: Classification and definition of terms related to clay formations (basically from /HOR 96/)

		Distribution of clay-size particles (< 2 µm), %		
		0-32	33-65	66-100
Non-indurated clay formations	Beds	Bedded Silt	Bedded Mud	Bedded Clay
		Laminated Silt	Laminated Mud	Laminated Clay
Indurated clay formations	Beds	Siltstone	Mudstone	Claystone
			Mudshale	Clayshale
Metamorphosed clay formations	Low	Siltstone	Mudstone	Argillite
	Medium	Siltshale	Slate	Slate
	High		Phyllite/Mica Shist	
Bentonite, backfill	Commercial		Montmorillonite	

Contrary to the discrepancies on the terminology related to clay formations, the terminology and definitions about the safety considerations of an underground waste repository are rather exact. In related literature the gas or gases being generated by the waste migrate in a cascade like barrier network and reach the biosphere if it has sufficient energy and buoyancy. The components of an underground repository system as discussed and presented in many of the earlier studies are schematically shown in Figure 2-1. These components are used with the same terminology in this study as listed in Table 2-2.

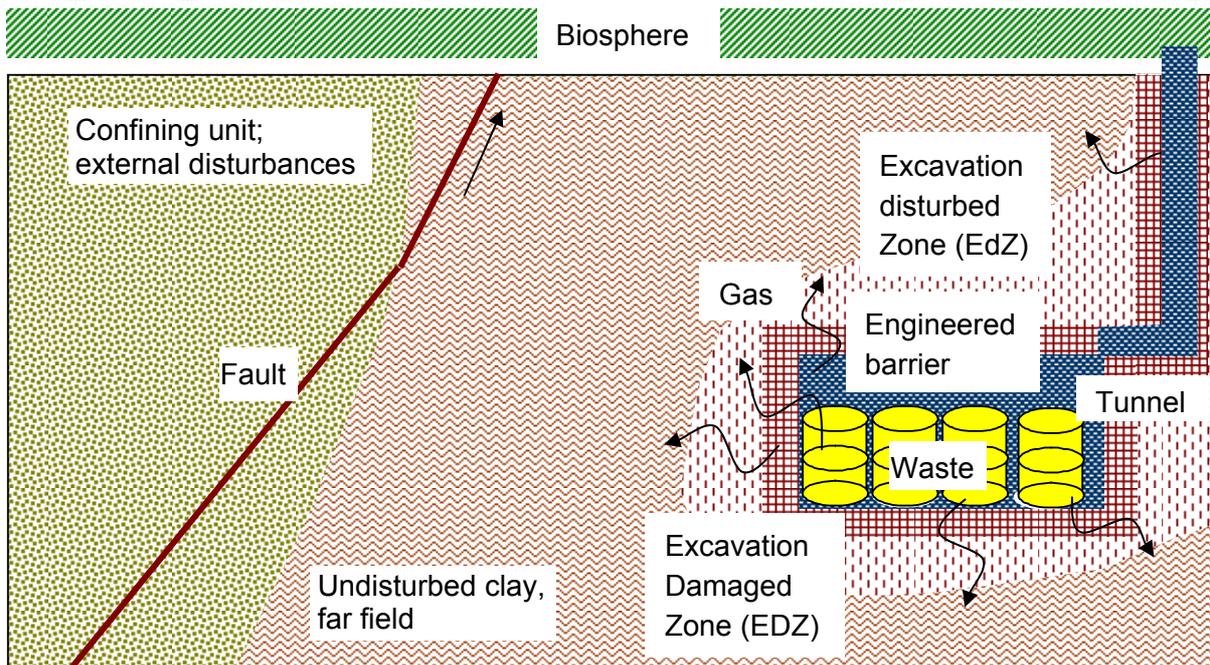


Figure 2-1: System components of a deep geological repository

Table 2-2: Definition of the system components of an underground waste repository

System component	Definition
Waste	Radioactive or chemical; gas source
Geological barrier	Geologic formations with low hydraulic conductivity serving as barriers to the underground waste emplacement
Engineered barriers	Synthetical barriers against transport designed mainly from salt, clay, portlandite, sand
Emplacement room, cavern, borehole	The excavated part of repository for waste emplacement
Excavation Damaged Zone (EDZ)	Zone where the host rock is mechanically affected und irreversibly damaged by tunnel-cavern excavation
Excavation Disturbed Zone (EDZ)	Zone where the host rock is mechanically affected by tunnel-cavern excavation
Affected Field (AF)	Zone in host rock beyond the EDZ that is affected by the presence of the repository (e.g. chemical and hydraulical effects)
Far Field (FF)	Zone in host rock unaffected by the presence of the repository with the exception of some transient effects
External influences, disturbances, perturbations	Processes originating from outside the host rock and including the geological long term evolution, climatic and human effects
Faults	A break or planar surface in brittle rock across which there is observable displacement. The faults forms the main potential leakage element
Tunnel, shafts and seals	Access openings to the repository

3 CLAY AS HOST ROCK FOR REPOSITORIES; BASIC PROPERTIES

3.1 Definitions; Clay as Host Rock

Clay rich formations are the most abundant sediments on the earth comprising between 50 to 75 % of the geological column. They hold a special place in scientific research because their wide spectrum of applications. Clays are applied for farming activities and civil engineering works; they are formed in diagenetic series prospected for petroleum resources; they crystallise in geothermal fields whose energy and mineral deposits prove valuable. Clays play very important roles in every day life, in pharmaceuticals, in cosmetics and in painting. Their sealing properties permit to serve as cap rocks for petroleum and geothermal reservoirs as well as for the isolation of the hazardous wastes. In the following the basic properties of clay formations as host rock for repository are summarized based on predominant literature on the subject.

3.1.1 Structural Aspects

Clay minerals belong to the phyllosilicate group (from the Greek “phylon”: leaf, and from the Latin “silic”: flint). As a distinctive feature, they are very small (a few micrometers maximum) and their preferred formation occurs under surface (alterides, soils, sediments) or subsurface (diagenesis, hydrothermal alterations) conditions. Difficult to observe without using electron microscopy (scanning and transmission), they have been abundantly studied by X-Ray diffraction, which is the basic tool for their identification. While the number of their species is relatively small, clay minerals exhibit a great diversity in their composition because of their large compositional ranges of solid solutions and their ability to form polyphased crystals by interstratification. An understanding of the crystal structure is essential for understanding their properties.

The elementary level structures of the clays are the layers which are determined with atomic planes exhibiting determined inter-distances. As with any mineral species, phyllosilicates are characterized by a “unit cell”. As a first step the unit cell can be considered at the scale of a single layer and its dimension is determined in 3D spaces. The a and b dimensions are in the x-y plane (the plane in which the largest faces are oriented) The c dimension along the z-axis corresponds to the “thickness” of the layer. A simple geometrical calculation provides approximate values for these three dimensions. These elementary levels are in forms of tetrahedral and octahedral “sheets” are formed by cation-anion bonds (bonds intermediate between ionic and covalent bonds) whose length is used as a reference in the calculation of the cell dimensions. Ionic diameters which are measured to be in the range of 0,4 to 2 Angström (Å, 1 Å=0,1 nm) are used for the determination of cation coordination. Three types of coordination determine the elementary polyhedra that make up various sheets of the crystal structure:

- 4-fold coordination (SiO₄ 4-or AlO₄ 5- Tetrahedron)
- 6-fold coordination (Octahedron whose centre is occupied by a Al³⁺, Fe³⁺, Fe²⁺ or Mg²⁺ cation for most part – the vertices being formed by O²⁻ or OH⁻ anions)

- 12-fold coordination (Dodecahedron whose centre is occupied by a cation with a wide diameter: K^+ , Na^+ , Ca^{2+} and vertices are formed by O^{2-} anions of the two opposite tetrahedral sheets).

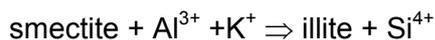
The crystal structure of all phyllosilicates is based on two types of layers:

- 1:1 layers in which one tetrahedral sheet is bonded to one octahedral sheet.
- 2:1 layers in which one octahedral sheet is sandwiched between two tetrahedral sheets.

The geometrical structures (without deformation) of both types of layers depend on the hexagonal symmetry of the tetrahedral and octahedral sheets which are linked to each other. However, the tetrahedral and octahedral sheets exhibit differing a and b dimensions. Thus, their linkage cannot possibly take place without deformation of the angles and lengths of some chemical bonds, as indicated previously. These deformations of the angles and lengths of some chemical bonds as indicated previously. These deformations are significant in trioctahedral layers. In all cases, the 6-fold symmetry becomes 3-fold symmetry.

Kaolinite and lizardite show 1:1 layer structure whereas micas and smectites have 2:1 layer structure for which the electrical neutrality of crystal structures is ensured by the addition of a cation interlayer sheet /MEU 05/.

The 2:1 and 1:1 layers of clay minerals are strongly bonded internally but relatively weakly bonded to each other. Because the surface planes of different kinds of layers are geometrically similar, the layers can stack together in numerous different ways. Minerals with such interstratifications are known as mixed-layer clays. The intergrowth may be regular or irregular, although the irregular type is most frequently encountered in sedimentary clays. The most common form of mixed-layer clay in clay formations is illite-smectite because the reaction



occurs during the burial diagenesis of clay sediments and the reverse reaction occurs during sub-aerial weathering. It is also noted that illite-smectite may be the most abundant clay mineral type in the lithosphere. Many other interstratified clays have been identified including kaolinite-smectite, chlorite-smectite and chlorite-vermiculite /HOR 96/.

3.1.2 Deposition

Subsequent to their transport in moving water, clays may be accumulated in a variety of environments, including marine, fluvial and lacustrine settings, and in water of varying depth, salinity and temperature. Thick sequences of clay sediments are found primarily in one particular form of geological structure, the sedimentary basin. Basin development is associated with very large-scale deformation of the earth's crust and mechanisms which include crustal downwarping, faulting and isostasy. Assuming sediment supply, the primary control on sediment accumulation is basin subsidence. Clay minerals in recent marine sediments have two major sources: detrital clays from sediment source areas and, to a lesser extent, authigenic

clays. The clay mineral assemblages of marine depositional basins are broadly related to the soil clays of adjacent land masses. The principal authigenic clays in modern marine sediments are Fe-rich smectites which probably formed by submarine alteration of volcanic debris or by precipitation from hydrothermal solutions. Apart from smectites, neo-formed clay minerals make only minor local contributions to marine clays. The clay minerals found in fluvial and lacustrine environments also broadly reflect the input of detrital material from source areas. However, authigenic clay minerals may represent a greater proportion of the total clay fraction in hypersaline lake environments /HOR 96/.

3.1.3 Burial Diagenesis

Diagenesis is the process by which sediments become lithified during burial and the extent of diagenetic alteration is, perhaps, the most significant factor in determining the physical, chemical and hydrogeological characteristics of a clay deposition. Diagenesis is primarily a response to the changes in temperature, stress, fluid pressure and chemical environment which are occasioned by burial /SHA 81/. Some of the principal diagenetic processes occurring during burial are:

- compaction and fluid migration,
- development of diagenetic bonds,
- mineralization and introduction of cements,
- organic reactions,
- clay mineral dehydration and transformation, and
- pressure solution and recrystallization.

Eventually diagenesis causes metamorphism, but there is no clear boundary between these two processes. The loss of pore fluid by the process of mechanical dewatering may be considered to be the first of the many diagenetic processes affecting a clay sediment upon burial /RIE 74/. Very large amounts of water are driven off during compaction and as a result of the smectite-illite transformation during deep burial. These waters may act as carriers for inorganic and organic ions and compounds formed during diagenesis. If the rate of burial is very high then there is a potential for pore waters to become overpressurized. Burial diagenesis can cause important mineralogical changes in the originally deposited clay mineral assemblages. Under the influence of alkaline pore waters kaolinites may transform to illite in the presence of K^+ , or to smectite or chlorite if Ca^{2+} , Na^+ or Mg^{2+} are present. At burial temperatures greater than 200° - $250^{\circ}C$ kaolinites will become unstable, even in an acid environment, and will be destroyed. In alkaline pore waters, smectite, vermiculite, illite and chlorite will be initially stable. In acid pore waters these minerals may be transformed to kaolinite. During deep burial diagenesis, smectites and vermiculites will dehydrate and be transformed, via mixed-layer clay phases, to illite and/or chlorite, depending on whether the pore water environment is enriched in K^+ and/or Mg^{2+} . These changes are thought to occur progressively over the temperature range 100° - $180^{\circ}C$ although smectite conversion is now known to occur at much lower temperatures in high pH, potassium-rich solutions. The illites and chlorites form more stable polymorphs with increasing burial diagenesis in the presence of alkaline pore waters. A proposed diagenetic zonation of marine clays which places emphasis on the geochemical processes occurring during burial including; in order of increasing depth and

temperature these are: oxidation, bacterial reduction of sulphate, organic fermentation reactions, decarboxylation, clay mineral dehydration and, ultimately, metamorphic reactions /HOR 96/.

Diagenesis of clay sediments is dependent upon many factors, including depositional environment, types of clay minerals, amount of organic matter, pore water chemistry geothermal gradient and burial history /NEA 96/. Because of diagenetic processes are linked to flowing fluids, which transport heat and ions, flow rates, duration of flow and fluid pathways are critical. During shallow burial pore water are expelled from compacting clay formation through the interparticle network. With increasing overburden and degree of particle orientation, accompanied by loss of porosity and permeability, flow is channelled along inhomogeneities such as sand layers, fractures and faults. Fluid inclusions often reveal precipitation of diagenetic minerals into fractures at temperatures less than 50 °C, as well as the presence of injected clay fillings. Both indicate that fractures may form during shallow burial. Fractures are the single most important conduits in tight shales and largely control cross-formational flow.

3.1.4 Tectonic Deformation

The character and properties of many clay formations are not exclusively determined by burial diagenesis, since a number of geological processes occurring subsequent to burial can play an important part in determining the structural attributes of these rocks (e.g. faults, folds, joints and fissures). The most important of these are tectonic deformation, uplift and exhumation and, not infrequently, all three processes are closely interrelated as surface erosion strips away sediments thrown up by large-scale deformation, bringing the clay rock stratum closer to the surface.

The combined effect of these processes is to impose a stress history on the clay formations and it is this history which is the second major modifier of the character and properties of many clay rocks. In some "tectonized" clay rocks, stress history may be exceedingly complex and almost impossible to unravel. In others, subject to a simple cycle of burial and exhumation, it may possible to reconstruct the stress history and use it to predict some of the main attributes and properties of the rock. The water content, strength, plasticity and rock mass characteristics of the less-indurated, overconsolidated clay rocks are often more or less quantifiable functions of their stress histories. Stress history is not only a modifier of clay rock properties, it may also have a dominant effect on the hydrogeology of low permeability argillaceous sequences /NEA 96/.

3.1.5 Degradation

The slow degradation of clay formations begins with their uplift and exhumation. In the less indurated rock-types, stress-relief may lead to jointing and fissuring, an increase in water content and possible softening. Loss of overconsolidation may be viewed as the process by which a clay rock which has been deeply buried and then uplifted gradually readjusts to the altered physico-chemical conditions prevailing at shallower depth. Minerals which were sta-

ble at maximum burial depth may not be so under the new conditions and some regression of the diagenetic rock-forming processes may occur. Increase in water content is only possible if interparticle bonds are broken, and the extent of swelling will depend on bond strength. Near surface, clay rock degradation is accelerated in the weathering zone, due to the penetration of oxygenated meteoric water. Joints and fissures, dilated by stress-relief, may provide channels for groundwater circulation and weathering. Secondary minerals such as pyrite may rapidly oxidize, releasing acid which can react with carbonates to produce major changes in both the fabric and the properties of the clay rock. Penetration of the clay by fresh water leads to swelling and softening and repeated movement of wetting and drying phases may produce air-breakdown or slaking.

3.2 Mechanical Behaviour

The deformation behaviour of a host rock is one of the most important parameters by considering its sealing and therefore hydraulic properties. If the degree of diagenetic alteration of the clay rock and the stress regime during deformation both favour brittle behaviour, fluid flow in the natural system is likely to be fracture dominated. Conversely, if the material properties and stresses tend to favour plasticity or ductility as modes of deformation, fracture flow may be much less important. However, the definition of the clay formations in terms of rock mechanics is relatively difficult. Mainly because of the higher porosity and the swelling ability of the consisting minerals, the stress dependent deformation of the clay formations could not be defined with basic mechanical laws. In most of the cases, the hydraulic, chemical and thermal effects should be taken into account and the definition of the mechanical behaviour should be made with the coupling of these effects.

Considerable amount of study on the mechanical properties of clay formations can be found in the international literature /NAG 02b/, /HOU 02/, /TSA 05/, /SCO 05/, /LUX 06/. The studies are mainly concentrated on the elastic and plastic deformation behaviour of the clay formations and the effect of the water content on the mechanical properties. There are limited data on the dilatancy and dilatancy boundary of the clay formations. In the following a summary of the mechanical behaviour of the clay formations is given based on the existing literature.

Laboratory studies demonstrate the extremes in mechanical behaviour. It is indicated that the most significant parameter on the mechanical properties of clay formations is the ratio of clay species to quartz plus feldspar. With increasing amounts of quartz and feldspar, the material becomes progressively more brittle and stronger. Studies on the frictional resistance to sliding have shown that a decrease in frictional strength only begins when the amount of clay approaches 25-30% of the rock volume. As the percentage of clay increases the frictional strength decreases monotonically until the amount reaches 70-75%, after which little change occurs. A second parameter is the nature of the phyllosilicate species. Illite and kaolinite have been found to have less affect in altering the strength of rocks than do species containing interlayer water such as the smectites. This is found in both the frictional strength as well as in the mechanical behaviour of samples that are 100% clay.

Mechanical behaviour common to many types of shale is illustrated in Figure 3-1 as observed in the tests on samples that are composed of quartz plus feldspar 37-45%, illite/mica 27-31%, kaolinite 10-17% and chlorite 10-16%. Specimens were deformed in triaxial compression at constant strain rates of 10^{-5} and 10^{-7} s^{-1} , at confining and pore pressure to 200 MPa and temperatures to 225 °C /NEA 96/. In experiments performed at room dry conditions and confining pressures to 200 MPa, a transition from brittle to semi-brittle behaviour is observed, with all specimens eventually failing in shear fractures. Figure 3-1 also shows a comparison of the strength behaviour compared some other brittle rocks. It is shown that the strength behaviour of the shales is not significantly different; they are generally stronger than the highly porous limestones, but weaker than some marbles.

The experimental studies show that the mechanical properties of clay are prescribed by the anisotropy, composition and water content. Elastic, plastic und viscose deformation (isotropic, anisotropic), failure- and residual strength, dilatancy, effect of the pore pressure, bedding are some other basic properties that are integrated to the mechanical studies of clay formations.

The following section consists of a generalized summary of the international experiences on the basic mechanical characteristics of clay formations.

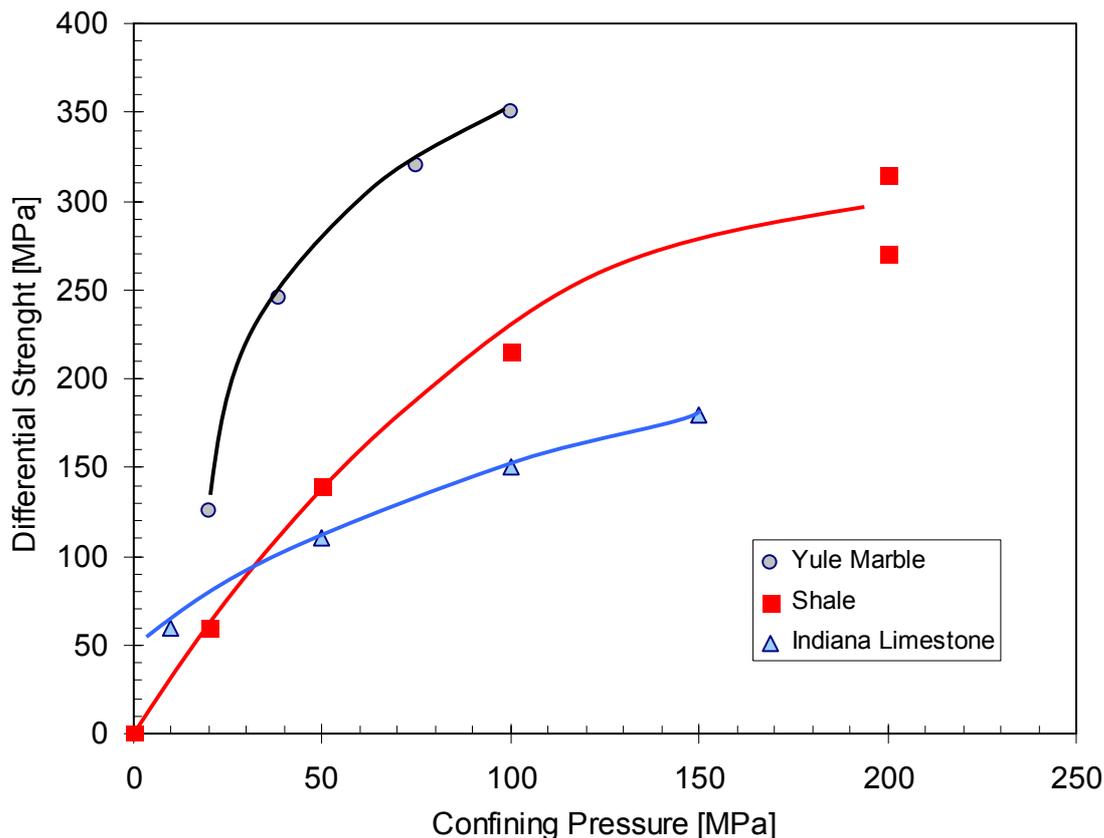


Figure 3-1: Mechanical behaviour of the shales compared to other rocks /NEA 96/

3.2.1 Elastic, Plastic and Viscoplastic Deformation of Clay Formations

After the short and long-time studies conducted by NAGRA /NAG 96/ on Palfris-formation at the location Wellenberg, the mechanical behaviour of this clay formation is observed to be dominated by the anisotropy, inhomogeneity and brittleness:

(1) The anisotropy is concluded based on experimental data on the elastic deformation as well as on the strength. Uniaxial and isostatical stress experiments show that the microcracks are oriented in parallel to the foliation. After the observation of the compressive wave velocity values conducted under uniaxial stress conditions, the orientation of the foliation and bedding dominates the anisotropy of the clay formations.

(2) The inhomogeneity of the clay formations is based on one side on the mineralogical composition, on the other side on the microcrack density.

(3) The deformation tests with radial/confining stress exhibit inelastic deformation as the result of the formation and/or opening of microcracks which are controlled by their interaction and coalescence.

The elasticity moduli that are measured in-situ or in laboratory with various methods provides in general detailed information on the mechanical behaviour of the geological formations and their comparison based on mechanical behaviour. However, the elasticity moduli measured in laboratory exhibit generally lower values as compared with intact rocks. The same situation is also observed for clay formations whereas even the experimental methodology and technology could change the measured elasticity modulus.

The best agreement between the in-situ and experimental data is obtained if the experiments are performed in the direction of foliation. This means that the measurements from the laboratory (with angles of 45°-90° to the bedding) contain the effect of the unloading on microcracks compared to the measurements conducted with the probes taken parallel to the bedding. This hypothesis is supported by the observations of the higher dynamic elastic parameters measured in-situ in comparison with the elastic parameters measured on the wellbore cores.

In conventional triaxial compression experiments, saturated clay formations exhibit a tendency to plastic deformation behaviour. To investigate the effect of the partial saturation and dehydration, coupled hydro-mechanical experiments were conducted. The results show that the deformation behaviour of the clay formations is greatly dependent on water content of the rock. The decreasing elastic parameters (elastic modulus, Poisson ratio) with increasing water saturation, begin to re-increase again after some saturation values. This behaviour is commented as a consequence of closing of existing microcracks and therefore changing mechanical behaviour of the material /SUK 03b/. On the other hand, the experiments show that the clay formation cores exhibit an obvious tendency to creep even at high water saturation. The temperature as well as the anisotropy is indicated to be the other relevant on this creeping behaviour.

As a result, it is mainly concluded that the stress-deformation behaviour of clay formations is very complex and the deformation is not only dependent on the facies (mineral composition, compaction degree, other structural and geological factors) but also on the water content and bedding. The experimental difficulties are an additional factor for the evaluation and determination of the mechanical behaviour of the clay formations.

3.2.2 Failure- and Tensile Strength

The failure and tensile strength and their dependence on the structural properties of clay formations are experimentally investigated. The measured failure strength behaviour of various cores of Palfris-Clay formation is given in Figure 3-2. The data points that are origins of the lines show a strong dispersion (low R^2) showing probably the effect of probing and structural variations. The averaged values determined for cohesion and friction angles of various clay cores result in various tendencies by low and higher minimum stresses (σ_3). The transition takes place at a minimum stress component of approximately $\sigma_3=25$ MPa. It is indicated that this two-step behaviour is a result of differences in failure processes. Figure 3-3 shows the results of the experiments conducted for determining the compressions strength of the clay cores from the location KONRAD /DÜS 88/.

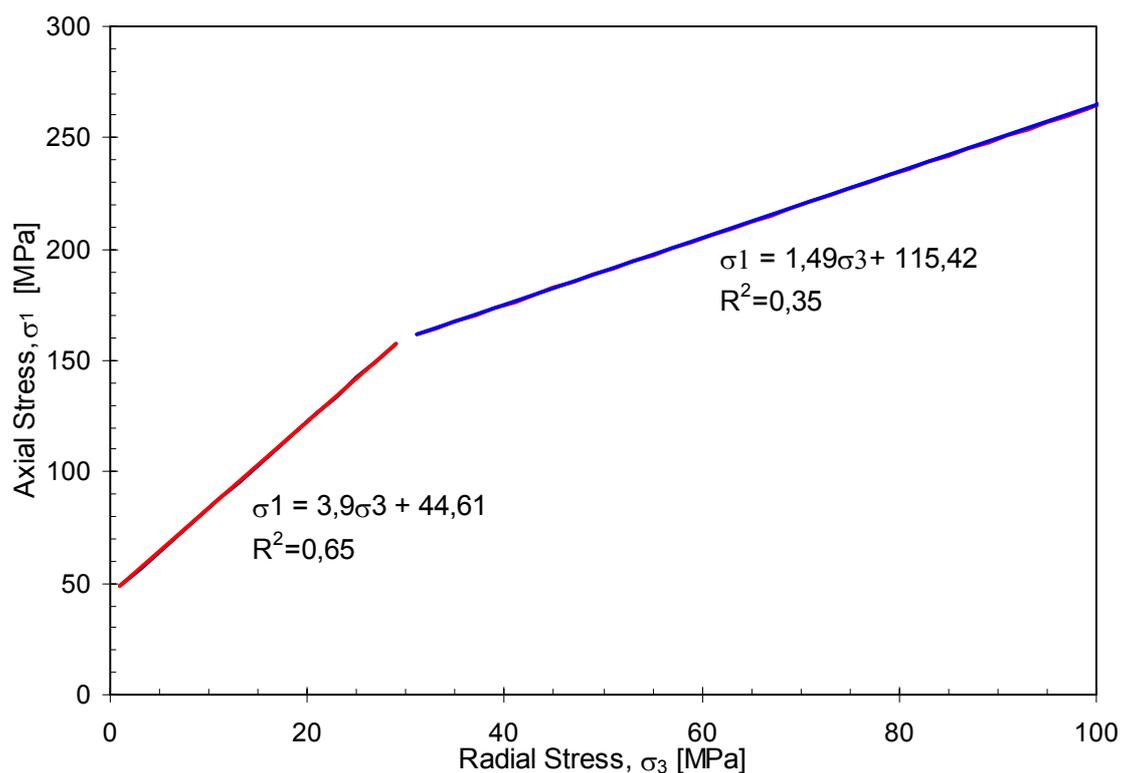


Figure 3-2: Failure strength evaluation for Palfris-Clay formation, experimental data correlated with linear regression /NAG 96/

The effect of the microstructure on the failure strength of clay formation cores are experimentally investigated /NAG 01/. Various cores taken from Benken formation parallel, vertically and inclined to the foliation are tested with triaxial equipment for their maximum strength. The results show that the anisotropy as well as the water content has considerable effect on the friction angle. The samples inclined cored to the foliation have a lower tendency for cohesion i.e. lower strength. The tendency for lower failure strength increases with increasing water content. A conclusion of all these kinds of experiments is that the effect of bedding and water content on the mechanical properties of clay formation is not negligible as very often done for other rock types.

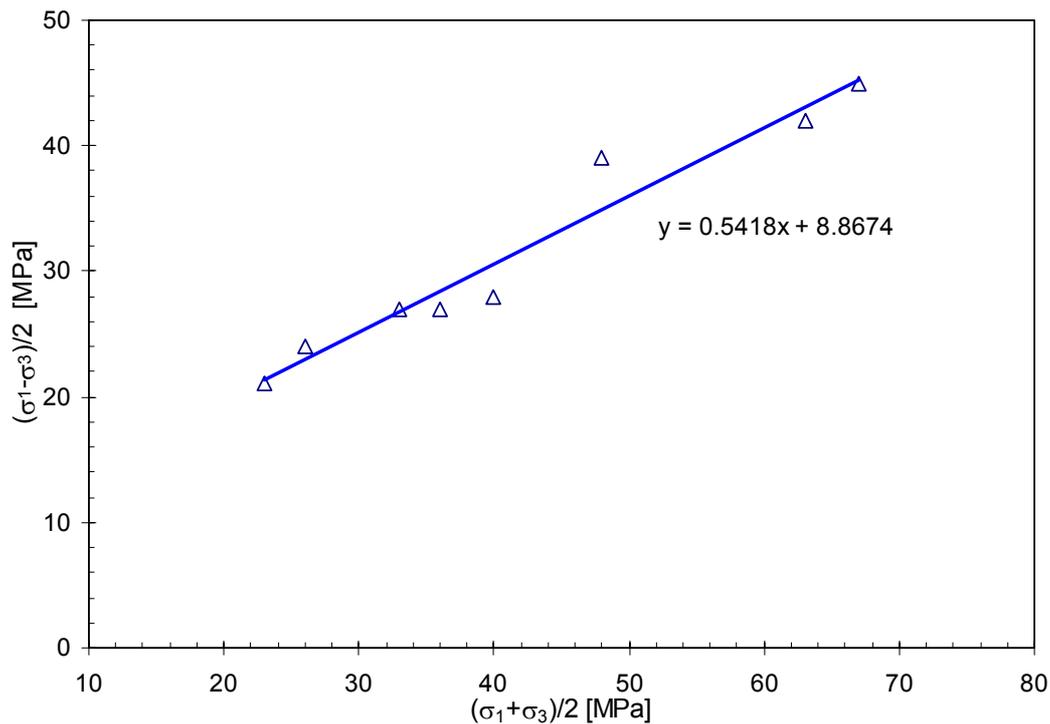


Figure 3-3: Measured compression strength of clay cores from the location KONRAD, /DÜS 88/

3.2.3 The Effect of the Water Content

The mechanical properties of the geological formations are strong function of microstructure which is determined by various geological processes such as compaction and bedding. In addition, the water content is a factor that causes considerable changes in the mechanical properties of the clay formations. Figure 3-4 shows the mechanical behaviour of Opalinus Clay with various water contents. Figure 3-5 presents on the other hand, the uniaxial strength of samples from various clay formations as function of water content. At low water saturation the cores exhibit higher compressive strength and stiffness probably due to higher compaction and smaller intervals between the particles with increasing capillary forces. At high water saturations clay behaves more plastic. From this point of view, it can be concluded that the

drying out of the clay formations in repository systems by planned or unplanned ventilation can have positive effects on the mechanical properties by reducing the water content. The decreasing water saturation is expected to increase the strength of at least in the near vicinity of opened galleries and caverns. However this is a critical situation while the higher degree of drying causes fracturing due to shrinkage which can end the consolidation with a total disintegration. The experiments performed on the cores taken from Tournemire clay formation show similar results, in this case taking the structural respectively the anisotropic properties into account /VAL 04/. The gain or loss of water has an impact on the opening or closing of the space interlayers. In a dry atmosphere, the average values of elastic modulus, the compressive strengths and the cohesion increase, while the Poisson's ratio decreases. Figure 3-6 and Figure 3-7 illustrate the evolutions of the elastic coefficients and triaxial compressive strengths with saturation. For modulus E1, values are quite constant (close to 20,000 MPa) for the range of saturation between 0,95 and 0,5; for lower values of saturation, modulus E1 increases with suction. For the other elastic modulus E2, there is a quite linear correlation between the modulus and the degree of saturation; the modulus is divided by two when the saturation decreases. The Poisson's ratios decrease with suction. On the other hand, as can be concluded from the Figure 3-7 for all directions, there is an important decrease in triaxial compressive strength with the degree of saturation. Values for compressive strength are close to 20–40 MPa for saturated samples and reach 70–90 MPa for the driest samples. The axial strain when compressive strength is reached, is not sensitive to the degree of saturation in the case of the $\theta = 45$ direction, and in the case of other directions, there is a significant increase in maximum axial strain when increases the degree of saturation.

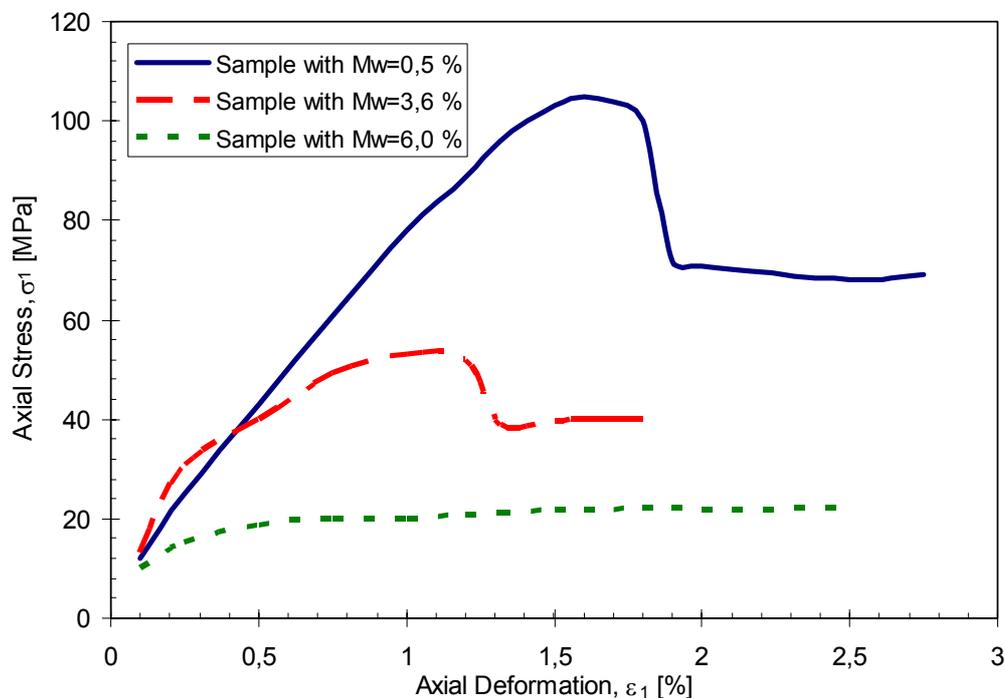


Figure 3-4: Deformation behaviour of the Opalinus Clay with various water contents /NAG 02a/

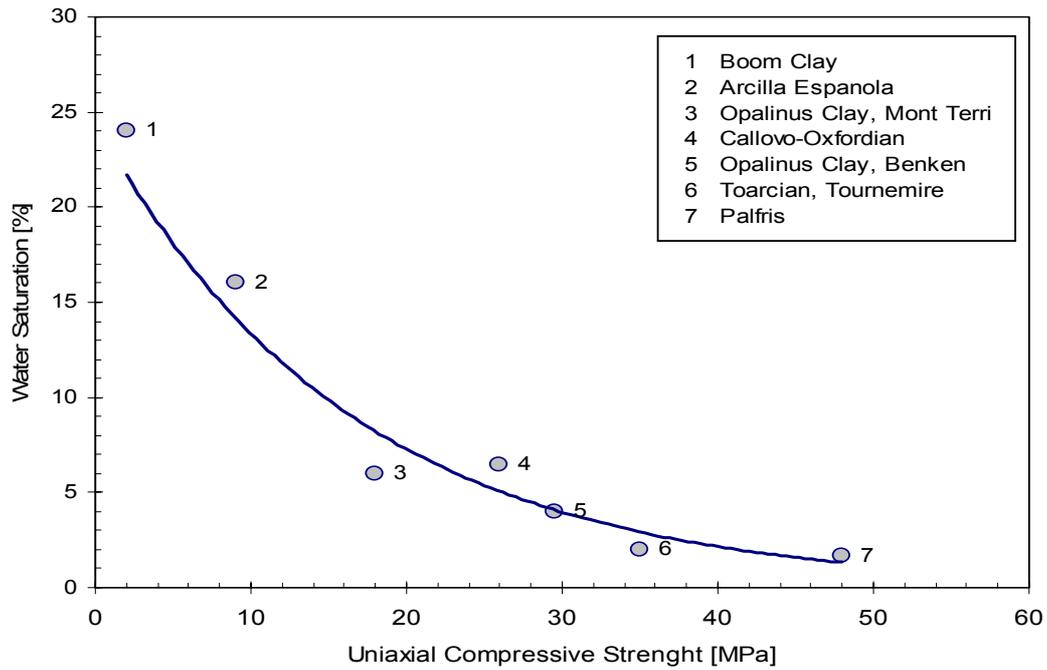


Figure 3-5: Effect of the water content on the compressive strength of various clay formations /NAG 02a/

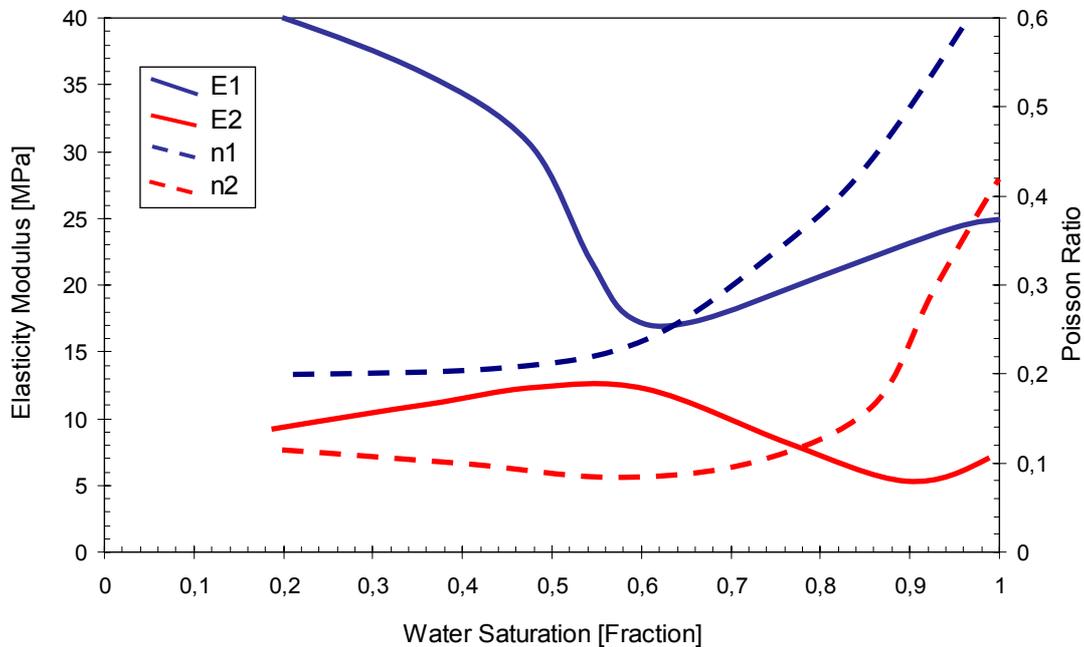


Figure 3-6: Mechanical properties of Tournemire clay formation as function of the water saturation and sampling orientation (2: parallel to plane of isotropy, 1: perpendicular to the plane of isotropy) /VAL 04/

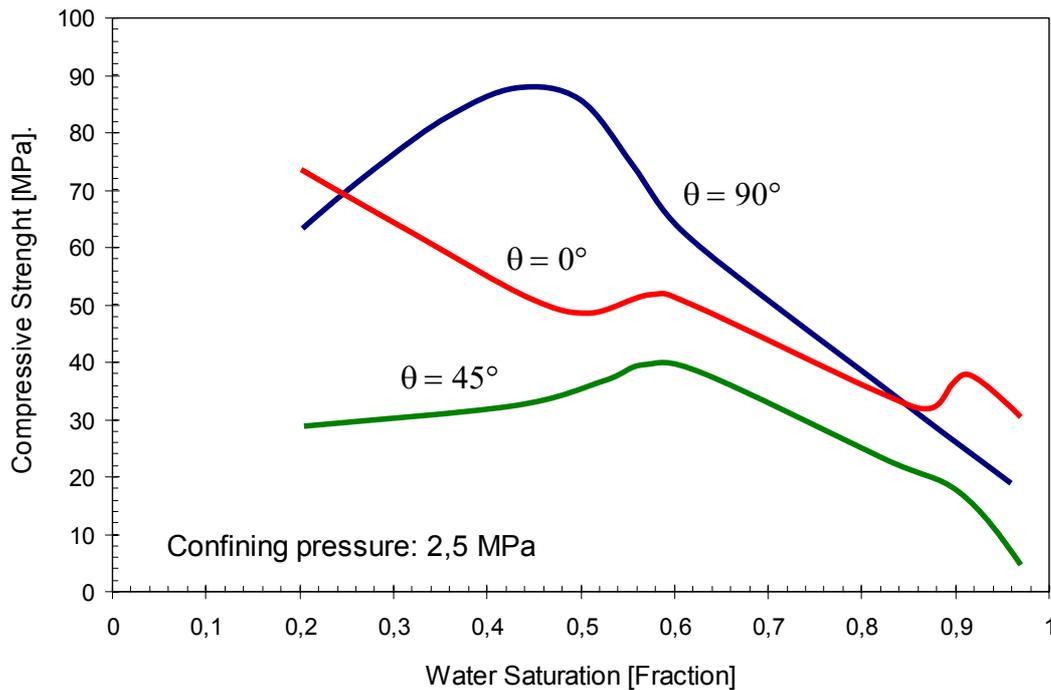


Figure 3-7: Measured triaxial compressive strength of Tournemire clay formation as function of water saturation and sampling orientation (0° : parallel to plane of isotropy, 90° : perpendicular to the plane of isotropy) /VAL 04/

3.2.4 Effect of Bedding-/ Foliation

The previous discussion on the mechanics of clay formations reveals a strong and basic dependency of the mechanical behaviour to the bedding and foliation (Figure 3-6, Figure 3-7). This is an obvious result of the anisotropy created by the structure due to the deposition and other geologic processes. The structural anisotropy is highly dominated in clay formation and the neglecting of this aspect has to cause deficits on the evaluation of the mechanical behaviour. Therefore it is suggested that all experimental as well as numerical studies should consider the effect of the anisotropy. The effect of the anisotropy on the mechanical properties of the clay formations especially on their elastic respectively on thermo-elasto-plastic behaviour is demonstrated in some related studies /VAL 04/,/COR 07/. Relevant measured mechanical properties of some clay formations are given in Table 3-1 as function of orientation to bedding.

Table 3-1: Measured strength and deformation properties of some clay formations (in-situ or close to in-situ condition)

	Opalinus /COR 07/, /NAG 02a/		Tournemire /REJ 06/, /VAL 04/		Boom (Mol) ¹ /MEN 04/, /BOU 96/	
Orientation to bedding	Parallel	Perpend.	Parallel	Perpend.	Parallel	Perpend.
Un. Comp. Strength, MPa	10	16	13	32	2	4
Tensile Strength, MPa	2	1	3,6	-	-	-
Elasticity Modulus, GPa	10	4	27,7	9,3	0,3	0,2
Poisson ratio	0,33	0,24	0,40	0,23	0,125	-
Cohesion, MPa	2,2	5	0,40	-	0,3	-
Shear Angle, °	25	25	23	22	47-52	-

¹ No reliable information on the effect of the foliation

3.2.5 The Effect of the Pore Pressure on Material Properties

If any rock has an interconnected porous or fracture system defining a pore volume, the effect of pressure of the fluid filling this network on the mechanical properties of this rock should be considered. This is also the case for clay formations. The effective stress formulation can be used for calculating the dependency of the total stress acting on the rock to the pore pressure /BIO 41/

$$\sigma_e = \sigma - \alpha \cdot p \quad (3-1)$$

where

σ_e = effective stress, MPa

σ = total stress applied to the rock, MPa

p = pore pressure, MPa

α = Biot Coefficient which is dependent on the structure of the rock and porous medium. This coefficient is given between 0 and 1 /BIO 41/.

The experiments on the mechanical properties of the clay formations are due to the correction of the effect applied by the pore pressure. This is related obviously to the saturation of the core as well as to the average pressure of the fluids. If the neglected pore pressure in the mechanical experiment is higher than expected, lower shear strength values will be observed

because of reduced effective stress. In the contrary, if the pore pressure is lower than expected the estimated shear strength is higher than estimated.

Studies on the effect of the pore pressure on estimating the mechanical properties are intensifying especially on determining the poroelastic parameters. After /BEM 04/ poromechanical behaviour of clay formations appears to depend on the rock saturation state. Samples with a greater initial saturation seem to show a less apparent degree of overconsolidation and a higher compressibility. The results also show the influence of the applied stress on the poroelastic parameters. Biot's coefficient decreases when the axial stress increases, while the drained bulk modulus and the shear modulus increase. The effect of the applied stress on Biot's modulus is more difficult to explain because its measure strongly depends on the saturation level of the sample.

In a numerical study the Biot coefficient is assumed to be 1 which is speculative if the low permeability and microstructure of compacted clay formation is taken into account /XIE 05/.

The effect of pore pressure on the shear-strain behaviour of the Boom clay can be observed from Figure 3-8 as typical example for plastic clays. The stress-strain curves of the reconstituted samples exhibit a brittle behaviour with distinct undrained peak strength. All the samples initially showed a stiff response. A slow continuous decrease of deviatoric stress is also observed (after peak conditions) with an increase of axial strain. The tests are performed with various effective stresses. The increasing effective stress thus increasing effect of the pore pressure increases the hardening effect. This is coupled with a slight increase in the excess pore water pressure up to peak deviator stress before the end of the test, suggesting they are approaching the critical state /BOU 96/.

3.2.6 EDZ, Dilatancy Behaviour, Dilatancy Boundary

Underground excavation disturbs the original stress equilibrium of the rock. The result is a deviatoric stress distribution around the caverns with a maximal and a minimal stress. Rocks under uniaxial or triaxial compression undergo volumetric changes, which are negative (compression) in earlier stages and positive (dilatancy) in later stages of loading. The experiments conducted on several brittle and ductile materials have shown that there is compression followed by expansion. The dilatancy is caused by the deviator of normal and transversal stresses. This acts on the rock and leads to a positive shear deformation that occurs at micro level by the initiation and formation of microcracks.

A typical stress-dilatancy behaviour for crystalline rocks is given in Figure 3-9 for rock salt /ALK 02/. At the initial stage of the deviatoric deformation process for crystalline rocks, the pore volume decreases gradually due to a visco-elastic compaction, this closes the existing primary pore network. After the elastic deformation phase, the cracks begin to reopen, or new cracks form because the shear stress increases. This transition from compression, crack closure and reduction in pore volume towards crack reopening, micro-fracturing and pore volume expansion takes place near a dilatancy boundary. The dilatancy boundary is a turnover region where very important structural changes in the crystalline aggregates of the rock occur as deviatoric stress increases. After passing the dilatancy boundary, a rapid in-

crease in porosity and permeability is expected. A percolative flow cluster is formed along the hydraulic pathways because the cracks are interconnected. This behaviour which is very important for commenting the transport properties of the host rock in a repository is relatively less investigated for clay formations.

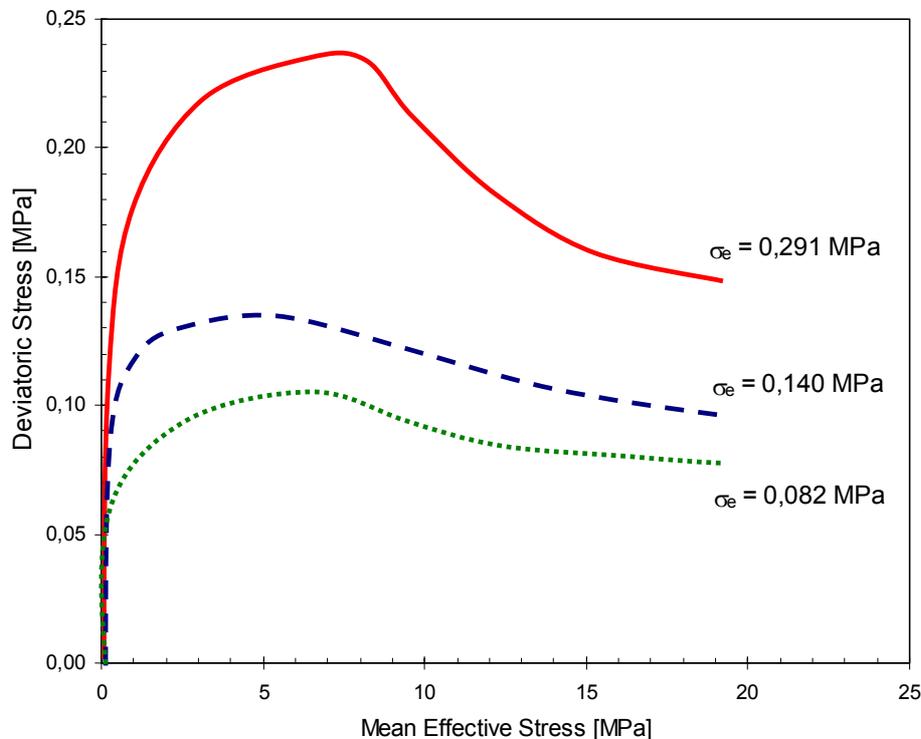


Figure 3-8: Stress-strain curves observed in the tests on reconstituted isotropically consolidated Boom clay /BOU 96/

The triaxial stress-strain relationship of the Callovo-Oxfordian clay is compared with the stress-strain behaviour of the Asse salt taken from a similar experiment in triaxial conditions. As shown in the Figure 3-10 the lateral strain is minor up to the higher stress levels indicating a small volumetric dilatancy. The axial strain, on the other hand indicates a high visco-elastic compression with increasing axial stress. A cumulative volumetric dilatancy begins relatively later indicating a higher dilatancy boundary for the Callovo-Oxfordian clay. The viscoplastic behaviour for the clay formation is expected after the axial pressure reaches 35 MPa.

Investigations at different sites (e.g. HADES/Belgium, Mont Terri/Switzerland and Tournemire/France) have shown that an EDZ occurs in soft or plastic clays as well as in indurated and more brittle claystones or argillites. Most discrete features in the EDZ are caused directly by the instantaneous unloading during excavation (undrained elasto-plastic response) and are of extensional nature. Sometimes, especially for weaker rocks, these features can be accompanied by shear failure. In case of anisotropic rocks (e.g. bedded rocks, low-grade metamorphic rocks), an activation of the planes of weakness can be observed. This failure process can be of extensional or shear origin.

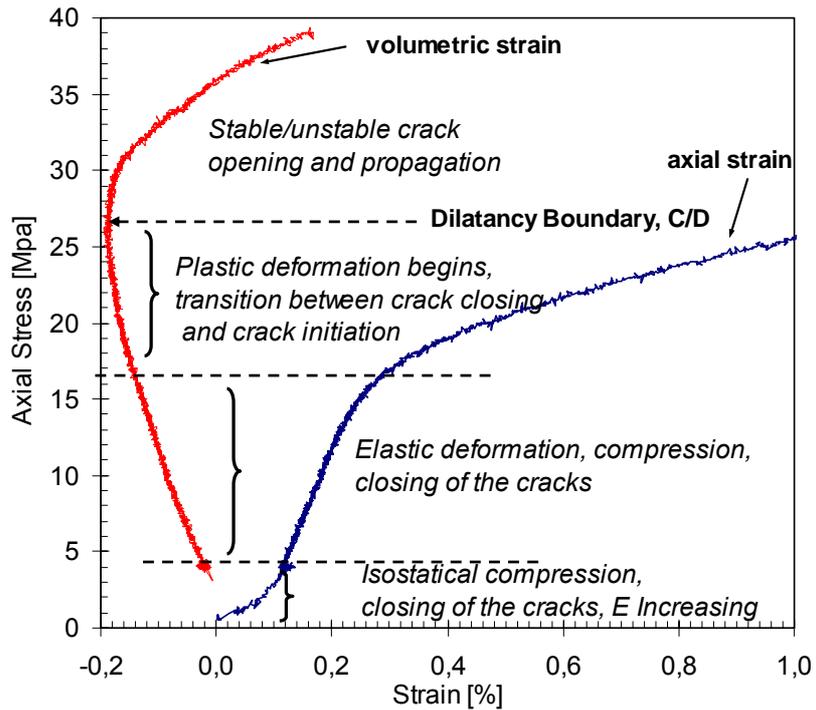


Figure 3-9: Stress-strain behaviour of crystalline rocks /ALK 02/

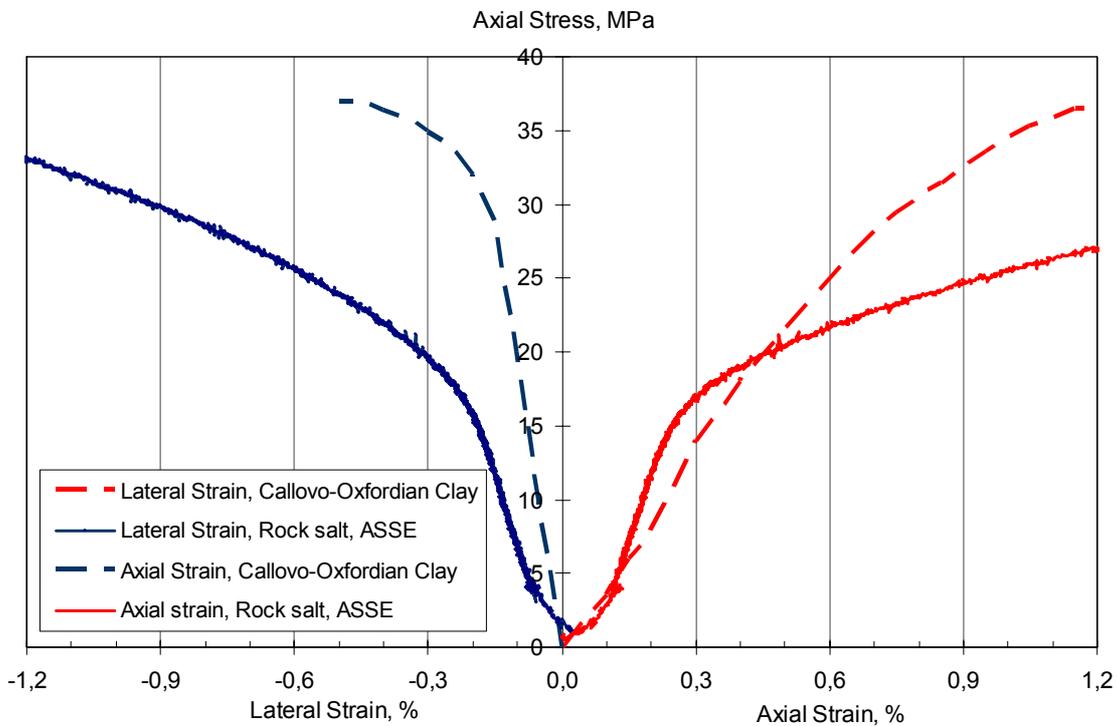


Figure 3-10: Comparison of the dilatancy behaviour of the Callovo-Oxfordian clay with rock salt ASSE

The most important parameter of the EDZ with respect to waste disposal is the effective dilatancy induced permeability increase. In claystones like Opalinus Clay in Switzerland an increase from a homogeneous hydraulic conductivity of about 10^{-13} m/s to local maximum fracture transmissivities of 5×10^{-7} m/s has been observed in the initial phase of the EDZ creation. The effective increase in permeability, which is controlled by several factors (e.g. the interconnectivity of individual features), has not been measured so far. There are indications from *in-situ* tests that this property of the EDZ is much lower than the locally measured values. Investigations on Opalinus Clay formation at Mont Terri exhibit new results by giving new data on the height of the dilatancy boundary. The Dilatancy of the Opalinus Clay as function of minimum stress and bedding is given with the following relationships /LUX 06/:

$$\Delta V/V = (-2100 \pm 1800) \times 10^{-6} \text{ for the samples parallel to the bedding} \quad (3-2)$$

and

$$\Delta V/V = (-4100 \pm 4100) \times 10^{-6} \text{ for the samples vertical to the bedding} \quad (3-3)$$

In a recent study it is indicated that the presence of the microcracks in Opalinus Clay is obvious and that the opening, re-opening of the microcracks is controlled by a mechanical process at EDZ similar to those affirmed for crystalline rocks /COR 07/. Figure 3-11 shows the effect of the microcracks on the stress-strain curves of a sample of Opalinus Clay in an unconfined compression tests. As in other rock types used as repository, the stress-strain curves of the clay formations give good indications on their dilatancy behaviour. The stress-strain curve of Opalinus Clay, although it is considered to be a relatively weak rock, is similar to that of brittle rocks. The approximate divisions of the five regions of the stress-strain curve are shown in Figure 3-11 for a typical uniaxial test on Opalinus Clay with unload-reload cycles.

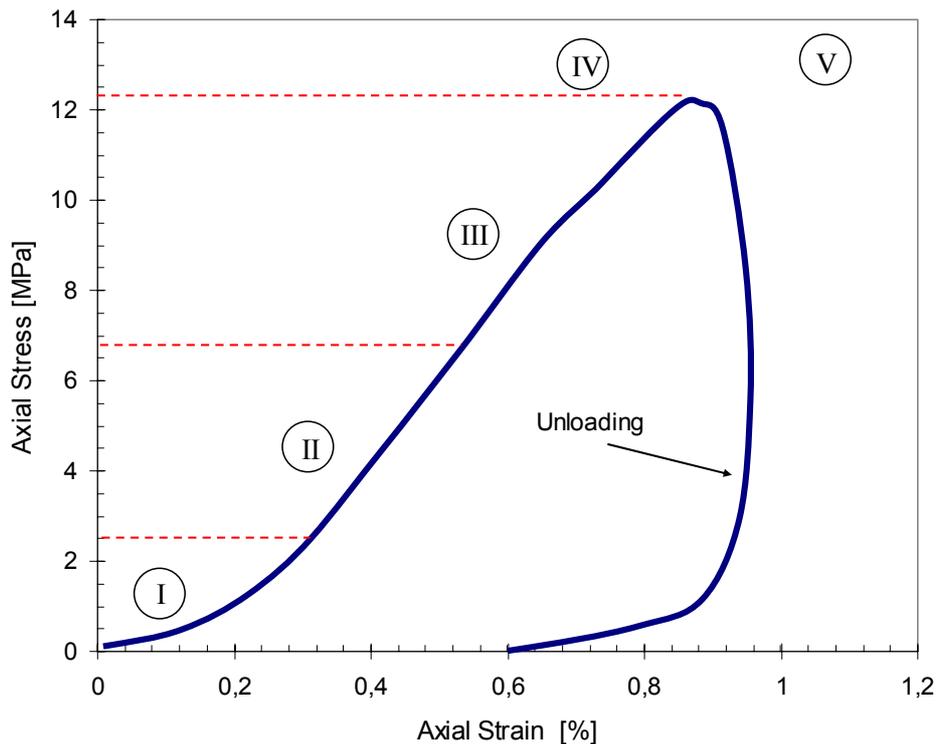


Figure 3-11: Effect of the microcracks on the stress-strain curve for Opalinus Clay /COR 07/

The five regions of stress-strain behaviour are determined as done for the crystalline and salt rocks:

- Region I—closure of existing micro-cracks and crushing of asperities
- Region II—linear elastic
- Region III—onset of dilation (crack initiation)
- Region IV—unstable crack growth
- Region V—post-peak.

In this classification of the stress-strain region the transition between region II and III determines the dilatancy boundary, a boundary showing the structural damage for clay formations, too.

Small scale heterogeneity in the clay composition can initiate microfracturing during loading even before the peak strength of the material is reached. For Callovo-Oxfordian clay, the potential host rock for a repository for radioactive waste in France, differences in stiffness of clay minerals on the one hand, and quartz and calcite on the other hand lead to local strain accumulation (2% in clay agglomerates for a mean strain of 0,76%). This process induces micro-cracks at crystalline interfaces mainly clay/calcite, or even cleavage of minerals. Their general direction is related to the stress field.

The stress damage threshold seems to be correlated to the strength of the clay formations but the carbonate content controls the damage – the higher the carbonate content the more severe the damage. For the Callovo-Oxfordian clay the following relations were observed:

$$\sigma_{\text{dam}} = 0,9 \sigma_c - 13 \text{ (MPa) in the carbonate-rich formation} \quad (3-4)$$

$$\sigma_{\text{dam}} = 0,6 \sigma_c - 2 \text{ (MPa) in the clay-rich formation} \quad (3-5)$$

where σ_{dam} = threshold of deviatoric stress for the onset of damage and σ_c = peak deviatoric strength

The observed non-linear behaviour can be described by elasto-plastic models including anisotropic damage criteria. When the deviatoric stress reaches 90% of the peak strength, the propagation of cracks becomes unstable. They coalesce in shear bands, creating macro fractures /BLÜ 05/.

After waste emplacement the heat generating waste may cause the increase of stresses because of thermal expansion of solids and porewater and heating-related reduction of strength. Numerical calculations indicate that this transient effect is quite limited as the temperature increase at some distance from the emplacement tunnel is quite moderate. This process could further increase the size of the EDZ but in turn, heating may also increase creep rates and thus accelerate the closure of open fractures and reduce the influence of the EDZ.

The re-saturation of the tunnel near-field and the bentonite buffer will cause additional processes, such as:

- Swelling of the host rock in the unloaded area
- Disintegration of the rock in part of the EDZ
- Increase of host rock creep
- Swelling of the buffer and therefore increase of radial pressure on the tunnel wall (in case of smectitic clay buffer material)

These processes cause self-sealing effects leading to a significant reduction of the EDZ permeability (up to 4 orders of magnitude within about 3 years for clay formations) as demonstrated in several large scale *in-situ* tests in underground laboratories and laboratory tests. Supporting evidence for such self-sealing processes in clay formations under a certain effective normal stress is given by hydraulic test results on natural fractures or fracture zones in clay formations. Therefore, it can be expected that the increased hydraulic conductivity, which was created due to the excavation-induced unloading process may approach the original in-situ values during the equilibrium process after repository backfill and closure. This process happens very rapidly in plastic clays but also within a few years in the indurated clays /BLÜ 05/.

An in-situ EDZ characterization study in URF HADES was realised. The EDZ around test gallery was characterised by studying various topics: fracturing, mechanical parameters and hydraulic parameters. During the excavation works, an extensive fracture observation programme was carried out. The front and sidewalls were systematically observed and this re-

sulted in a description of the excavation induced fracture pattern. Cores were drilled and these revealed that the radial extent of the fractures is about 1 m into the host rock /BAS 05/.

The hydraulic disturbed zone of EDZ, around the gallery was also studied using multi-piezometers. These instruments allow long-term follow-up of pore pressures and measurement of the hydraulic conductivity “k”. The influenced zone is anisotropic: the influenced zone is ~20 m in a horizontal cross section and ~40 m in a vertical cross section. The anisotropy of the hydraulically affected zone can be explained by the anisotropic stress state ($K_0 < 1$) as is shown by numerical modelling and analytical calculations. The same anisotropy is measured during the first years after excavation. But as time passes, the pressures in the horizontal piezometer drop, the pressures in the vertical one rise and after ~10 years the anisotropy is inverted. This effect is due to the anisotropy of the hydraulic conductivity in Boom clay ($k_H \approx 2 \cdot k_V$) which causes a larger draining effect horizontally. The in-situ value of k is low ($\sim 10^{-12}$ m/s) so the characteristic time for the drainage effect is high. An other observation is that piezo-filters as few as 60 cm into the host rock are measuring positive water pressures, which means that the converging borehole has sealed off the piezometer (no packers are used) and that no interconnected fracture network exists (at least) beyond 60 cm. Measurements also showed that the hydraulic conductivity is influenced up to 6 m into the host rock. At 1m $k_H \sim 3 \cdot 10^{-11}$ m/s was obtained, in the far field $k_H \sim 6 \cdot 10^{-12}$ m/s /BAS 05/.

Within the framework of several projects at different locations at the URL Mont Terri seismic measurements were carried out to detect the EDZ. The application and combined interpretation of different seismic techniques and the methodology used for the characterisation of the EDZ with the help of seismic parameters are proved to be a good tool for routinely in-situ application /SCH 05/.

The distribution of seismic P-wave velocities and damping of amplitudes along the borehole depth are used primarily for the detection and determination of the extent of the EDZ. In terms of a relative assessment different degrees of damage can be identified. The extent of the EDZ varies between several centimetres and around 2 meters, depending on the location and orientation (roof, floor, and wall) as well as on the type of excavation (tunnel bore machine, pneumatic hammer, blasting technique).

Cross hole measurements between two parallel boreholes at a distance of 1 m and depths of 1,7 m gave very good results about the seismic anisotropy behaviour of the Opalinus Clay. Derived P-wave velocities vary systematically between 2400 m/s and 3100 m/s which results in a remarkable anisotropy factor of 1,3.

A comparison of the EDZ for all possible host rocks are made by /TSA 05/. The comparison shows that all rock types have an undisturbed rock permeability of 10^{-19} - 10^{-21} m². The stress redistribution created by the excavated tunnel or drift is the key cause of the EDZ in all four rock types, giving rise to tension, compression, and shear or deviatoric stresses in different parts of the rock around the opening. The responses of the different rock types to these stresses depend on their properties and structure. Shear stresses also act to open fractures or create new ones through shear displacement and dilation. The effect is largest at the drift wall and extends about one drift radius into the rock. For the much softer indurated clays, owing to their bedding structure, the responses are different in the side walls compared to

the ceiling and floor. Above the ceiling and below the floor, there is a predominant opening of bedding planes, while on the two walls layers of vertical fractures are formed. For plastic clays, because of anisotropy, the induced fractures form an eye-shaped set of curved fractures, much like onion skins, around boreholes. However, many of the fractures are not hydraulically conductive. Thus, a 4,8 m drift in plastic clay may have fractures extending several metres beyond its wall. After a few weeks, however, piezometric measurements indicate that open fractures do not extend beyond a zone of about 1 m. A very important component of excavation activity is the emplacement of support, which is of particular importance for plastic clay. Much consideration has been given to minimise the over-excavation gap between the shield and the excavated rock wall, and to emplace an expanded lining system as soon as possible. In this way, a back-pressure quickly develops and prevents further wall convergence and larger EDZ development. Similarly, a back-pressure from a rock support system can help to limit EDZ development in indurated clays.

In contrast to crystalline rock, once the drift-chamber is constructed, an EDZ still evolves under the stress-strain conditions for plastic and indurated clays and for salt. Ventilation reduces drift humidity and dehydrates the rock near the drift surfaces. This dehydration has obviously a significant effect on clay properties. For indurated clay, dehydration strengthens the rock so that it may be self-supporting at the drift wall. But it also causes contraction and thus could induce tensile fractures. For plastic as well as indurated clays, ventilation changes suction, changing in turn the clay creep properties and retarding self-sealing /TSA 05/.

Mechanically, rock creep is a significant process for plastic clay, indurated clays as well as for salt. Where support has been emplaced, the rock moves against the support, which provides a back pressure. In plastic clay, unsupported axial movement at the front of a drift can be as much as 10 cm per year. Further, its deformation, coupled with its low permeability, can result locally in larger pore sizes, with an enhanced suction even without desaturation.

After the closing of the excavated chambers with the swelling of the backfill, a back-pressure is applied to the rock that will tend to close fractures in the EDZ for all rock types of repository. For certain repository designs in plastic clay a non-swelling backfill is sometimes chosen to avoid such reloading, since one can depend on rock creep to close up the fractures. For indurated clay, data suggest that the largest permeability values are not found at the drift rock surface, but at about 0,6 m into the rock, probably as a result of the back-pressure. Similarly for salt, the expression of the EDZ around a room at WIPP (waste isolation pilot plant) assumes an ovoid shape, wherein the largest fractures occur at a nominal depth, as noted for the indurated clay. At the backfill-rock interface, there is also a subtle effect involving the capillarity of the rock versus that of the backfill, based on the local saturation in the two media. In this instance, water exchange between the two will occur through suction. The implications of this dynamic process, with an associated potential change in rock strength, are yet to be studied carefully.

3.2.6.1 Time Effects on EDZ

The disturbed or damaged properties of the EDZ are due to the significant changes with time. Within the EDZ the stress redistribution may lead to localized consolidation and swell-

ing in the post-closure phase. For example in the region of tangential stress concentration the maximum stress may exceed the previous overconsolidation stress and the material may behave more like normally consolidated sediment rather than an overconsolidated one. In the unloaded areas, suction may attract moisture and these materials may locally swell. Hence the EDZ may experience several complex processes and the material properties may significantly alter with time. Hence as for example the water content changes within the EDZ, as it adjusts to the new stress conditions, the strength and deformation properties will also change. In general, the water content is a very important parameter to characterise the mechanical behaviour of clay rocks but it may affect the rock in very different ways:

- In a saturated stage the water content describes the total porosity of the rock and therefore the distance between clay particles which strongly influences the distance-dependent inter-particle forces (repulsive and attractive forces)
- Swelling due to water uptake or compaction may change the total porosity and distances between particles and therefore weaken or strengthen the rock, respectively.
- De-saturation may result in large suction pressure which increases the apparent strength while re-saturation of partly saturated samples will have the opposite effect.

Regardless of the detailed process, rock-water interaction will have a severe effect on the mechanical behaviour and the sensitivity of these weak rocks to changing water content or the degree of saturation should not be underestimated. For example Little reported on the performance of an 11,1-m-wide, 7,5-m-high and 45-m-long test chamber in weak shale /LIT 89/. The extensive monitoring revealed that the rock mass response to excavation was essentially elastic with no indication of time-dependent movement and that nominal concrete and rock bolt support was an adequate support system. Approximately one year after excavation the lower portion of the test tunnel was flooded. Upon dewatering one year later, major portions of the test chamber had collapsed. Although this example does not directly describe the processes expected during the slow re-saturation of a backfilled tunnel in a repository, it reemphasizes and highlights the role of water in the determining behaviour and strength of such materials.

It must be anticipated that the characteristics of the EDZ in these materials will change with time and that these changes can be accelerated if the environmental conditions (e.g., humidity) are also changed. These changes are currently being monitored at Mol and at the Mont Terri underground research laboratory in several experiments /BAS 05/.

3.2.6.2 Self-Healing of the EDZ

Healing of the damaged zone may be important for clay formations /ALH 03//BEN 03/ /BER 03/. Some field information shows that the EDZ permeability for plastic clay recovers to intact rock value within 15 years, though the fracture traces can still be seen. In this case, the healing process involves not only closing up of fractures due to swelling and creep, but also volume increase around large cracks with an increasing plasticity index. For both plastic and indurated clays, changes in stress state, dilatancy, swelling, and newly formed minerals all

may play a role in healing. A series of experiments are being conducted at the Mont Terri underground laboratory in Switzerland to investigate the healing of excavation-induced fractures as well as gas-pressure-induced fractures. Lessons learned from these experiments may be transferable to salt and plastic clay case.

The self sealing of the microcracks and fractures in EDZ zones of clay formations are more emphasized and studied than other host rocks. /DEB 04/, /BAS 05/, /FRÖ 05/, /MEI 00/. In the framework of SELFRAC project fracturing, self-sealing and self-healing processes of Opalinus and Boom Clay were studied in laboratory and in-situ experiments /BAR 00/, /BAR 03/, /BAS 05/, /COL 04/. The origin and extent of excavation induced fractures are discussed and sealing and (partial) healing of these fractures is demonstrated. The main conclusion gives valuable information on the fracturing and healing processes in both indurated (Opalinus Clay) and plastic clays (HADES, Boom Clay) /KOV 05/.

The tests at Mont Terri, suggest that hydraulic conductivity of fractured Opalinus Clay is restored when the host rock is saturated and pressure is applied. With respect to healing, only indications of weak or partial healing have been observed for Boom Clay in the framework of the SELFRAC project: several of the artificially fractured samples showed some fracture cohesion after dismantling of the experiment. However, the cohesion was low and it was not possible to quantify it. Partial healing was also observed in-situ in HADES. For Opalinus Clay, healing was not observed during SELFRAC. Sealing (and healing) is in general the result of several mechanisms. The main mechanisms for sealing (and healing) in clays are swelling, consolidation and creep. Each of these mechanisms makes a more or less important contribution to the overall process, depending on the properties of the rock and the state it is in; it is however often difficult to distinguish the quantitative contribution of each of them. In geotechnical and mining engineering, the evolution and geometry of the “Plastic Zone” as part of an EDZ is a key issue in the design of tunnels and other underground openings. Many theories have been developed, but the availability of appropriate data is still a major issue. In-depth information from various underground research laboratories constitutes a very valuable set of much needed new *in situ* data. Moreover, purpose-designed innovative tools were developed which enable an accurate delineation of the geometry, extent and evolution of the plastic zone. An example is the Interval Velocity Measuring Method in boreholes developed by Alheid and co-workers, which was employed e.g. in Tournemire and Mont Terri /SCH 05/ The investigations carried out in the New Gallery of the underground research laboratory at Mont Terri revealed the extent and degree of fracturing of the EDZ and the changes with time in a detail which, in the opinion of the Expert Group, is without precedent in underground construction. The evolution of the EDZ after repository closure is affected by a number of processes, such as resaturation, pressure build-up, swelling and disintegration/homogenisation on a nanometric scale. These processes contribute to self-sealing, i.e. the reduction of hydraulic conductivity of fractures with time. Self-sealing is of key importance to PA and is often cited as an important factor favouring the choice of argillaceous formations as host rocks for deep disposal. Self-sealing directly addresses the functionality of the clay host rocks as a migration barrier. When the self-sealing process proceeds in reasonable time, fractures created by the construction of the repository will not persist as preferential pathways for radionuclide migration, and thus the system becomes diffusion-dominated. Self-sealing also occurs in natural fractures and faults penetrating argillaceous rocks. Substantial

evidence exists that natural fractures are not hydraulically active and have not been active over geological periods of time. This set of observations constitutes a strong geological argument for the self-sealing capabilities of argillaceous formations, addressing both sealing of natural fractures as well as the EDZ around underground openings. Self-sealing mechanisms have been widely observed in a variety of clay rocks, and the basic physico-chemical and hydro-mechanical processes leading to self-sealing are well understood. In plastic clays, self-sealing is expected to be a rather quick process. In more indurated clay rocks, self-sealing is expected to be slower. However, the currently available knowledge is not yet sufficient to permit detailed predictions concerning the kinetics of the self-sealing process in various types of argillaceous media. In spite of the existing data and observations, understanding still needs to be improved.

One question is whether the observed self-sealing of natural fractures can be extrapolated to the sometimes geometrically different fracture arrays in an EDZ. Wedge-shaped and composite fracture planes, for instance, may develop in the roof of tunnels excavated in horizontally bedded argillaceous rocks. For this case geological analogues may be of limited value, as natural and EDZ fracture planes may be different in shape. The resistance to closure of composite and wedge-shaped fracture planes, particularly in response to swelling pressures originating in the formation and/or in the backfill, should be carefully investigated. Besides the hydro-mechanical evolution of the EDZ, chemical reactions may occur in the EDZ during the operational phase of the repository. For example, EDZ fractures create pathways for oxygen. The most relevant chemical effect is the oxidation of pyrite, which occurs as an accessory phase in all formations considered (except for the Boda Clay Formation). There is substantial evidence that pyrite oxidation will not have detrimental effects on the geochemical and geomechanical properties of the EDZ. Evidence from laboratory experiments and from natural analogues (such as tunnels penetrating argillaceous formations or surface-near decompaction fractures) indicates that oxidation penetrates only a few cm into the rock matrix even if exposure to air occurs over decades. The acid produced due to pyrite oxidation will be consumed by a small degree of calcite dissolution, thus pH will be buffered by the carbonate system and will not drop substantially (all formations considered contain calcite). As the EDZ self-seals, the access of oxygen to the rock gets blocked. Thus the kinetics of the self-sealing process will influence the magnitude of oxidation and, by consequence, the geochemistry in the affected field of the repository.

The design and technical parameters of EDZ in indurated and plastic clay formations are given in Table 3-2 for various operational stages.

3.2.7 Swelling

Bentonites are considered to be favourable sealing and backfilling materials because of their swelling capacity. The swelling property of clay minerals adds some additional features to the mechanics of clay formations. The unsaturated bentonite as engineered barrier for example experience large strain when they are wetted. High volumetric expansions create a swelling pressure which can be very advantageous in terms of the sealing capacity of the engineered barrier systems. On the other hand, laboratory experiments show that the gas permeation of an initially water-saturated clay buffer occurs when the gas pressure slightly exceeds the

sum of the swelling pressure and the hydrostatic pressure. Consequently, in order to cause the gas to flow preferentially through the seal and not into the host rock, the swelling pressure should not exceed the gas entry pressure of the host rock. The swelling properties of bentonite can be significantly reduced in the case of presence of high salinity systems. Therefore the swelling properties of the clay formations, especially of the bentonite buffer should be sufficiently examined for the performance assessment as barriers system.

Table 3-2: Property - design and technical parameters of EDZ in indurated and plastic clay formations (after /TSA 05/, /CHA 03/, /BER 03/)

Stages	Indurated Clay	Plastic Clay
Excavation	<p>Rock property parameters; anisotropy (bedding planes)</p> <ul style="list-style-type: none"> • <i>In situ</i> stress state, including stress anisotropy • Drift orientation relative to bedding plane directions and to fracture directions • Drift (gallery) shape, • Methods of excavation with emplacement of support, • Moisture content in rock and transient pore pressure <p>Indurated clays exhibit several features of both -soft rocks (creep-prone, strength related to moisture -Martin et al.)-hard rocks (brittle behaviour), complexity of the EDZ in indurated clays is high.</p> <p>Medium characterized by dependence on moisture content: low moisture case corresponds to harder rock and high case corresponds to ductile (soft) behaviour</p> <ul style="list-style-type: none"> • Role of structures (bedding planes), weathering (drying), dissolution and oxidation; • Nonlinear stress-strain behaviour dependent on stress level, suction (water content) and weathering conditions; • Stress and strain localization: onset and propagation of discontinuity; effect of heterogeneity. 	<p><i>In situ</i> stress-strength ratio;</p> <ul style="list-style-type: none"> • Excavation and lining installation procedure to limit wall convergence • Parameters related to shear and extensional fracturing • Presence of bedding planes or planes of weakness. • Excavation shape and initial stress state <p><u>Mechanical</u> Naturally occurring fractures are found in outcrops with spacing 0,5 to several metres; mostly <i>extensional fractures</i> with a small part <i>shear fractures</i>. However, they are not seen at depth. Confining pressure, as well as moisture content, is reason for absence of fractures.</p> <p><u>Geochemical</u> Geochemical changes at local scale, calcite precipitation?</p> <p><u>Thermal</u> Modification of material properties, increased creep rate, enhanced plasticity?</p>
Open Drift Stage	<p>Process has 4 stages in stress-strain development</p> <ol style="list-style-type: none"> 1. Closing of pre-existing fractures 2. Elastic deformation of material 3. Plastic deformation; occurrence and 	<p>EDZ is still changing;</p> <p><u>Mechanical</u></p> <ul style="list-style-type: none"> • Fractures develop several metres in rock, but if convergence is limited, fractures can be limited to less than

Stages	Indurated Clay	Plastic Clay
	<p>growth of micro cracks</p> <p>4. Localization of stress strain and initiation and propagation of macro fractures</p> <p><u>Mechanical</u></p> <ul style="list-style-type: none"> • Peak of Δk is behind peak of stress as a function of strain • Effect of heterogeneity in rock property (clay content and hence rock strength not uniform). • Swelling due to humidity increase <p><u>Hydraulic</u></p> <ul style="list-style-type: none"> • Sealing of EDZ by emplacement of backfill after removal of EDZ damage materials or by radial cuts that are filled with bentonite—yet to be studied <p><u>Geochemical</u></p> <ul style="list-style-type: none"> • Geochemical changes at various levels • Transport of chemical species (carbonate precipitation) • Oxidation of pyrites (Bure), Production of Sulphuric Acid) 	<p>1 m from rock wall.</p> <ul style="list-style-type: none"> • Ventilation drying changes EDZ properties near drift wall <p><u>Hydraulic</u></p> <p>Combination of low k and deformation (undrained) causes changes in suction and in apparent mechanical properties.</p> <p><u>Geochemical</u></p> <ul style="list-style-type: none"> • Geochemical changes at various levels • Transport of chemical species (carbonate precipitation) • Enhance cohesion (strength)? • Clay oxidation in open fractures • Corrosion • Degradation, ageing, chemical effect on clay minerals
<p>Early Closure Stage</p>	<p><u>Mechanical-hydraulic</u></p> <p>Resaturation weakens rock, enhances creep, and induces closure, especially normal to bedding planes</p> <ul style="list-style-type: none"> • Resaturation is a slow process; effects of spatially and temporally varying saturation yet to understand. • Heating may cause near-field drying in EDZ, working opposite resaturation from the rock, resulting in varying wetting and pore pressures in EDZ • Sealing bentonite provides loading on EDZ and reduces k • Fluid pressure in the galleries (filled with water? water pressure in the gallery?) • Gas pressure build up generated by corrosion and wastes <p><u>Geochemical</u></p> <ul style="list-style-type: none"> • Geochemical changes at various levels 	<p>Resaturation causes suction to disappear.</p> <p><u>Mechanical-hydraulic</u></p> <ul style="list-style-type: none"> • Open fractures start to heal. • After a few weeks, piezometric measurement indicates open fractures do not extend beyond 1 m of wall <p><u>Geochemical</u></p> <ul style="list-style-type: none"> • Geochemical changes at various levels • Transport of chemical species (carbonate precipitation) • geochemically damaged zone? <p><u>Thermal</u></p> <ul style="list-style-type: none"> • Temperature assists in healing; may also cause pore water pressure build-up in pores. • Temperature with saturated conditions increases creep.

Stages	Indurated Clay	Plastic Clay
	<ul style="list-style-type: none"> • Transport of chemical species • Swelling induced by changes in fluid chemistry, precipitation of infilling minerals, etc <p><u>Thermal</u></p> <ul style="list-style-type: none"> • Effect of desaturation (bond failure) followed by resaturation • Temperature and humidity varying both with respect to time and space 	
Late Closure Stage	<p><u>Mechanical-hydraulic</u></p> <ul style="list-style-type: none"> • Sealing is a time-dependent process; stress state for contractancy; dilatancy, swelling, newly formed minerals • With saturation, Δk of fracture network reduces by factor of 50 in 110 days. • With gas injection, fractures open. When gas depressurizes, fracture remains open and closes slowly over 5 months • Sealing needs more studies to confirm. • Lining degradation rate is considered a key factor 	<p><u>Mechanical-hydraulic</u></p> <p>Observed: k in EDZ restored in several years: (a) clay closes spontaneously against borehole casings; (b) open boreholes closed completely, and (c) clay flows into open boreholes</p> <ul style="list-style-type: none"> • Fractures closed by increase in stress; swelling and creep. • Discontinuities are still present, but k restored. <p><u>Geochemical</u></p> <p>Geochemically damaged zone?</p> <p><u>Thermal</u></p> <ul style="list-style-type: none"> • Temperature assists in healing; may also cause pore water pressure build-up in pores. • Temperature with saturated conditions increases creep.

Isotropic total stress in clays can be taken as the total of the interparticle stress σ_i acting in the solid skeleton and the water-film pressure p_{fm} consisting of the disjoining pressure p_D and the pressure p_w of free water:

$$\sigma_t = \sigma_e + p_{fm} = (\sigma_i + p_D) + p_w \quad (3-6)$$

where the effective stress σ_e is defined as the sum of the interparticle stress and disjoining pressure, and osmotic effects are not considered. If the pores occupied by free water are interconnected and open to external water, the free water pressure is then equivalent to the external pressure. The swelling pressure for saturated clays where the interparticle stress can be taken as zero (assuming that the saturated clays may behave as perfect colloids), the isotropic effective stress is equal to disjoining pressure p_D of the interparticle water-films, this is also called as swelling pressure:

$$\sigma_e = p_D \quad (3-7)$$

The relevant properties of mechanical response of the clay layers on swelling is summarized in /SAN 05b/ as follows:

- Large swelling strains when they are wetted
- High swelling pressure when they are wetted
- Dependence of the swelling thus the mechanical response on the initial state (density, water saturation, etc.)
- Dependence of the swelling strain on stress path
- Swelling pressure reaching to a maximum for an intermediate suction
- Strain accumulation during suction cycles
- Secondary swelling

Numerous studies were and are conducted on the swelling properties of various bentonites as well as clay formations under various thermophysical conditions /FEB 98/, /ZHA 04/, /SAN 05a/. Figure 3-12 shows the measured swelling pressure for Febex bentonite on the dependency of the applied load in a swelling cell /FEB 98/. The dependency of the swelling pressure on various initial and boundary conditions for compacted bentonite as well as clay formations are experimentally investigated. The expansive behaviour of the clays is calculated using constitutive models based on elasto-plastic formulations.

3.2.8 Long-term Mechanical Behaviour

The long-term behaviour of the clay formations is one of the most important mechanical parameters for the safety assessments. Creep tests were performed for some clay formations like Callovo-Oxfordian and Opalinus /ZHA 02/, /NAG 02b/. The creep behaviour of Callovo-Oxfordian clay formation was investigated by the experiments conducted in uniaxial testing rigs allowing for two and five simultaneous creep tests. The effect of temperature, specimen size, water content, anisotropy and axial stress on creep behaviour are reported in /ZHA 02/. Creep rates between $1 \cdot 10^{-9}$ and $1 \cdot 10^{-10} \text{ s}^{-1}$ are obtained for various experimental cases.

The experiments conducted on Callovo-Oxfordian clay by using a uniaxial stress cell show the importance of anisotropy on creeping behaviour /GRS 01/. As shown in Figure 3-13 the creep tests were performed with stepwise increase of the stress at ambient temperature. Before each increase of the stress, the samples were unloaded to examine the reversible elastic part of the deformation. Generally, the creep deformation and the creep rate increase non-linearly with increasing stress. It has been found that the clay samples creep soon at very low stress levels of less than 2 MPa. Due to an anisotropic micro-crack distribution – existing with longer cracks oriented parallel to the bedding plane and smaller cracks perpendicular to the bedding plane – the creep deformation and creep rate perpendicular to the bedding plane are higher than those parallel to the bedding plane.

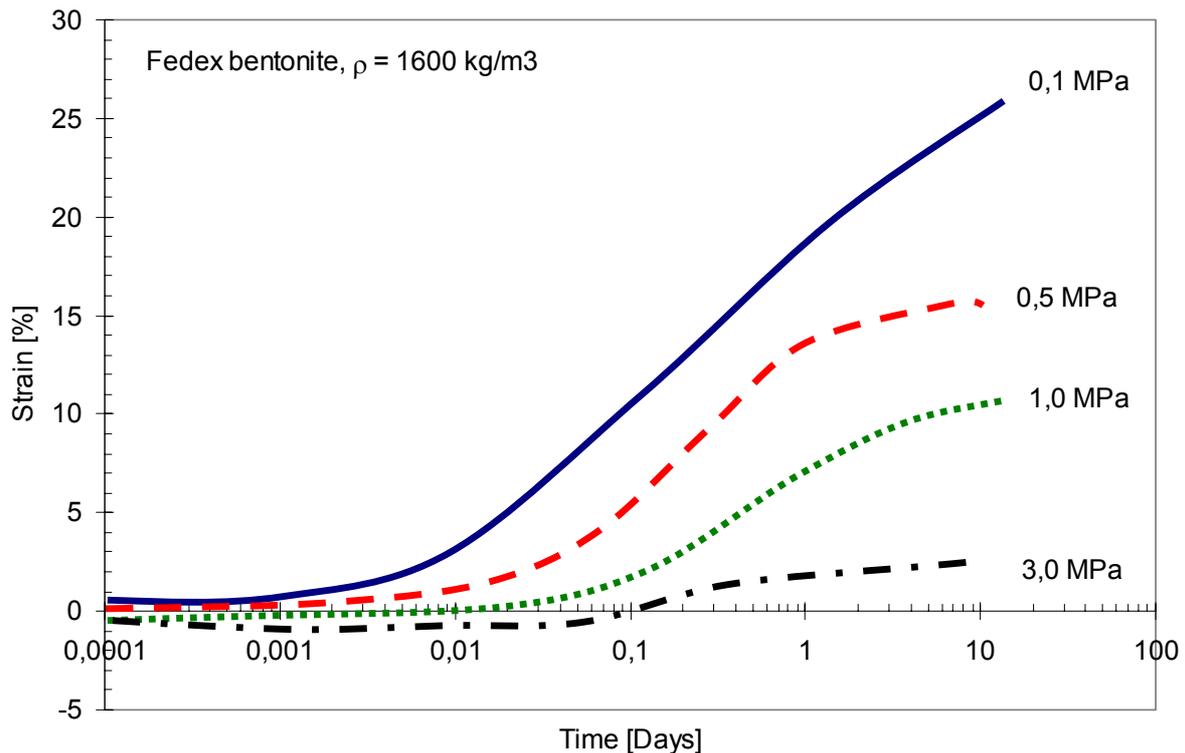


Figure 3-12: Swelling of the Febex bentonite with dependency on the applied load /FEB 98/

As the existing literature provides limited data on the creep behaviour of the clay formations, it is worth to list some of the conclusions of the study on the creep behaviour of Callovo-Oxfordian clay:

- The Callovo-Oxfordian clay rock creeps even under very low of 2-3 MPa indicating the absence of a lower creep limit.
- The pure creep strains and the creep rates are similar, independently from the specimen size.
- Total deformation perpendicular to the bedding plane is larger than parallel to the bedding. However, no significant differences in creep deformation and creep rate were found for the both loading directions
- Creep deformation after the stress reduction from 12 MPa down to 10 MPa can be recovered after several days.
- During the creep duration of several months, quasi-steady creep seems to be reached beyond the transient creep. The following linear relation between the quasi-steady state creep rate, $\dot{\varepsilon}$ and the stress, σ was found, but the creep parameter slightly depending on the origin of the rock which is parameterized with a factor:

$$\dot{\varepsilon} = A \cdot \sigma \quad (3-8)$$

The relaxation behaviour of Callovo-Oxfordian clay rock was also experimentally studied /ZHA 02/. A steady state relaxation i.e. a relaxation with a constant stress rate can not be observed. The relaxation of the stress in the saturated conditions was found faster than in

the air-dried conditions. The relaxed stress increases with increasing the starting stress of the relaxation or with increasing the axial-deformation. The relaxation of the air-dried specimens is nearly independent on the periodic change of the temperature in the cell whereas the fluctuations of the relaxation curves of the saturated specimens are correlated to the temperature change. As temperature rose, the stress increased.

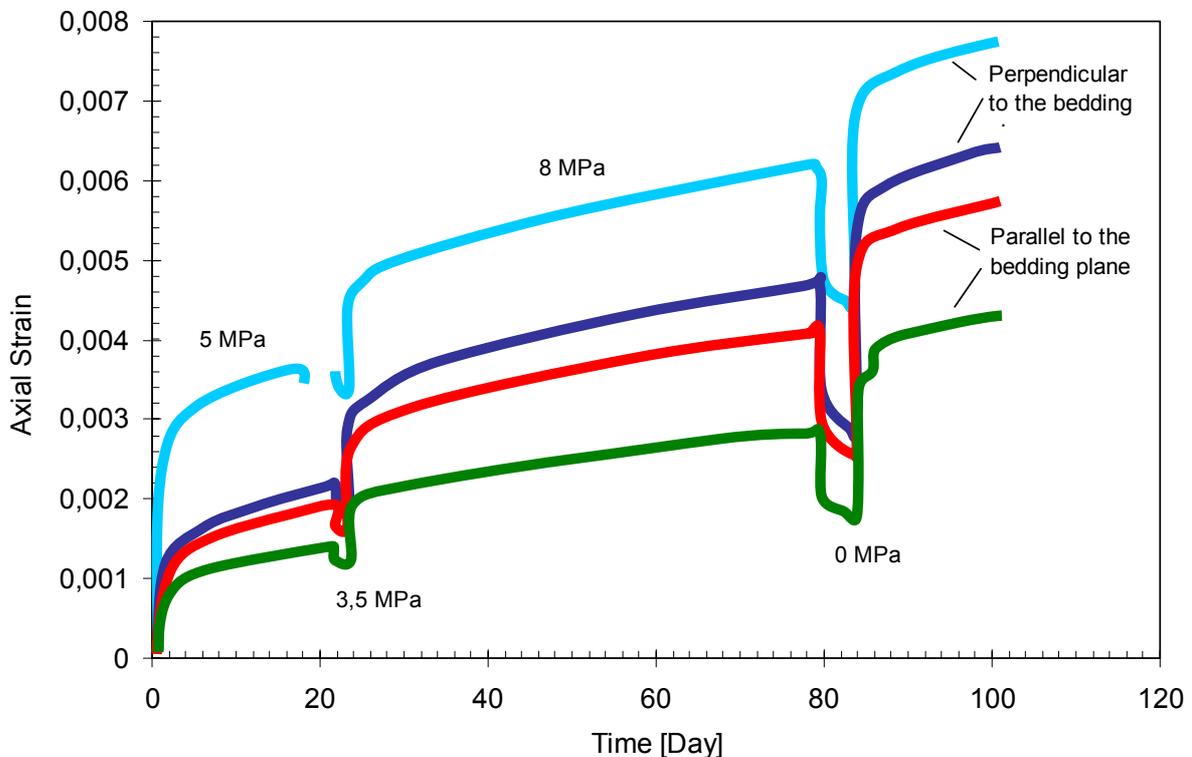


Figure 3-13: Creep behaviour of Callovo-Oxfordian argillite samples from the Bure site /GRS 01/

3.3 Physico-Chemical and Chemical Considerations

The clay formations are chemical rock dominated. That is, the majority of the chemical species dissolved in pore-water are buffered by minerals. The combination of fine grain size and extended pore-water residence times typical of clay formations assures that changes to pore-water chemistry that might be brought about by the repository construction or operation will be strongly buffered by rock-water reactions /MAZ 03/. Many important physical and chemical processes occur at the interface between solid matter and an aqueous phase. Because of the large total surface area and the correspondingly large solid-liquid interface, the colloidal fraction of a clay soil or rock is most active in binding chemical species and compounds.

The interactions between solutes and mineral surfaces are fundamental to our understanding of the transport processes in natural clays. There is a very substantial volume of literature on this topic, stemming from colloid chemistry, soil science and specific research studies on contaminant transport. Clay-water-solute interactions also play a dominant role in determin-

ing the geotechnical and hydrodynamic properties and responses of natural clay systems such as plasticity, consolidation, swelling and thermal behaviour. Some of the physico-chemical and chemical processes in clay-water system are described in the following sections based on previous studies /HOR 96/, /ROD 99/, /MAZ 03/.

3.3.1 Adsorption

Water is adsorbed on the clay mineral surfaces by hydrogen bonding between the water molecules and exposed hydroxyls or oxygen atoms and by the hydration of exchangeable ions. The exact arrangement of the bound water is disputed, but it is certain that the molecules adjacent to the crystal faces are tightly bound in a fairly regular pattern.

The adsorption-desorption isotherms for water-clay interaction are based on a set of measurements at constant temperature of the mass of water sorbed per unit mass of dry clay. Measurements of this type generally show fairly strong hysteresis over an adsorption desorption cycle. Calorimetry provides an alternative method of investigating the thermodynamic properties of adsorbed water. It can be quantified from a set of isotherms established over a range of temperatures. During the deep burial and compaction of an argillaceous rock, the water on the internal and external surfaces of the clay minerals is desorbed as discrete layers of water molecules.

If a solvated ion does not form a complex with a charged surface functional group, but instead neutralizes surface charge only in a non-local sense, it is said to be adsorbed in the diffuse ion-swarm. The diffuse ion-swarm and the outer-sphere surface complex mechanism of adsorption involve almost exclusively electrostatic bonding, whereas inner-sphere complex mechanisms are likely to involve ionic as well as covalent bonding. Inner-sphere complexation is, therefore, termed specific adsorption and outer-sphere complexation, together with diffuse ion association are called non-specific adsorption. Readily-exchangeable ions are those that can be replaced easily by leaching with an electrolyte of prescribed composition, concentration and pH value. Ions sorbed specifically are not normally considered readily-exchangeable. Readily-exchanged ions adsorb and desorb very rapidly with a rate governed by film diffusion. Specifically adsorbed ions show much more complicated behaviour, in that they often adsorb by multiple mechanisms that differ from those involved in their desorptions. These adsorption reactions are often slow. Cation sorption can be rationalised in terms of inner-sphere, outer-sphere and diffuse ion-swarm concepts. The relative order of decreasing interaction strength is: inner-sphere > outer-sphere > diffuse ion-swarm. For the inner-sphere surface complex, the electronic structures of the cation and the surface functional group are important, whereas for the diffuse ion-swarm only the metal cation valence and surface charge should be critical. The outersphere complex is intermediate with valence probably the most important factor. The relative affinity of an adsorbent for a free metal cation increases with the tendency of a cation to form inner-sphere surface complexes. For a series of metal cations of a given valence, this correlates positively with the ionic radius giving the well-known selectivity series: The mechanisms by which small anions adsorb are, as for cations, surface complexation and diffuse ion-swarm association. An estimate of the size of the interfacial region over which the electrostatic repulsion of the charged surface is effective can be made by defining an exclusion volume V which is the total volume of the soil solution (per

kilogram of dry soil) in which the concentration of the anion is lower than its bulk concentration.

3.3.2 Swelling

Swelling is the increase in volume which occurs when clay minerals or natural clay systems are exposed to water or other polar liquids. If volume change is constrained, then a swelling pressure develops which acts against the constraint. It is important to distinguish between the interlayer (intraparticle) swelling which is specific to certain 2:1 layer-silicates, notably smectite and vermiculite, and the interparticle swelling which occurs in most compact clays rocks, regardless of their precise mineralogy.

Fundamental studies are made on the interlayer swelling in montmorillonite and vermiculite and on the sensitivity of this mechanism to the exchangeable cation, electrolyte concentration and inter layer spacing. It is generally agreed that interlayer swelling, or lack of it, is controlled by the balance of attractive and repulsive forces between adjacent 2:1 layers /MEU 05/. However, there are several schools of thought on the precise nature of the repulsive force. The physico-chemical forces acting across the narrow, water-filled spaces between aligned clay particles are also probably responsible for the interparticle swelling observed in very compact argillaceous rocks such as shales. In clay formations which do not contain any significant quantity of expansive clay minerals, it seems likely that the swelling forces are developed between the external surfaces of closely-packed platy clay minerals such as illite by mechanisms which are not dissimilar to those which operate during interlayer swelling /NEA 96/.

The swelling property is determined by the ability of cations to retain their polar molecule "shell" (water, glycol, glycerol) within the interlayer environment. This property does not exist if the charge of the layer is too high (micas, chlorites) or zero (pyrophyllite, talc). More simply, this property is characteristic of di- and trioctahedral smectites and vermiculites. Polar molecules are organised into layers whose number varies inversely with the interlayer charge:

1. Charge contained between 0,8 and 0,6: 1 layer of polar molecules. High-charge polar saponites adsorb 1-2 layers of polar molecules.
2. Charge contained between 0,6 and 0,3: 2 to 3 layers of polar molecules.

3.3.3 Diffusion

With the assumption that the concentration gradient is essentially constant, diffusion may be described with Fick's Law:

$$\frac{\partial N}{A \partial t} = -D \frac{\partial N}{\partial z} \quad (3-9)$$

where N the number of particles which pass through a plane of area A within the unit of time t . The velocity of diffusion is dependent of the gradient in concentration i.e. the change of the particle number within a distance z , and the diffusion coefficient D . The flux of particles is

given as mol/m²s in SI units therefore the unit of diffusion constant is m²/s. The diffusion constant can be experimentally defined for a given temperature and materials. This means that the diffusion constant is given specific to the defined thermodynamic conditions for defined materials. This concludes the necessity of experimental values for each couple of fluid-rock.

In related literature there exist data for the diffusion constants of the gases in liquids or gases or liquids in clay rocks. The diffusion of CO₂ or methane in saline solutions is especially investigated for the modelling efforts.

The diffusion of the saline solution containing several species related to the transport in radioactive repositories is investigated in several studies experimentally. For example the diffusion constants of I⁻, Cs⁺ and SeO₄²⁻ are given in /ZHA 04/ successively as follows: 4,8 10⁻⁹ m²/s, 2,0 10⁻⁹ m²/s, 4,4 10⁻⁹ m²/s.

3.3.4 Surface Complexation

When a surface functional group reacts with an ion or a molecule dissolved in the pore solution to form a stable molecular unit, a surface complex is said to exist and the formation reaction is termed surface complexation. If no water molecule is interposed between the surface functional group and the ion or molecule that it binds, the complex is termed inner sphere. If at least one water molecule is interposed, then the complex is outer-sphere. Generally outer-sphere complexes involve electrostatic bonding and are less stable than inner-sphere surface complexes which involve ionic and/or covalent bonding. The zone adjacent to the surface where these complexes are located is referred to as the Inner Helmholtz Zone (IHZ) which is equivalent to the Stern layer and is bounded by the Outer Helmholtz Plane (OHP) at distance *d* from the solid surface.

3.3.5 Surface Charge

The surfaces of minerals present in natural clays develop an electrical charge in two principal ways: either from isomorphous substitutions among ions of differing valence within the clay lattice or from the reactions of surface functional groups with ions in the pore solution. Surface charge may be expressed per unit mass of solids or per unit area of solid surface. The latter quantity is referred to as surface charge density. Four different types of surface charge are considered to contribute to σ_p , the net total particle charge:

$$\sigma_p = \sigma_o + \sigma_H + \sigma_{IS} + \sigma_{OS} \quad (3-10)$$

The first term, σ_o , is the permanent structural charge due to isomorphous substitutions in the clay lattice. This ranges from -0,7 to -1,7 mol·kg⁻¹ for smectites, -1,9 to -2,8 mol·kg⁻¹ for illites and from -1,6 to -2,5 mol·kg⁻¹ for vermiculites. It is very small in hydrous oxides and 1:1 clays such as kaolinite, typically less than 0,02 mol·kg⁻¹. The second term, σ_H , is the net proton charge which is the difference between the number of moles of protons and the number of moles of hydroxide ions complexed by surface functional groups. Diffuse-swarm protons lying outside the σ_{HP} are not included in σ_H . The most important surface functional

groups, which complex protons, are organic compounds, hydrous oxides and the 1:1 clay minerals. The sum ($\sigma_o + \sigma_H$) is known as the intrinsic surface charge. The remaining terms, σ_{IS} and σ_{OS} , are the inner-sphere and the outer sphere complex charges, respectively. Contributing to σ_{IS} and σ_{OS} are the net total charge of the ions, other than H^+ or OH^- , which are bound into the surface complexes.

3.3.6 Double-Layer in Compact Clay

Transport processes, including advection and the diffusion of solutes involve the movement of chemical species within the interfacial regions of compact clay. This has very profound effects on these processes. A flux of water will tend to drag diffuse layer counter-ions along the flow channels, producing the electrokinetic phenomenon of streaming potentials. A flux of ions moving under an imposed electrical potential gradient will also tend to move water molecules, providing an explanation of electro-osmotic transport in clays. Since the diffuse-layer in clays is cation-dominated, the diffusion of chemical species through the clay takes place in an aqueous phase which has high concentration of cations. This concentration is non-uniform in a plane transverse to the direction of transport. Because of the distribution of electrical potential between closely-spaced, negatively charged clay particles, anions will tend to diffuse along paths which are remote from the clay surfaces, possibly along the centerlines of pore channels. It is noted that the water flow velocity will be greater towards the centre of a pore channel, leading to enhanced movement of anions /MEU 05/. Conversely, cations will tend to move along paths which are much closer to the charged surfaces. This interpenetration of double-layers produces an interparticle repulsive force between clay particles which resists compaction and which is, at least partly, responsible for the osmotic swelling of natural clays. The decrease in the thickness of the double-layer with increasing electrolyte concentration and with increasing temperature is probably an underlying mechanism of chemico-osmotic consolidation and thermo-consolidation in clays. In these forms of consolidation, pore volume decreases are associated with a change in the chemical and physical environment of the clay. At the very close interparticle spacings (≈ 1.5 nm), typical of a very compact shale, there is probably insufficient space for diffuse layers to form. However, the requirement for overall electron neutrality of the medium remains. In this case, the permanent structural charge of the clay surface must be balanced by the charge associated with a very dense arrangement of closely held cations. The diffusion of solutes within the shale matrix occurs in these molecular-scale pathways and, by definition, must be regarded as a surface diffusion process.

While many clay formations have demonstrably very low hydraulic conductivities, which result in very small advective fluxes, diffusive fluxes may be more substantial over relatively short geological time scales. As an example, Cl contents of pore-waters in clay units of the Benken borehole (Opalinus Clay and underlying Liassic) can be shown to have decreased by a factor of ca. 3 close to the contact with the underlying aquifer. Exchange processes between pore waters in argillaceous formations and embedding aquifers are relevant topics both for the future evolution of hydrochemistry and the understanding of present-day pore-water compositions. Modelling of such exchange processes could contribute to our current understanding of controls of pore-water chemistry, buffering capacity and thus the geo-

chemical stability of the host formations. Pore waters in clay formations are typically in chemical equilibrium with the minerals present in the formation. The geochemical stability of the formation and its pore water can be altered by changes in such boundary conditions as pressure, temperature and the pore-water chemistry of adjacent formations. Changes in boundary conditions may result from regional tectonic or erosional changes or other processes such as salt-water intrusion in near-coastal sites. These will be reflected by changes in the pore-water chemistry (and possibly the mineralogical properties) of a formation. The rates of change of these conditions for a site can often be evaluated from the geologic history of the region and (or) from modelling profiles of chemical tracers, as described above. The immediate past rate of change in formation chemistry may be applicable to the immediate future as well and so be useful in developing a base-case scenario for site evolution for performance assessment. An added contribution to the geochemical stability of argillaceous rocks is that they are chemically rock-dominated. That is, the majority of the chemical species dissolved in pore-water are buffered by minerals. The combination of fine grain size and extended pore-water residence times typical of argillaceous rocks assures that changes to pore-water chemistry that might be brought about by repository construction or operation will be strongly buffered by rock-water reactions. For example, this aspect of the Opalinus Clay at Mont Terri is described with particular relevance to its redox buffer capacity /MAZ 03/.

3.3.7 Ion Exchange

In its most general meaning an ion-exchange reaction is one in which one ionic species in a solid phase is replaced by another ionic species taken from an aqueous solution in contact with the solid. For an exchange reaction between cations M and N this can be represented by the equation:



Therefore, ion exchange can involve any kind of bonding mechanism, electrostatic, ionic or covalent. However, the usual meaning of the term ion-exchange reaction in soil chemistry is the replacement of one adsorbed, readily-exchangeable ion by another. Ion exchange, therefore involves only diffuse-swarm and outer-sphere ions held by electrostatic forces. The counter-ions associated with clay particles are in a state of dynamic equilibrium with the ions in the surrounding solution. If the composition of the bulk solution changes, the ionic content of the double-layers also changes in accordance with the law of mass action. Exchange reactions are reversible, stoichiometric and diffusion rate controlled, since the kinetics depend on the rate of diffusion of one ion relative to another. Morphology, the nature of crystal edges and the presence of precipitated coatings may affect reaction rates. Ion selectivity is often shown in exchange reactions, the preference being for cations of smaller hydrated radius, other factors such as ionic charge being equal. Monovalent cations are generally replaced by divalent cations, suggesting that higher ionic charge leads to stronger bonds with the clay surfaces /HOR 96/.

The ion-exchange capacity of a clay or soil is defined as the number of moles of adsorbed ion charge that can be desorbed from a unit mass of clay under given conditions of temperature, pressure, soil composition and soil mass ratio. In most applications this is the maximum

adsorption of readily-exchangeable ions (i.e. the ions adsorbed solely via the outer sphere complex and diffuse ion-swarm mechanisms). The ion-exchange capacity is specified in terms of the cation-exchange capacity (CEC) and the anion-exchange capacity (AEC).

3.4 Thermal Effects

The heat generation from the disposed waste is one of the most important aspects of the safety analysis of the radioactive repositories. When a heat source such as a canister of radioactive waste is buried in a saturated rock, the heat source will cause a temperature increment in the rock. The rock skeleton and the pore water will expand. However, the thermal dilatation coefficient is larger than the skeleton coefficient. As a result pore water pressure will increase. The magnitude of the water pressure depends on the rate of temperature increase and also on a number of rock parameters such as stiffness, permeability and porosity. The increase of rock parameters may lead in extreme conditions to rock fracturing.

Thermal processes are controlled by a temperature field, which is needed to (i) calculate the thermal-mechanical environment to predict preclosure underground opening stability and postclosure stability of emplacement boreholes (ii) model the thermal-hydraulic environment during operation and after closure of the repository to predict performance of the engineered barrier systems, and (iii) predict the THC environment for radionuclide transport to the accessible environment through the geologic setting.

The thermal loading influences the hydrologic, mechanical and chemical processes significantly which then affect the underground opening stability and the performance objectives of the repository. It is expected that heat generating HLW will elevate the temperature field, cause a redistribution of the in-situ fluid saturation, create thermal-mechanical stresses in the rock, affect container corrosion processes and alter the geochemical transport of radionuclides. Likewise, the hydraulic, mechanical and chemical processes have the possibility of influencing the temperature distribution.

Experimental studies investigating the thermal effect on clay formations are found in the literature. Recent publications about the subject are concentrated on the coupling of the thermal processes with hydraulic and mechanical properties.

The thermal properties as well as the effect of the temperature on the physical properties of the FEBEX bentonite is investigated in an experimental work /VIL 05/. FEDEX bentonite mainly consists of montmorillonite and is being used in the form of compacted blocks in the big scale experiments of the FEBEX Project. In both big scale tests, the bentonite blocks have been manufactured by uniaxial compaction of the granulated clay with its hygroscopic water content at dry densities close to $1,6 \text{ g/cm}^3$. Experimental results obtained in the laboratory on compacted specimens subjected to temperature, suction and stress changes are presented in this paper.

In the retention curves at constant volume, the influence of the initial dry density on the value of water content reached is more obvious as suction decreases. The hysteretic behaviour of the clay has also become evident. The temperature effects on water retention curves in confined and unconfined conditions have been determined and it can be concluded that the re-

tention capacity at higher temperature seems to be slightly lower: at a constant degree of saturation, the higher the temperature of the sample the lower its suction.

The hydraulic conductivity as a function of dry density and temperature has been successfully measured. It was possible to measure how the temperature increases the water saturated permeability of FEBEX bentonite, although this measured increase is slightly lower than what would be expected on the basis of the thermal changes in water kinematic viscosity. In addition, modifications of the intrinsic permeability due to structural changes caused by bentonite hydration have been detected by the measurement of the gas permeability.

The effect of dry density and temperature on the mechanical behaviour has been studied using swelling under load, swelling pressure, conventional oedometer and suction controlled oedometer tests. The results indicate that at high temperatures the swelling capacity of the clay decreases. In the same way, a clear decrease of swelling pressure as a function of temperature was observed. Oedometric tests have shown that saturation seems to induce a decrease in the apparent preconsolidation pressure regardless the temperature of the tests. On the other hand, temperature increases the compressibility of bentonite, both saturated and unsaturated, which would imply that a certain reduction in the size of the elastic domain takes place with temperature. Nevertheless, it seems that the deformation of bentonite is more dependent on the stress and suction path than on temperature. In tests with suction reduction, structure changes due to hydration are more relevant in the subsequent mechanical behaviour of bentonite than the effects of temperature.

Research activities are conducted at Mont Terri underground laboratory aiming at characterizing the THM response of the clay host rock and the effect of thermal expansion on the deformation of underground cavities /KUL 05/,/GÖB 05/,/JOB 05/.

A heating experiment named HE-D is being conducted by Andra, GRS and other partners in the Opalinus clay at the Mont Terri Rock Laboratory in Switzerland /KUL 05/. Two electrical heaters were installed in a horizontal borehole of 30 cm diameter and 13 m length drilled from the HE-D niche parallel to the existing MI niche. Since April 2004, the surrounding rock was heated by electric power input of 650 Watt in the first heating phase and 1950 Watt in the second phase. A third heating phase was carried out for reaching a maximum temperature of 150°C at the interface between heater and rock, depending on the conditions of the testing equipments. Finally, after heater shut-down, the rock cooled down to ambient temperature. To observe responses of the clay rock to the thermal loading, a large number of measuring instruments was installed in the near field around the heaters to measure temperature, pore water pressure, gas migration and deformation of the clay during the experiment.

Before drilling the heater borehole BHE-D0, eleven GRS mini-packer systems with sensors for measuring temperature and pore pressure were installed into slim boreholes of 20 mm diameter drilled from the MI niche to different positions up to 11 m deep in the rock, while other sensors of the Métro-Mesures were set up in a borehole parallel to the heater borehole. Figure 3-14 illustrates a typical example of the measurements at a position 1,35 m distant to heater 2. From this figure, it can be seen that:

(a) The initial pore water pressure of 1,2 MPa was constant over 3 months before drilling the heater borehole;

(b) Drilling the heater borehole BHE-D0 caused an insignificant sudden decrease of the pore water pressure, and then it remained unchanged;

(c) The constant power input of 650 Watt from both heaters to the rock generated a gradual increase of the temperature from 15 to 23,5°C over 3 months, and a rapid increase of the pore water pressure over the first month, and then maintained relatively constant at 2,3 MPa over further 2 months;

(d) The second heating phase with a power input of 1950 Watt increased the temperature to 40,5°C over about 3 months. At the very beginning of the heating phase, a transient drop down of the pore water pressure was observed. Afterwards, it increased to a maximum of 4 MPa and then decreased slowly to 3,7 MPa over about 1 month.

For investigating thermally-induced gas migration in the clay rock, two injection and four extraction boreholes were drilled from the MI niche perpendicular to the heater borehole. These measurements indicate that the Opalinus clay in the vicinity of the heaters is almost impermeable because, so far it has been observed any significant pressure decrease, neither before nor during the heating phases.

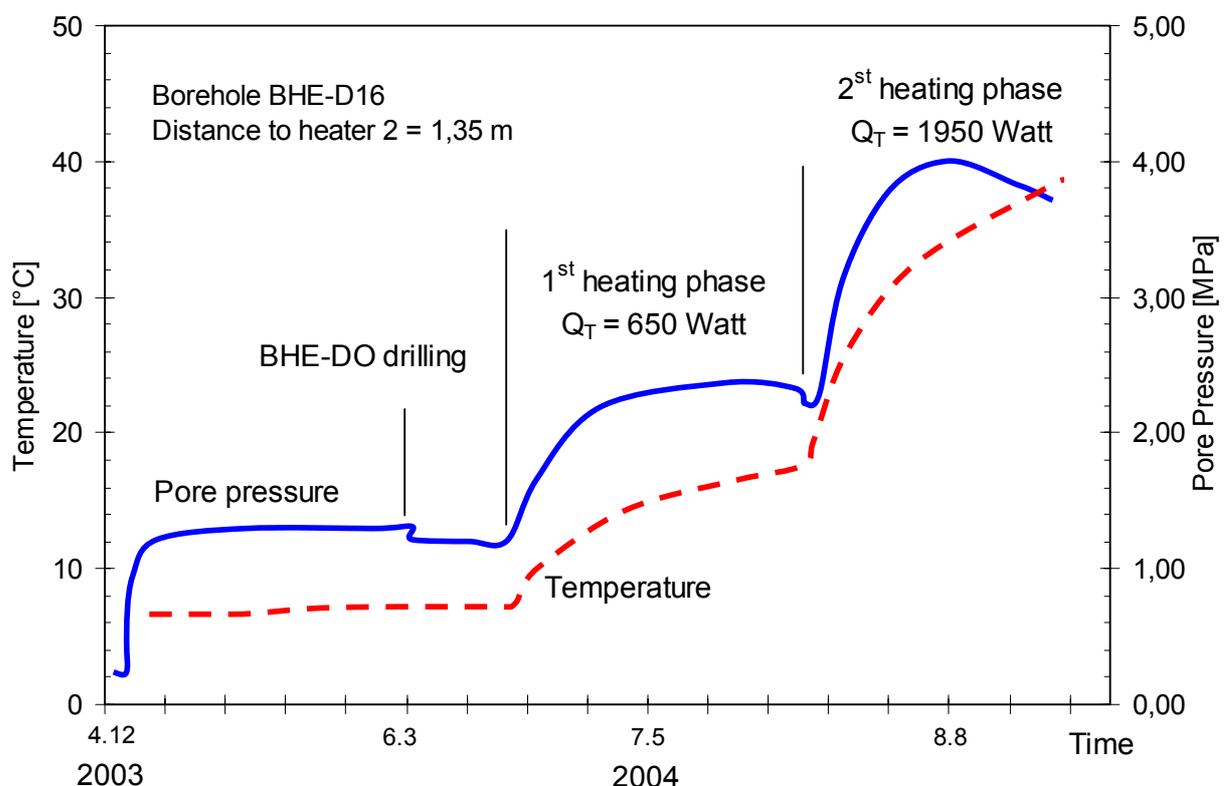


Figure 3-14: Measurements of temperature and pore water pressure during the heating experiment in the Opalinus clay at Mont Terri/KUL 05/

Difference in thermal expansion between pore water and solid particles in saturated clay is the driving force in the case of heating. Because the very low hydraulic conductivity of the clays does not allow the thermally-desorbed pore water so fast to disperse, heating results in an increase in pore water pressure which reaches the maximum under fully saturated undrained conditions. Under the external stress of 18,8 MPa and undrained conditions, a pore water pressure of 12,5 MPa was observed by heating the Callovo-Oxfordian specimens from 32°C to 91°C. Under the external stress of 15 MPa and partly drained conditions, heating the Opalinus specimen from 25°C to 120°C caused pore water pressure to rise up to 10 MPa. Additionally, increasing temperature results in expansion of the clays under undrained conditions. Even under high external stresses up to 15 MPa and partly drained conditions, significant thermal expansions were also observed by heating the Opalinus specimen from 25 to 60, 90 120 and 150 °C. However, under unsaturated and drained conditions, volumetric reduction of the clays was observed due to release of the pore water and collapse of unsaturated pores during the heating phases. In contrast to heating, cooling causes contraction of the pore water and reduces the pore water pressure. Correspondingly, the effective stress under a constant external stress is increased. Consequently, the clays can be compacted if drained conditions prevail. Under undrained conditions, the consolidation is negligible.

For predicting the effects of thermal processes mathematical models need to be established and accepted as accurately representing the thermal physics.

3.5 Transport Aspects

The transport properties of the clay formations and bentonite based back-fill materials are investigated and documented in the following sections.

4 GAS TRANSPORT IN CLAY FORMATIONS

Fluid movement in an underground repository system is examined generally as transport through geological and engineered barriers. The fluid movement through this barrier system has various and synergistic aspects which make the modelling of the transport processes very complex. To conceptualize this complexity, the compartmentalization of the total system into the smaller elements in space and in methodology can be a convenient way. To begin, the repository system and the mechanisms and processes contributing to fluid transport, geological repository systems and probable transport phenomena as well as processes proved to influence the transport can be illustrated as in Figure 4-1.

As can be concluded from the Figure and related literature the transport of gas from the repository to the biosphere –if is the case- is a result of transport processes affected by thermal, mechanical and chemical processes acting separately or interactively. In the following sections a description of these processes is given. For the transport of a gas to begin, the gas must be generated at first. Gas generation processes and rates in a repository system are briefly discussed based on the related literature.

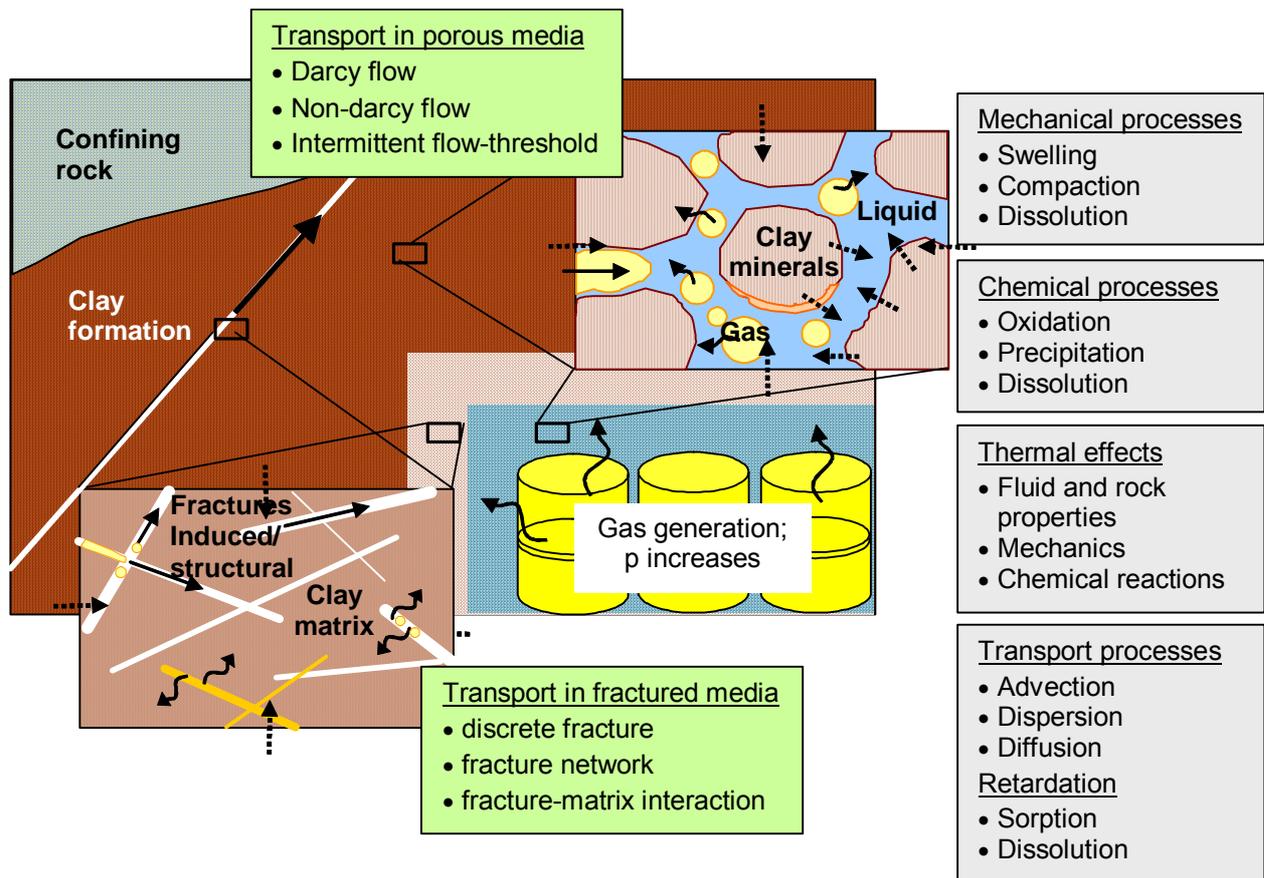


Figure 4-1: Schematic of the processes and mechanisms contributing to the transport of the gases in clay formations

4.1 Gas Generation

Gas generation from the disposed wastes is a well known phenomenon of waste management. At conventional landfills, the gases, if sufficient and in good quality may even be collected and used as energy resource. However the gas generation in underground waste deposits are one of the main concerns of safety management because of their toxicity, interaction with groundwater and ignitability. In this framework the characterization of the gas production mechanisms and of the physical as well as chemical properties of the generated gases is extremely important.

4.1.1 Gas Generation Mechanisms

A number of mechanisms that can contribute to the gas generation are identified in the literature. Their importance is relative to the physico-chemical, thermodynamical, geological milieu and waste characteristics. These parameters are the critical parameters for the determination of the various processes contributing to the total gas generation rate and gas types. The main mechanisms of gas generation in an underground waste repository are corrosion of metals in the waste, radiolysis of water and organic materials and microbial degradation. Studies can be found in the literature on the mechanisms and rates of the gas generation in the underground waste repositories /KID 92/, /KAN 99/, /MÜL 00/, /BRA 03/. These mechanisms are cited in the following sections with their importance for clay formations.

4.1.1.1 Corrosion

Possible contributions to the corrosion mechanisms are due to the presence of oxygen in the repository atmosphere, the presence of water in the waste and in the repository rock as saturation of various degrees and the groundwater being migrated to the surroundings. In addition corroding media may develop from the waste product, the backfill material and the host rock by secondary reaction such as radiolysis and microbial degradation.

The main parameters controlling the gas generation by corrosion are the temperature, pressure and radiation. Reaction rates are increasing with increasing temperature thus increasing the gas generation rates. For high level waste in crystalline rocks, salt and tuff, temperature above the boiling point of water may occur and in this case corrosion takes place for an extended period as corrosion by steam. This can be tolerated in repository design. For clay formations, however, this may be avoided because of the drying out processes of the host rock.

Pressure increase is expected due to the gas generation in waste repository units where the permeability of the host rock is low. However recent investigations showed that the effect of pressure on corrosion rates are of minor concern and can diminishing the corrosion rates only at high pressures well above the breakthrough pressure of the sealing properties /ROD 99/. The radiation is especially important for determining corrosion rates in high-level waste. The experiments show that for high level waste containers, steel corrosion may be enhanced only for limited high range of radiation that arises only limited time periods.

The chemical basics of the corrosion are defined in many sources /JOS 93/, /ROD 99/. The chemical conditions for corrosion are determined by the waste components, the water supply and the host rock. Heterogeneous waste like compacted solid mixed wastes can be characterized only in broad intervals with respect to their chemical compositions. Thus prediction of corrosion-induced gas generation should be done based on very conservative estimates for safety analyses or on statistical analyses of measured empirical values. The availability of water as the major corroding medium is obviously the decisive prerequisite for any gas generation by corrosion. In fractured rock, groundwater is an essential unlimited source. In clay formations, the host rock itself contains sufficient water to sustain corrosion reactions. Water enables certain other electrolytic reactions to occur. One of the best known corrosion mechanisms is the galvanic corrosion of the base metals in the presence of more noble metals. In assessing the availability of water, it has to be further taken into account that most wastes contain water themselves. In the case where the host rock supplies essentially unlimited amounts of water, water determines the chemical environment at least in the long term. The main parameters involved are the pH and Eh values, and the nature and concentrations of the dissolved species, notably various salts.

Corrosion of the candidate container materials for high level waste disposal in clay have been experimentally investigated in Boom Clay /KUR 97/. Measurements indicate low corrosion rates in the range of 1,8 $\mu\text{m}/\text{year}$ in carbon steel material. For materials such as nickel and titanium the corrosion rate decreases up to 0,03 $\mu\text{m}/\text{year}$. Experiments performed at laboratory conditions give higher values up to 50 $\mu\text{m}/\text{year}$ for carbon steel and up to 1 $\mu\text{m}/\text{year}$ for nickel and titanium /DEB 90/. In bentonite as engineered barriers, the corrosion rates are rather low due to alkaline environment. Short-term measurements have to be treated with care, because corrosion by dissolved oxygen in the bentonite water is the rate dominating process. These rates should not be used directly used for the assessment of gas generation.

4.1.1.2 Radiolysis

The decomposition of chemical compounds by radiation is termed radiolysis. Internal and external radiolysis is distinguished due to the location in radioactive water disposal. Internal radiolysis is the processes taking place in the waste product and its package. External radiolysis concerns the backfill and the host rock. Inside the waste packages all kind of radiation (α, β, γ) may contribute to gas generation by radiolysis. In the backfill γ -radiation dominates because of the shielding properties. Gas generation by radiolysis implies that gases are produced as primary or secondary decomposition products of the radiolytic processes. The leading examples for this kind of reaction is the decomposition of water (H_2O) resulting under idealized conditions in the formation of stoichiometric amount of hydrogen and oxygen gas. Since oxygen is generated in atomic form, it normally reacts immediately with its environment. Therefore, gas generation by radiolysis of water is commonly characterized by the amount of hydrogen produced per unit of substrate and applied radiation dose. Since the generation rates of H_2 are in a range comparable to that observed for internal effects, similar conclusions can be drawn for the external radiolysis.

4.1.1.3 Microbial Degradation

The first and most obvious condition of the microbial degradation in a repository is the existence of micro-organisms. It has been questioned in the past whether microbes exist in deep geological repositories. However, their capacity of surviving in deep groundwater is experimental confirmed. They are also present in clay formations. In any event, microbes will be present in the waste packages and will be brought into a repository by ventilation and by the operating staff. An essential prerequisite for microbial activity and thus microbial gas generation is the availability of water. In fractured rock and clay rock this is provided by the water in the geological formation. A second condition for microbial activity is the presence of nutrients. This concerns, in the first place, the availability of organic material providing the carbon. In addition, nutrients like nitrates, sulphates have a strong influence on microbial activity. Further environmental factors influencing the microbial degradation are pH value, temperature, pressure, oxygen supply, salinity or impurities in water, radiation and pressure.

Measurements of microbial gas generation are rare therefore the validation of the corresponding models is the main problem. All measurements so far demonstrate rather swift saturation behaviour of the CO₂ production, which is followed by lower generation rates with mostly CH₄ and CO₂ as the major gas components. For long-term safety considerations, the ¹⁴C content in these components is of particular interests. The estimation of the gas generation rates from waste in geologic repositories is due mainly to the measurement of the real wastes in laboratories or in-situ. The Table 4-1 gives mean measured values for generation rates from compacted mixed wastes.

Table 4-1: Averaged values of gas generation rates for compacted mixed waste /ROD 99/.

Gas type	Generation rate [l/(m ³ •a)] at STP
H ₂	25
CO ₂	0,75
CH ₄	0,35
C ₂ H ₆	7,5

4.1.2 Modelling of Gas Generation

A number of codes are available for the estimation of the gas generation in various waste environments. The codes calculate the expected rates of gas generation for various types of wastes in various milieus. A comparison of these software is given in /ROD 99/.

The modelling of gas generation most advanced for corrosion, although the difficulty remains that the metallic contents of the waste and the available corroding media have to be characterized in some detail. The modelling efforts for microbial degradation need more validation

and qualification studies. Some benchmark studies have been performed in order to test and validate the capacity of the software have been published in the literature /NYK 98/, /ROD 95/, /YIM 96/.

4.2 Gas Transport; Definitions and Properties

Gas transport through geologic and engineered barrier systems related to a deep radioactive waste repository typically involves flow through various types of media, from compacted backfill material to loose porous media and/or fractures. To be realistic and representative the flow processes should be coupled with thermal, mechanical and chemical disturbances arising in the whole system. As discussed in previous sections too, because of their structural complexities clay formations exhibit more difficulties in describing the flow physics.

The physical and numerical modelling of flow of any fluid in clay formations and backfill necessitates first of all the knowledge of the classical terminology of fluid flow in porous media as well as in fractures. The thermo and flow dynamics are two important disciplines dominating the modelling of the gas transport.

The thermodynamical aspects of gas transport deals with the phase behaviour and thermodynamic and physical properties of the gas. Gas can be a mixture of various gases such as CO₂, H₂, CH₄ and steam. The physical properties of these individual components are generally well known from the literature therefore, to seek simplicity the general assumption of the physical and numerical modelling studies is to consider the gas mixture as to one component lumped gas. The main component is introduced for determining the thermodynamical-thermophysical properties of the gas neglecting the minor components. In many of the cases air and/or steam are the gases taken in the modelling into consideration. It should also be noted that this simplification is not acceptable if the chemical reactions between fluid and rock are simultaneously modelled. In most of the cases gas is not the only phase in a repository and their physical as well as chemical interactions with liquid and solid phase should also be considered in modelling studies. In this framework the modelling studies have to be performed as two-phase transport taking the dynamic petrophysical changes into account.

The petrophysical and mechanical properties of the host rock and backfill material are other components of gas transport modelling in geologic repository. As previously discussed these properties differ greatly based on the location and time. The typical example of these variations occurs especially in EDZ where the permeability and porosity are expected to change dramatically shortly after the excavation and at long term.

In the following sections the properties of the fluids and rocks dealing with transport of gas in clay formations are classified and summarized.

4.2.1 Thermodynamics; Phase and Physical Properties of the Fluids

As thermodynamics describes how systems respond to changes in their surroundings, it is one of the elementary points of gas transport in clay formations. The classical thermodynamics as well as statistical or chemical thermodynamics find their places in modelling studies.

The first and most important concept that is used in this framework is the phase and related physical properties of the phases present in the system. The thermodynamical system in a repository is generally assumed to consist from air-steam as gas, saline water and rock. The physical properties of air or steam or a mixture of both is generally well known and can be described with simple half-empirical and empirical correlations.

For a system consisting of water, steam and air the phase changes are calculated generally with the Clapeyron Equation that determines the saturation as function of pressure and temperature:

$$S^n = S^n(\psi) \quad (4-1)$$

$$\psi = A.p + BT$$

Where ψ may be interpreted as a mean curvature of the phase interface, p and T are the characteristic pressure and temperature of the system, and A and B are empirical constants. However, the Clapeyron phase change relations are applicable in a more general sense and the coefficients need not be interpreted on the basis of surface curvature. The characteristic saturation relationship, often termed the "soil moisture characteristic", is a basic soil (or rock) property for multi-phase flow and is usually based on empirical measurements. Furthermore, these relationships are generally expressed in terms of cumulative relative saturation, S^n , rather than as the absolute value of the saturation, S .

The formation of steam should be taken into account depending on variations in pressure and temperature as equilibrium and non-equilibrium cases. In the equilibrium mode, the rate of vapour formation is automatically estimated from the equilibrium value of the vapour pressure and the thermal energy available for heat of formation of the vapour. In the non-equilibrium mode, the vapour formation equation is based on mass-transfer equilibrium. All water properties are presented by the empirical steam table equations generally. Air or any other gas is approximated as an ideal gas and additivity is assumed for air, a and vapour, v partial pressures in the gas phase, p_g :

$$p_g = p_a + p_v \quad (4-2)$$

The solubility of air or other possible gases in liquid water is presented by Henry's law as partial pressure:

$$p_a = K_h \cdot x_h \quad (4-3)$$

The Henry's law coefficient K_h for dissolution of air (gases) in water is strongly dependent on temperature. On the other hand for volatile species present as a very dilute solute in the liquid phase, Henry's law states that the partial pressure of the species in the vapour phase is directly proportional to its liquid-phase mole fraction.

$$y_i P = x_i K_{Hi} \quad (4-4)$$

Experimental data on the solubility of CO₂ in H₂O shows that the two previous models-Raoult's and Henry's law fail to accurately represent the equilibrium between phases, therefore a more rigorous approach needs to be taken.

Henry's law (Eq. 4-3) assumes that the gas fugacity is equal to the partial pressure. This assumption is not necessary and is removed by including the gas phase fugacity coefficient:

$$f_2 = \Phi_2 y_2 P = K_{H_2,1} x_2 \quad (4-5)$$

Where 1 represents the solvent (H₂O) and 2 represents the solute (CO₂). In general the fugacity coefficient of component i , Φ_i is defined:

$$\Phi_i = \frac{f_i}{y_i P} \quad (4-6)$$

Under ideal gas conditions the fugacity coefficient is equal to unity. The more the fugacity coefficient deviates from the unity, the greater the system deviates from ideal gas behaviour.

If other gases than air and/or steam are present in the system the effect of these gases on the thermodynamic properties should be taken into considerations if their fraction in the total composition is relevant. The calculation of the thermodynamic properties of individual gases and mixture of gases is relatively simple and accurate compared with the calculations for the liquid and gas mixtures. For individual gases the application of ideal gas law is sufficient for the calculation of the phase properties. At thermodynamical conditions where high pressures dominate the system, the thermodynamic behaviour should be corrected by applying the real gas law. The use of more complex equation of states can also be applied if insufficiencies in describing the thermodynamical behaviour occur. From the literature it is known that the three parameter half empirical equations of states (EOS) such as Peng-Robinson and Redlich-Kwong-Soave give good results in modelling the phase behaviour of light gas mixtures. The Peng-Robinson EOS is the EOS most widely used in chemical engineering thermodynamics. It is known to give slightly better predictions of liquid densities than the Soave-Redlich-Kwong EOS. The EOS requires three inputs per compound: T_c , P_c and the acentric factor ω .

$$p = \frac{RT}{v-b} - \frac{a(T)}{v^2 + 2bv - b^2} \quad (4-7)$$

where p , R , T and v are the pressure, temperature, gas constant and specific volume. The equation parameters, a and b are the sum of the semi-empirical parameters calculated for each gas component separately. The thermodynamics of saline water in equilibrium with non condensable gases like CO₂ exhibit complexities compared to air-steam-water systems. The use of Henry's law for modelling the solubility behaviour of the gas is generally applied and for the equilibrium of the gases with liquid fugacity concept is used. Especially in the last years many studies on the phase behaviour of water-saline water-CO₂ and/or CH₄ are published based on increasing importance of geological CO₂ sequestration /DUA 92/, /DUA 03/. The solubility of CO₂ in saline solutions is given in /DUA 03/ with the following equations as function of dissolved salt type and ionic strength:

$$\ln(m_{CO_2}) = \ln y_{CO_2} \phi_{CO_2} p - \mu_{CO_2} / RT - 2\lambda_{CO_2-Na} (m_{Na} + m_K + 2m_{Ca} + 2m_{Mg}) - \zeta_{CO_2-Na-Cl} m_{Cl} (m_{Na} + m_K + m_{Mg} + m_{Ca}) + 0.07m_{SO_4} \quad (4-8)$$

where T is absolute temperature in Kelvin, p represents the total pressure of the system in bar, R is the universal gas constant, m is the molality of components dissolved in water, y_{CO_2} is the mole fraction of CO_2 in vapour phase, ϕ_{CO_2} is the fugacity coefficient of CO_2 , μ_{CO_2} is the standard chemical potential of CO_2 in liquid phase, λ_{CO_2-Na} is the interaction parameter between CO_2 and Na^+ , and $\zeta_{CO_2-Na-Cl}$ is the interaction parameter between CO_2 and Na^+ , Cl^- . The fugacity coefficient of CO_2 , ϕ_{CO_2} , is calculated as a function of temperature and pressure, as proposed in the same study.

Figure 4-2 shows a comparison of the CO_2 solubility in NaCl and $MgCl_2$ brines with various salt concentrations. The thermophysical properties of CO_2 and other possible gases in the repository are calculated with equations of states of various complexities or based on experimental correlations. The estimation of the density of CO_2 rich solutions i.e. water with various salt and gas content is especially important because of the retrograde behaviour of such solutions. It is affirmed that the density of CO_2 rich solutions increases with increasing dissolved CO_2 which is an unconventional behaviour /GAR 01/.

Figure 4-3 shows the solubility of CO_2 and CH_4 in water for 4 molar NaCl salinity and 50 °C temperature. As can be concluded from the Figure the solubility of CH_4 is much lower than the solubility of CO_2 . The ionic activity, on the other hand, is another factor which should be taken into account by calculating the solubility of the gases in brines. The solubility of gases is lower in the solutions with higher dissolved salt content.

The density and viscosity of water and saline water are two important parameters. They are calculated as function of temperature and pressure if their variations are not negligible in terms of their effect on corresponding properties. Various empirical and half-empirical correlations are used for this purpose. The effect of salt and gas content, if not negligible, should be taken into consideration in all modelling studies. Figure 4-4 shows the density of water and saline water with 0,10 equivalent NaCl mass fraction as function of pressure at a temperature of 60 °C.

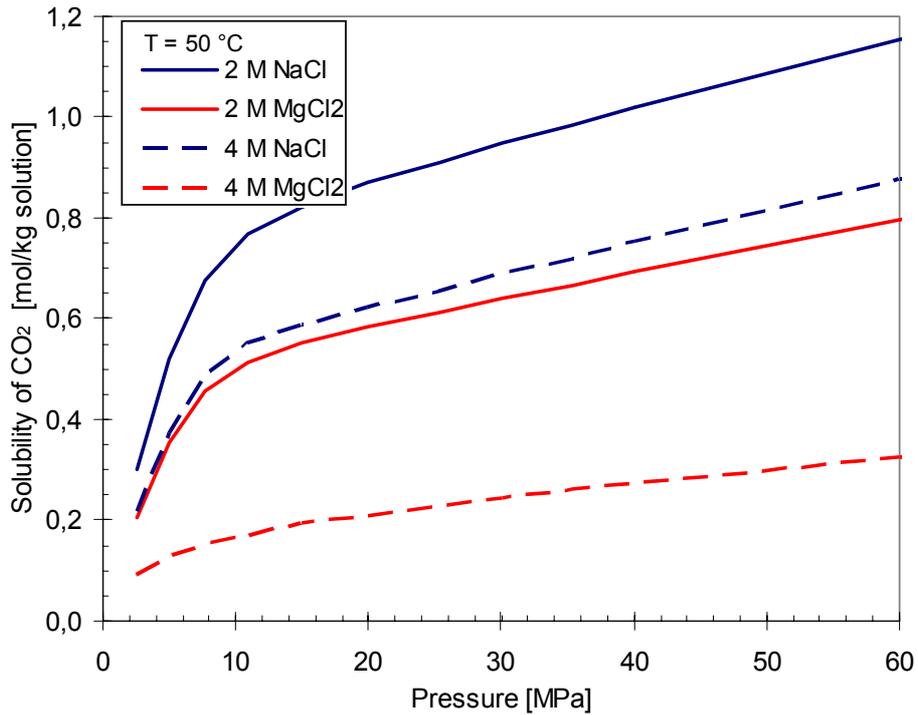


Figure 4-2: Solubility of CO₂ in brine with various salt type and strength /DUA 03/

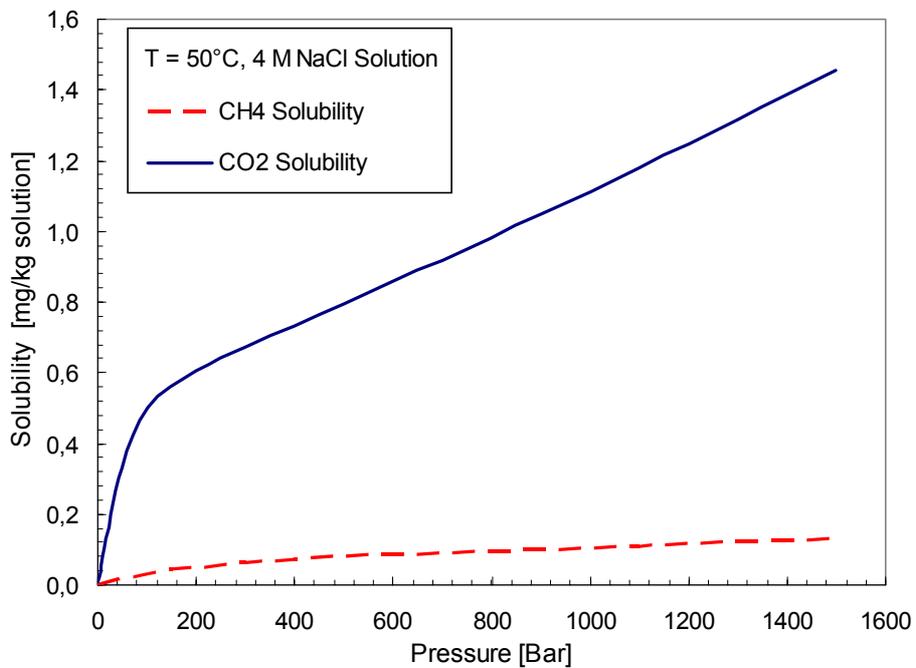


Figure 4-3: Solubility of CO₂ and CH₄ in 4 M NaCl at 50 °C /DUA 03/

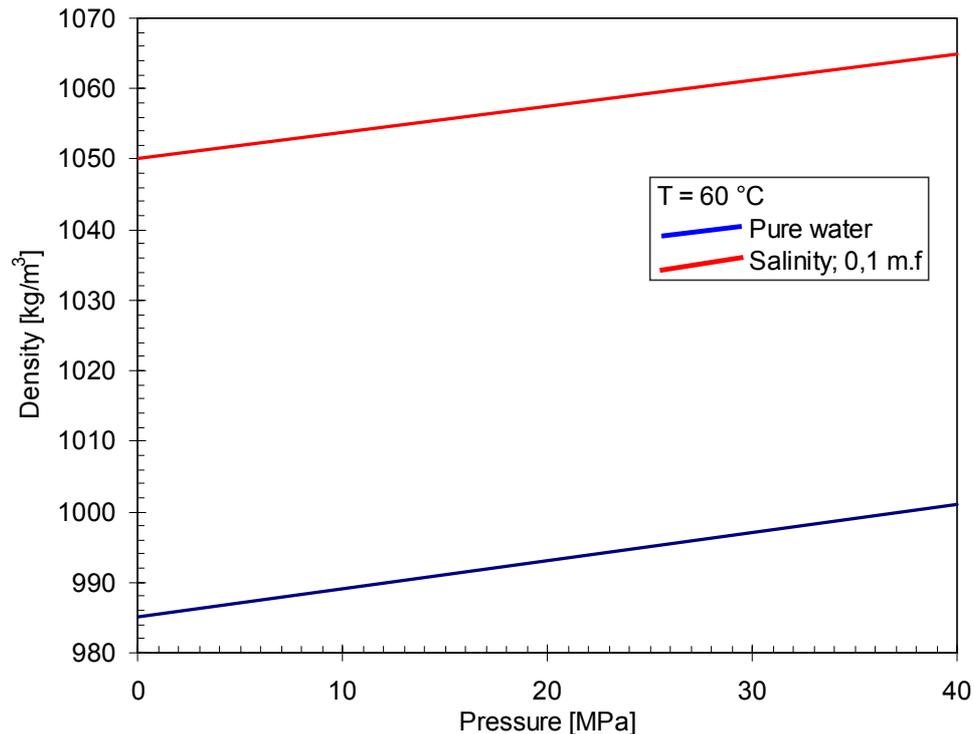


Figure 4-4: Density of pure and saline water as function of pressure /BAT 92/

4.2.2 Petrophysical Properties, Definitions

4.2.2.1 Pore-size Classification

Pores with diameters less than 2 nm (i.e. molecular dimensions) are called micropores. It is highly improbable that pores of this size can accommodate normal viscous flow. Pores with a diameter between 2 and 50 nm are mesopores. Capillary forces are most important for pores in this size-range. The pore diameter can be equated with the smallest dimension of a slot-shaped pore. For reference, the thickness of a single molecular layer of water is approximately 0,3 nm. The term "open pores" in this context means the total matrix porosity of clay, which may be considered to be the sum of the porosities associated with each of these size classes.

Clays largely accumulate by settling-out from aqueous suspensions. The salinity of the depositional waters is a particularly important factor in the early stages of fabric development, since it affects the interactions between colloidal particles, leading to a variety of flocculated or dispersed particle arrangements. All "rock-like", rather than "soil-like", natural clays would fall in the category of very low void ratio materials. The typical void ratio of a plastic, over-consolidated clay (e.g. Boom Clay of Belgium and London Clay of UK) is around 0,65.

At modest levels of compaction, the primary particles in natural clay may be arranged in groups variously known as aggregates, packets, clusters or domains. The term domain is

used to describe arrays of clay particles in face-to-face arrangements. For clays exhibiting this type of fabric, the total porosity is distributed among inter- and intra-group components.

In contrary of pore size, the grain size is an important property in terms of hydraulic characterization of the bentonite based buffer materials. In FEDEX experiments, for example, the fraction of the grains sized less than 2 μm is given as 65%, the fraction of the grain size between 2 mm and 74 μm (silt size) as 28%. The remaining 7% is given as sand size (>74 μm) /FEB 98/.

4.2.2.2 Porosity

Porosity is a basic parameter in mass transport theory describing the open, fluid filled voids in a rock. Numerically, total porosity is the ratio of the total volume of voids to the total volume. In general, the total porosity is the sum of the total matrix porosity and the fracture porosity. Recognising that the values assigned to these quantities will depend on scale, a representative elementary volume (REV) is selected, appropriate to the problem under consideration, for corresponding definition. In the absence of fracturing and other forms of inhomogeneity, the total porosity of the material within the REV is equal to the total matrix porosity. For saturated clays, the total porosity of the matrix, ϕ is usually calculated from bulk dry density and the average grain density of the mineral solids or from the void ratio.

Porosity can be a relic of deposition (primary porosity, such as space between grains that were not compacted together completely) or can develop through alteration of the rock (secondary porosity, such as when feldspar grains or fossils are preferentially dissolved from sandstones). Effective porosity is the interconnected pore volume in a rock that contributes to fluid flow in a reservoir. It excludes isolated pores. Total porosity is the total void space in the rock whether or not it contributes to fluid flow. Thus, effective porosity is typically less than total porosity.

The mathematical formulation of the porosity, ϕ , is given as:

$$\phi = \frac{V_p}{V} \quad (4-9)$$

In effective porosity V_p is the interconnected pore volume. The unit of the porosity is fraction; it can also be given as percentage.

Porosity is generally measured with saturation method. As a standard way, the material is saturated with a fluid for which the density is known, the difference in weight before and after the saturation is taken as the weight of the fluid present in the pores of the material. The volume of the fluid in the pores is calculated using the density and the ration of the fluid volume to the total volume is equal to the porosity. This measurement technique determines the effective porosity. Because of its probable chemical and/or structural effects on the rock the selection of a suitable fluid for the saturation is essential for the success of this method. The use of inert, apolar fluids (gas or liquid) are common especially for measuring porosity on clays.

Because of the sensitivity of the mechanical and hydraulic properties of the clay formations to the water/fluid content some other conventional and unconventional porosity measurement methods can be applied. Therefore, the porosity of the clay formations is also dependent on the measurement technique.

The pore volume determined by using the pycnometer method is obviously the total pore volume which includes the dead volume which does not permit any flow. Another difficulty on determining the porosity of the clay samples with pycnometer lies on drying and determining the volume of the matrix.

The porosity of the clay samples can also be determined based on the evaluation of the transient diffusion experiments. However this method can be erroneous due to the experimental problems. The dead volumes of the experimental apparatus and the structural changes (swelling) of the clay due to the time required process are the main problems.

The measurement of the porosity with the mercury injection into the pore volume is the most precise method for measuring the porosity. In this method the mercury is injected into the pores as function of inlet pressures. Therefore, this method gives not only the porosity but also a definition of the pore structure via pore diameter distribution and capillary properties. However this sophisticated technique of measuring the porosity and pore distribution could not give the desired result for clay formations. High injection pressures cause structural changes in microscopic levels affecting the measurement precision considerably.

Microcrack porosity

Although much of the fluid in a compact clay formation is present as thin interparticle and interlayer films, the possibility that a small fraction actually resides in microcracks or microfissures should not be excluded. Although the distinction between these two types of flaw is somewhat arbitrary, the term *microcrack* is probably best applied to the more indurated rocks (shales) which are capable of undergoing brittle fracturing, while the term microfissure might be used more appropriately in relation to the plastic clays. The biggest difficulty in assessing whether or not microcracks or microfissures are present naturally in any particular mudrock is that these features are very sensitive to sample disturbance, in particular, the de-stressing, dessication, oxidation and damage which accompany sampling and specimen preparation.

After some studies the interparticle spaces of a deeply buried shale are so small that the shale matrix should be virtually (if not totally) impermeable under in situ stress conditions and representative hydraulic gradients. However, the combined effects of burial diagenesis and overpressurization might make these materials susceptible to brittle fracturing. Scanning electron microscopy of the Boom Clay (Tertiary) of Belgium /HOR 94/ has revealed several types of microfissure in this plastic clay, ranging in aperture from a few microns to 50 μm . Linear fissures were observed parallel to the bedding. The biggest of these, with apertures exceeding 20 μm , were found to be lined with authigenic pyrite and to continue through the mudrock for several millimetres. Smaller aperture fissures occurred more frequently and were lined with detrital clay components. A few irregular fissures disrupted the uniformity the clayey plateaux (i.e. bedding surfaces comprising the basal surfaces of numerous clay platelets). With a maximum aperture of 10 μm , these features were lined with bigger detrital com-

ponents coated with clays, quartz and other minerals. Microfissure apertures were demonstrably sensitive to the aqueous vapour pressure used in environmental scanning electron microscopy (ESEM), once again raising the question whether or not such features would be open under in situ conditions.

Diffusion accessible porosity

Research on compact clays suggests that only a fraction of the total water-filled porosity is available for diffusive transport. As being observed in the last chapter, the mechanism of Donnan exclusion can cause negatively-charged ions to be excluded from the narrower interparticle spaces of the clay. This, together with possible size-exclusion effects, has prompted the use of a *diffusion accessible porosity* term in transport modelling. The accessible porosity of Boom Clay under *in situ* conditions is measured to be 0,087 for I⁻ and 0,34 for tritiated water (HTO), which compares with a total porosity of about 0,4 for this clay /PRE 91/

Effect of depth of burial on total porosity

From the earlier studies of petroleum engineering it is known the dependency of the petrophysical properties of the geological formations on depth is known. A commonly used relationship for determining the depth dependent porosity is:

$$\phi = \phi_0 \exp(-c.z) \quad (4-10)$$

where z is depth below surface. The parameters ϕ_0 and c may depend on a variety of factors such as mineralogy, formation age, position within the sedimentary basin and the presence or absence of tectonic stresses. The porosity measurement for Callovo-Oxfordian Clay formation given in Figure 4-5 shows an obvious dependency of the porosity on the depth of the cores sampled as well as on the saturation.

The porosities of clay formations measured with various methods depend greatly on the sampling depth as well as on the water content of the original or saturated sample. Table 4-2 gives a collection of data from related literature.

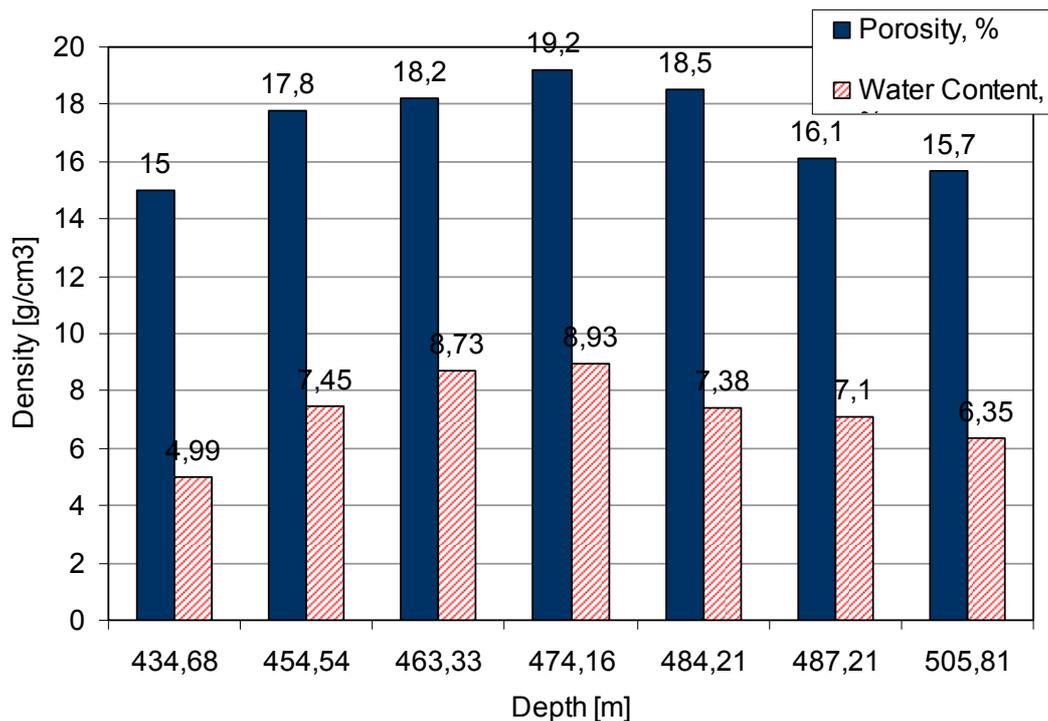


Figure 4-5: Porosity values of Callovo-Oxfordian Clay as function of water saturation and depth /GRS 01/

4.2.2.3 Permeability

Formations that transmit fluids readily, such as sandstones, are described as permeable and tend to have many large, well-connected pores. Impermeable formations, such as shales and siltstones, tend to be finer grained or of a mixed grain size, with smaller, fewer, or less interconnected pores. Absolute permeability is the measurement of the permeability conducted when a single fluid, or phase, is present in the rock and is mathematically defined in flow equation experimentally concluded by H. Darcy.

The original units of the Darcy equation are CGS and in these units the unit of the permeability is named as Darcy. The main assumptions of the Darcy equation are the laminar and isotropic, incompressible flow as well as the full saturation of the porosities with the fluid. Permeability varies with direction of flow through the porous medium. Permeability varies with direction of flow through the porous medium. Lateral permeability contrast can be particularly important in fractured formations, where effective permeability in the direction of the fractures may be many times greater than the matrix permeability. If the permeability in one direction is significantly more than in the other, the flow pattern may more closely approximate linear flow than radial flow. This can be detected from well-test data. Likewise, laminations in most clastic formations cause the permeability normal to the bedding plane to be less than the lateral permeability parallel to bedding. This is called vertical to horizontal permeability anisotropy.

Table 4-2: Porosity data for clay formations and some bentonite based buffers

Formation / Site	Source	Method/Remarks	Value
Opalinus, Benken	/NAG 02a/	Water loss porosity by drying at 105 °C. The physical porosity is estimated to be 1,1-1,2 times the water loss porosity.	0,053-0,137
Opalinus, Benken	/NAG 02a/	Measured with pycnometer	0,074-0,169
Opalinus, Mont-terri	/NAG 02a/	Water loss porosity by drying at 105 °C.	0,08-0,191
Opalinus, Mont-terri	/ZHA 04/	Measured with pycnometer, water content: 5,8 %	0,18
Opalinus, Herden	/NAG 02a/	Saturation method, apolar liquid	0,003-0,045
Opalinus, Well Benken	/NAG 02a/	Measured with pycnometer	0,108±0,02 (average)
Opalinus, Well Benken	/NAG 02a/	Water loss porosity	0,053-0,137
Callovo-Oxfordian	/ZHA 04/	EST05481-01-II, Sample depth: 434,5 m, water content: 4,99, measured with pycnometer	0,15
Callovo-Oxfordian	/ZHA 04/	EST05630-02, Sample depth: 474,0 m, water content: 8,93, measured with pycnometer	0,192
Callovo-Oxfordian	/ZHA 04/	BVE1-01, test field, water content: 5,8, measured with pycnometer	0,18
Callovo-Oxfordian Bure	/NEA 05/	Measured with Hg injection, total	0,33
Callovo-Oxfordian Bure	/AND 99/	Primary Porosity	0,14
Tournemire, Toarcian-Domerian	/NEA 05/	Measured with Hg injection, min. value	0,02
Tournemire	/VAL 04/	Saturation of the cores from 250 m depth	0,068-0,071
Mol, HADES	/BAS 03/	Primary Porosity	0,33-0,40
Boom Clay	/NEA 05/	Measured with Hg injection, max. value	0,40
Boom Clay	/NEA 05/	Measured from water content, burial depth app.200 m	0,37
Boom Clay	/AER 04/	Diffusion accessible porosity	0,37± 0,03
Marls from Wellenberg, Switzerland	/MAZ 01/	Core measurement	0,01-0,02
Boda Claystone Formation	/MAZ 03/	In-situ determination (?)	0,006-0,017
Palfris-Formation	/MAZ 03/	Total Porosity	0,0143
Buffer, 50/50 Clay-sand	/ROT 05/	Bulk density 1756 kg/m ³	0,344
Buffer, 70/50 Clay-Sand	/ROT 05/	Bulk density 1603 kg/m ³	0,405

The intrinsic permeability (or coefficient of permeability) k (m^2) can be calculated from the hydraulic conductivity K ($\text{m}^2 \cdot \text{s}^{-1}$) used in most of the related studies to define the hydraulic conductivity of the clay formations using the relationship

$$k = K \frac{\mu}{\rho} \quad (4-11)$$

where μ and ρ are the absolute viscosity and density of water or flowing medium, respectively. Note that at 20°C the absolute viscosity of water is $1,002 \times 10^{-3} \text{ Pa}\cdot\text{s}$ and the density is $998,2 \text{ kg}\cdot\text{m}^{-3}$. Provided that flow is non-reactive with the porous medium, the intrinsic permeability should be a property of the medium alone. Since most fluids interact in some way or another with the clay-water-solute system, it is optimistic to believe that permeabilities derived from hydraulic tests would quantify the flow of a fluid with a chemistry which is quite different from that of pure water. A compilation of permeability values for a range of clay formations is given in Table 4-3.

The typical matrix permeability of a glacial till (close to surface) is in the range $10^{-17} - 10^{-19} \text{ m}^2$, of a typical unweathered (overconsolidated) plastic clay is around 10^{-19} m^2 , of a more compact clay shale in the range 10^{-20} m^2 , and the permeability of a deeply buried and very compact oil-field shale around 10^{-22} m^2 . The permeability of many clay formations as the case for other rocks is often found to be directionally-dependent, indicating that this material constant should be represented by a tensor quantity. As a scale, the ratio of the horizontal permeability to the vertical permeability of the Belgian Boom Clay is 2,4 /CAN 95/. Scale-effects may have a strong influence on the permeability values obtained for many clays and mudrocks, with laboratory tests frequently giving values for permeabilities which are substantially lower than medium and large-scale field values. This is closely linked with the issue of fracture flow in clays. These scale-effects may be less important in some of the more plastic clays.

Another very important effect on the permeability of the clay formations is the lithostatic pressure compacting the clays. Figure 4-6 shows the results of an experimental study on the effect of the confining pressure on the permeability.

The hydraulic conductivity of compacted bentonite-sand mixtures used as backfill materials are expressed by some authors with polynomial correlations as function of characteristic properties of the bentonites such as chemical concentrations and adsorption capacity /KOM 04/, /EBI 04/. A recent example of these attempts is given by /EBI 04/ to calculate hydraulic conductivity at 288 K:

$$\ln k = -19,57 + 0,0266 \text{ Ca} / \text{Na} + 12,76 \text{ Al} / \text{Si} + 0,746 \text{ MgO} + 0,866 \text{ K}_2\text{O} + 0,467 \text{ CaO} - 0,008 \text{ MB} - 0,184 \text{ Al}_2\text{O}_3 \quad (4-12)$$

where MgO, K_2O , CaO and Al_2O_3 are the chemical compositions determined by X-ray fluorescence analysis (wt. %). Ca/Na and Al/Si are the ratios of CaO to Na_2O , Al_2O_3 to SiO_2 and $\text{Na}_2\text{O}/\text{CaO}$, respectively. In this equation MB is a measure of cation exchange capacity (CEC) of the clay. The regression coefficient of this polynomial equation is given as 0,996.

Table 4-3: Permeability data for clay formations and clay based buffers

Formation / Site	Source	Method/Remarks	k, m ²
Callovo-Oxfordian / Bure	/NEA 05/	In-situ measurement, no information on the flow direction, calculated from K	2×10^{-21}
Callovo-Oxfordian / Bure	/LAV 05/	In-situ tests, ca 460 m depth	$< 1,7 \times 10^{-18}$
Callovo-Oxfordian	/MAL 05/	After healing of the radial cores 3 months	5×10^{-21}
Toarcian-Domerian / Tournemire	/NEA 05/	In-situ measurement, no information on the flow direction, calculated from K	3×10^{-21}
Opalinus, Laboratory Mont-Terri	/NEA 05/	In-situ measurement, no information on the flow direction, calculated from K	3×10^{-15}
Opalinus, Mont-Terri	/FRÖ 05/	Sample BLT-10/08/01, before drying	6×10^{-17}
Opalinus, Mont-Terri	/FRÖ 05/	Sample BLT-10/08/01, after drying	7×10^{-15}
Boom Clay	/AET 04/	Water based tracer, calculated from K values, perpendicular to bedding	2×10^{-18}
Boom Clay	/ORT 97a/	In-situ measurements, HADES,	$< 2 \times 10^{-18}$
Boom Clay	/MAL 05/	Measured with 4 MPa effective mean stress	3×10^{-19}
Boom Clay	/BEA 94/	Perpendicular to bedding Parallel to bedding	$1,7 \times 10^{-19}$ $4,5 \times 10^{-19}$
Boom Clay	/SAF 01/	Core measurements	$k_h = 8 \times 10^{-17}$ $k_v = 5 \times 10^{-17}$
Boom Clay, Putte	/SAF 01/	Pulse tests	$1-3 \times 10^{-18}$
Callovo-Oxfordian Bure	/AND 99/	Primary permeability, in-situ	1×10^{-19}
Mol, HADES	/BAS 03/	Calculated from measured hydraulical conductivity	$k_h = 3 \times 10^{-18}$ $k_v = 1 \times 10^{-18}$
Spanish Ref. Clay	/MAZ 01/	Hydraulic tests	$3,3 \times 10^{-18}$
Pleistocene, Louisiana	/HOR 96/	Laboratory test	$10^{-20} - 10^{-21}$
Shales, N. America	/NEA 96/	Core and borehole data	$10^{-15} - 10^{-19}$
Shale, Canada	/HOR 96/	Flow tests	$10^{-19} - 10^{-20}$
Shale, Kansas, Okl.	/HOR 96/	Laboratory tests	$1,7 \times 10^{-20}$
Elena Argillite	/HOR 96/	Transient or pulse test, in-situ	$10^{-20} - 10^{-23}$
Argille Scagliose Italian Clay	/BON 05/	In-Situ measurement	$10^{-13} - 10^{-15}$
Buffer, 50/50 bentonite-sand mix.	/ROT 05/	Gas permeability	$7,5 \times 10^{-14}$
Buffer, 70/50 bentonite-sand mix.	/ROT 05/	Gas permeability	$1,2 \times 10^{-15}$
Buffer, bentonite	/FEB 98/	Dry density: 1700 kg.m^{-3}	$8,1 \times 10^{-14}$

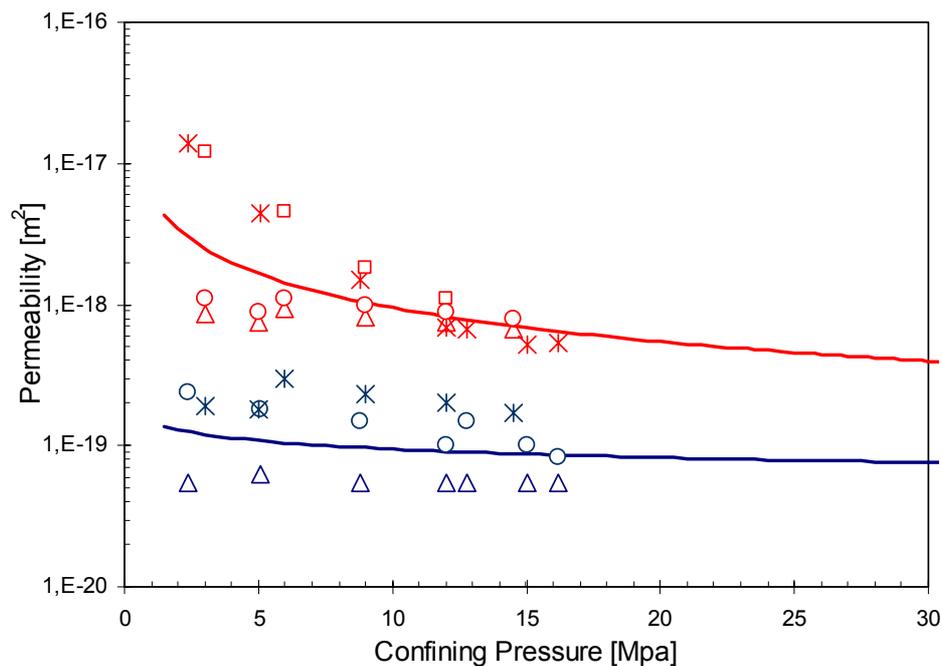


Figure 4-6: Effect of the confining pressure on the permeability of bentonite packs /ZHA 02/

4.2.2.4 Porosity - Permeability Relationship

The estimation of the permeability via porosity or vice-versa is necessary in the case of lack of experimental data or for relating the transient changes of the porosity to the permeability. Various attempts are made to express the permeability in terms of various pore properties such as pore diameter, capillary characteristics. Kozeny-Karman relationship is one of the most important of these efforts and gives the hydraulic conductivity as function of porosity, ϕ , and tortuosity, τ :

$$K = \left[\frac{\phi^3}{(1-\phi)^2} \right] \left[\frac{\rho_w g}{\tau^2 (\rho_s S)^2 C_s \mu_w} \right] \quad (4-13)$$

where ρ_w and μ_w are the density and viscosity of water, τ is the tortuosity, S and C_s are internal surface area and shape factor successively. The units are given in SI.

A study to investigate the validity of Kozeny-Karman relationship showed some deficits of describing hydraulic flow in compact clays which is attributed to unequal pore sizes caused by the grouping of clay particles in clusters or domains /OLS 62/.

The relationship between porosity and permeability for a wide variety of clay formations is experimentally investigated. A plot of $\log(k)$ against total porosity, ϕ gives a broadly linear trend across the entire range (Figure 4-7). As can be concluded from the Figure the data are considerably dispersed. A correlation is possible only with a very low degree of confidence

($R^2=0,6567$). From petrophysics it is known that there is no obvious relationship between porosity and permeability /DUL 79/. For the well determined cases, the porosity-permeability relationship of the reservoirs obeys to the following semi-logarithmic empirical equation:

$$\phi = a \text{Log}k + b \quad (4-14)$$

Both mineralogical composition and stress environments strongly influence permeability evolution through their effects on clay fabric. Field and laboratory studies suggest that shear zones in clay-rich sediments can both enhance and retard fluid flow. Faults in unlithified, clay-rich sediments are generally regarded as aquitards, and experimental studies have demonstrated that tectonised clays have low intergranular permeabilities /DEW 96/. A result of the experimental study on Callovo-Oxfordian clays is presented in Figure 4-8 showing the effect of confining pressure and time on measured permeability. The results of a study conducted by measuring the radial and vertical permeability on consolidated and sheared smectite-rich Barbados Clay is presented in /DEW 96/. Sheared under fully drained conditions, the clay develops permeability anisotropy with progressive consolidation and shear displacement. The consolidated clay had a comparable level of absolute permeability so that of the sheared clay in the direction parallel to the shear zone. Permeability across the shear zone was up to 1000 times less than along it (Figure 4-9). The results suggest that effective barriers to fluid migration can be produced by shearing in clays and that permeability anisotropy is probably dependent on shear displacement, clay content and mean grain size. The figure also shows that the permeability and its anisotropy remains approximately constant as effective stress decreases, while the permeability of the consolidated clay increases slightly.

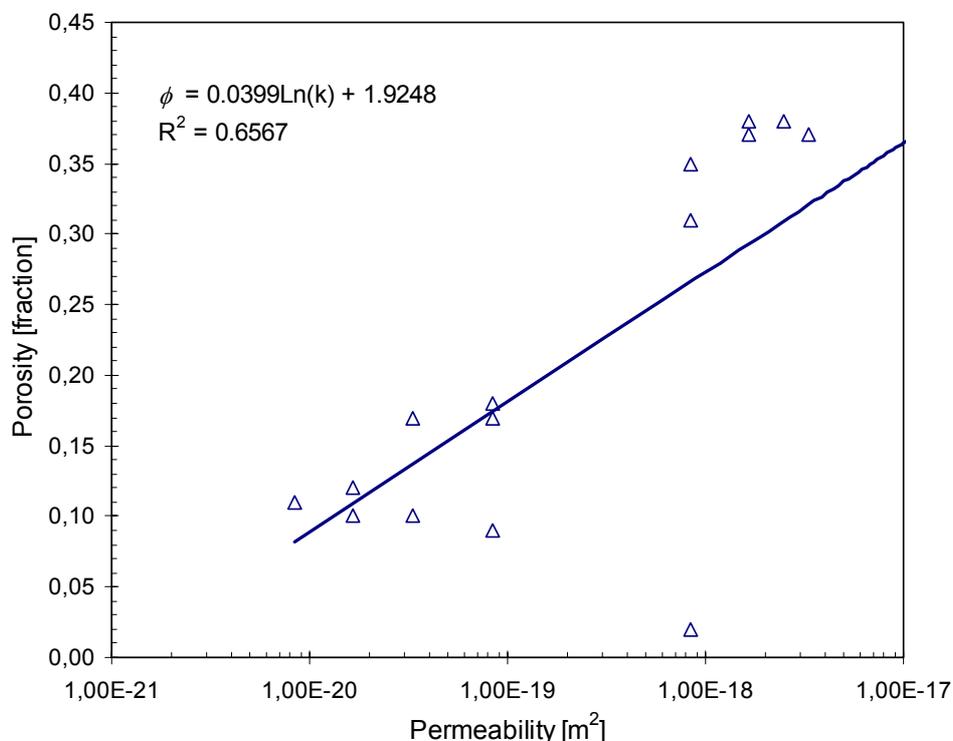


Figure 4-7: Porosity-permeability relationship for published clay formation data

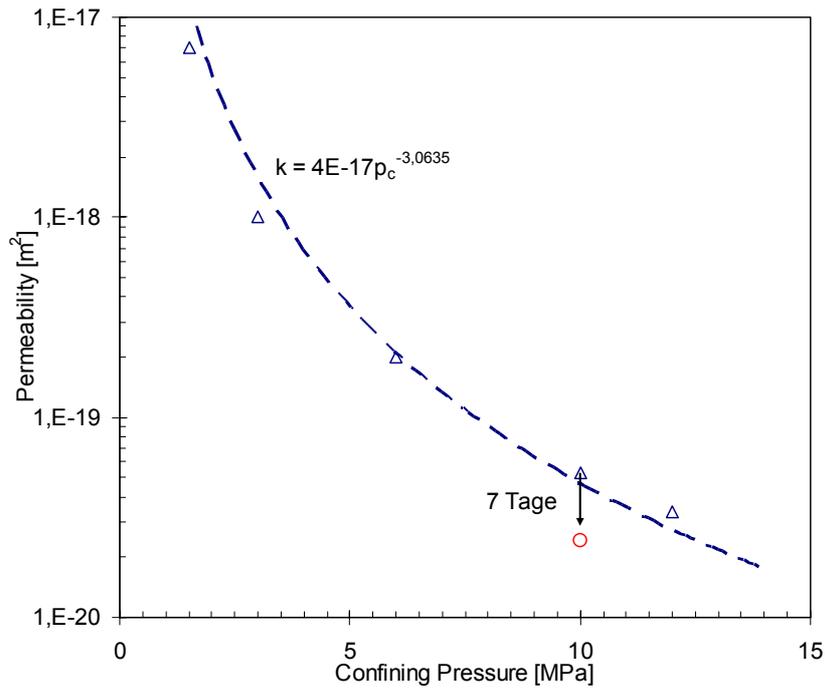


Figure 4-8: Effect of the confining pressure and time on permeability, Callovo-Oxfordian- Clay /ZHA 02/.

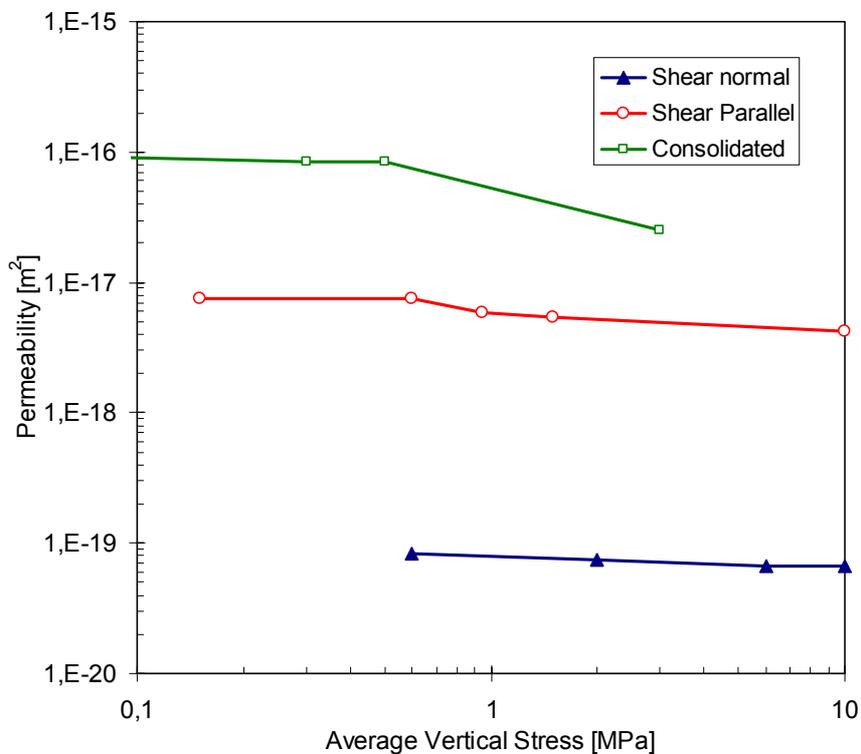


Figure 4-9: Effect of the anisotropy on the permeability of Barbados Clay as function of the effective stress conditions /DEW 96/

4.2.2.5 Tortuosity

For an actual porous medium, the interconnected void spaces can be assumed to be a number of tortuous pore channels. The tortuosity τ is defined as the average ratio of the microscopic path length L to the macroscopic path length X in the medium, or

$$\tau = \frac{L}{X} \quad (4-15)$$

Calculations for gas transport are fairly insensitive to τ and, in the absence of experimental data, this parameter is usually taken as 1,41 for clays. However, it has been suggested that clay mineral orientation and the overlapping of clay platelets in compact clays might lead to a tortuosity which is substantially larger than this value.

4.2.2.6 Saturation

Saturation is defined as the relative amount of water, oil and gas in the pores of a rock, usually as a percentage of pore volume.

$$S_x = \frac{V_f}{V_p} \times 100 \quad (4-16)$$

Where the pore volume and the fluid volume are given as V_p and V_f successively. The importance of water content on the mechanical and hydraulic properties of the clay formations is well determined. Therefore the saturation is especially emphasized for clay formations.

To define the water content of the clay formations, w in terms of mass units the following equation is sometimes preferred:

$$w = \frac{m_w}{m_s} \times 100 \quad (4-17)$$

where m_w is the mass of water and m_s is mass of the rock.

4.2.2.7 Surface Area

The specific surface of a particulate material is the surface area of the particles expressed in square metres per gram of dry solids. The generally high specific surfaces of clay minerals, when contrasted with those of other rock-forming minerals, is due to both the size and the shape of the particles, the area of the sheet surface (001 crystal faces) is generally much larger than that of the edge surfaces. Kaolinite is exceptional and the edges of these crystals can make up 10 - 20% of the surface area.

Specific surface may be estimated from vapour-phase isotherms by applying the Brunauer-Emmett-Teller (BET) theory. Commonly nitrogen gas is used in the routine BET analysis, and when applied to clays, the external surface area per gram of clay, including edge sur-

faces, is measured. Nitrogen molecules generally do not penetrate the interlayer regions of expandable clay minerals. The surface measured by nitrogen adsorption is not a unique property of the clay but depends on sample preparation and on the nature of the interlayer cations.

Methods which measure the total surface area (interlayer + external) of swelling clays are based on the adsorption of monolayers of polar organic compounds such as ethylene glycol glycerol or ethylene glycol monethyl ether (EGME). The assumption of monolayer adsorption is rather dubious from a theoretical standpoint since molecules of adsorbate tend to cluster around charge centres on the clay surface. Nevertheless, the techniques have had considerable empirical success, particular when calibration tests have been performed using a well-characterized clay such as montmorillonite. For non-swelling clay minerals the nitrogen- and EGME-determined values for specific surface are approximately the same. The surface areas of some clays are for Callovo-Oxfordian 30 m²/g, for Opalinus Clay 23-34 m²/g, for Boom Clay 44 m²/g /MAZ 03/. They are all measured with BET method.

4.2.2.8 Interfacial Tension

If gas and water are at one point in contact with the flat surface of a solid, then equilibrium is only possible if the interface between the gas and water forms a definite angle with the solid. This angle is known as the contact angle θ . High affinity of clay minerals for water suggests that clay surfaces are always naturally wet and that gas-mineral contact is impossible under normal circumstances. A film of adsorbed water will therefore always exist between the gas and the clay mineral. The thickness of the residual films after gas entry is of great importance since it may be of a similar order of magnitude as the interparticle spacing in a very compact argillaceous medium (e.g. shale or high-swelling bentonite). The difference in pressure between a gas and a liquid in a narrow capillary is given by the relationship:

$$p_c = p_g - p_w = \frac{2\sigma}{r} \cos\theta \quad (4-18)$$

where σ is the interfacial tension (N·m⁻¹) and r is the radius of a circular capillary or the half spacing between flat parallel plates /DUL 79/. This relationship forms the basis of most theoretical approaches to the problem of two-phase flow in porous media. Taking $\theta = 0$ for clay and assuming that the gas-water meniscus is a hemisphere of radius a , the basic form of the Young-Laplace equation can be written. The quantity $(p_g - p_w)$ is known as the capillary pressure in oil industry studies and the matrix suction in soil mechanics. Capillary pressure p_c is no longer a simple pore pressure term; (b) p , may not be constant over the cross-section of a capillary pathway; (c) the gas-water meniscus is probably not hemispherical and may be very distorted in a very narrow capillary; and (d) it is very uncertain whether the interfacial tension σ_{wg} remains constant across the pathway cross section.

4.2.2.9 Wettability

The wettability is defined as the preference of a solid to contact one liquid or gas, known as the wetting phase, rather than another. The wetting phase will tend to spread on the solid surface and a porous solid will tend to imbibe the wetting phase, in both cases displacing the non-wetting phase. In the case of water-gas systems rocks are essentially water-wet. The intermediate state between water-wet and gas-wet can be caused by a mixed-wet system, in which some surfaces or grains are water-wet and others are gas-wet, or a neutral-wet system, in which the surfaces are not strongly wet by either water or oil. Both water and oil wet most materials in preference to gas, but gas can wet sulphur, graphite and coal.

Wettability affects relative permeability, electrical properties, nuclear magnetic resonance relaxation times and saturation profiles in the reservoir. The wetting state impacts waterflooding and aquifer encroachment into a reservoir. Reservoir wetting preference can be determined by measuring the contact angle of crude oil and formation water on silica or calcite crystals or by measuring the characteristics of core plugs in either an Amott imbibition test or a USBM test.

4.2.2.10 Relative Permeability

This is a dimensionless term to adapt the Darcy equation to multiphase flow conditions. Effective permeability is the ability to preferentially flow or transmit a particular fluid through a rock when other immiscible fluids are present in the reservoir (for example, effective permeability of gas in a gas-water reservoir). The relative saturations of the fluids as well as the nature of the reservoir affect the effective permeability. Relative permeability is the ratio of effective permeability of a particular fluid at a particular saturation to absolute permeability of that fluid at total saturation. If a single fluid is present in a rock, its relative permeability is 1,0. Calculation of relative permeability allows for comparison of the different abilities of fluids to flow in the presence of each other, since the presence of more than one fluid generally inhibits flow:

$$k_r = \frac{k_f}{k} \quad (4-19)$$

The most reliable way of determining the relative permeabilities of the clay formations as well as of the bentonite buffers is measurements performed using two-phase flow experiments. Figure 4-10 shows relative permeability curves for Opalinus clay and compacted Serrata Bentonite. However such measurements are time consuming and difficult to perform therefore semi empirical numerical approaches are also used to estimate the relative permeability of the various porous media.

Modelling of two-phase flow in porous media requires the specification of the functional relationship between capillary pressure (p_c), relative permeability (k_r) and saturation (S). Various correlations exist in the literature to define these relationships. These are mainly semi-empirical equations.

Various correlations were developed to estimate gas-liquid relative permeability as function of gas-liquid saturations. Corey-Brooks correlation is commonly used for oilfield reservoir simulation; another is the Parker and Lenhard correlation adapted from Van Genuchten.

Corey-Brooks equations for a two phase system as function of the water saturation S_w are given as follows /BRO 64/:

$$k_{rw} = (S_w^*)^{\frac{2+3\lambda}{\lambda}}$$

$$k_{rg} = (1 - S_w^*)^2 \left(1 - (S_w^*)^{\frac{2+\lambda}{\lambda}} \right) \quad (4-20)$$

The superscript (*) refers to normalized saturations; that is saturation space that does not contain irreducible water.

$$S_w^* = \frac{S_w - S_{wir}}{1 - S_{wir}}$$

$$S_g^* = \frac{S_g}{1 - S_{wir}} \quad (4-21)$$

These equations can be written in terms of S_g^* , since for saline formations

$$S_g^* + S_w^* = 1 \quad (4-22)$$

The λ parameter is the pore size distribution index, and typically ranges from 0,5 for a wide range of pore sizes to 5 for a uniform pore size rock. Sensitivities on these exponents were also included in the simulation study. Variations were segregated to obtain a range of outcomes with relative permeability uncertainty.

The Parker and Lenhard correlation for relative permeabilities adapted from Van Genuchten is given as follows /PAR 87/:

$$k_{rl} = \sqrt{\bar{S}_l} \left[1 - \left(1 - \frac{S_{gt}}{1 - \bar{S}_l^\Delta} \right) \left(1 - (\bar{S}_l + \bar{S}_{gt})^{\frac{1}{m}} \right)^m - \left(\frac{\bar{S}_{gt}}{1 - \bar{S}_l^\Delta} \right) \left(1 - (\bar{S}_l^\Delta)^{\frac{1}{m}} \right)^m \right]^2$$

$$k_{rg} = (1 - \bar{S}_l - \bar{S}_{gt})^{\frac{1}{3}} \left(1 - (\bar{S}_l + \bar{S}_{gt})^{\frac{1}{m}} \right)^m \quad (4-22)$$

Where \bar{S}_l and \bar{S}_l^Δ are the effective values of liquid saturation S_l and turning-point saturation S_l^Δ , respectively, normalized with respect to irreducible liquid-phase saturation:

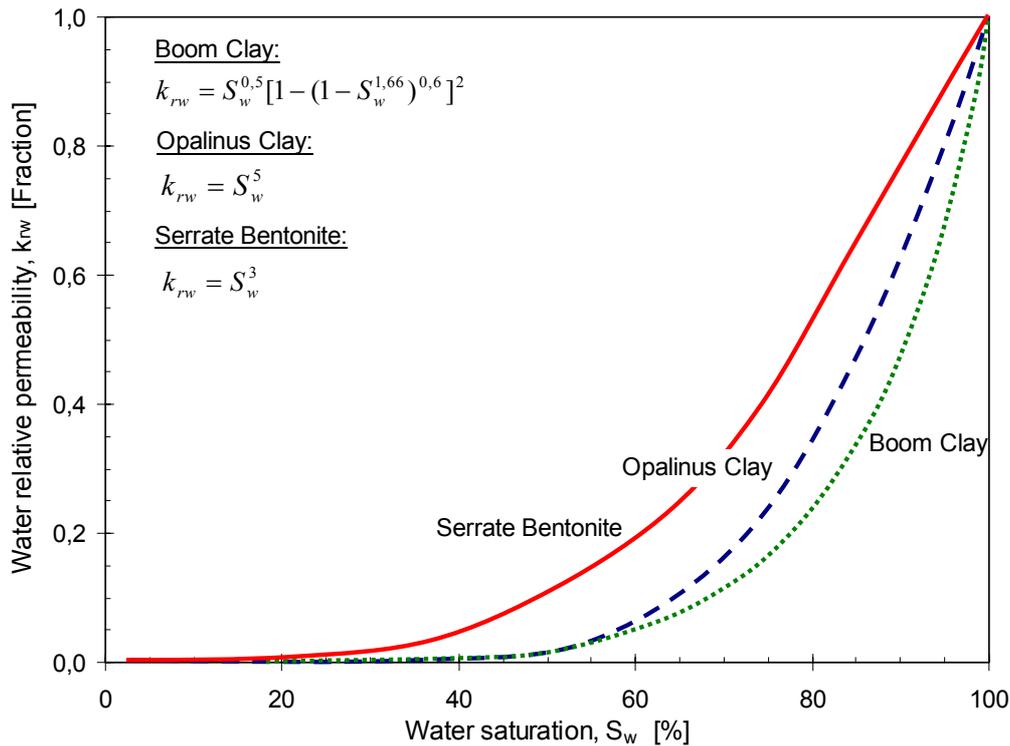


Figure 4-10: Relative permeability curves for Boom Clay, Opalinus Clay and Serrate Bentonite /ZHA 04/

$$\bar{S}_l = \frac{S_l - S_{lr}}{1 - S_{lr}}$$

$$\bar{S}_l^\Delta = \frac{S_l^\Delta - S_{lr}}{1 - S_{lr}} \quad (4-23)$$

The most important quantity determining the significance of hysteresis effect is the trapped gas saturation after a flow from drainage to imbibition. Most relative permeability hysteresis models make the use of the trapping model proposed by /LAN 68/.

For wetting curves, S_{gr}^Δ is given by modified version of the Land equation as:

$$S_{gr}^\Delta = \frac{1 - S_l^\Delta}{1 + \left[\frac{1}{S_{gr \max}} - \frac{1}{1 - S_{lr}} \right] (1 - S_l^\Delta)} \quad (4-24)$$

Where S_{lr} is the residual liquid saturation (the saturation below which the liquid phase is immobile, assumed to be a constant rock property), S_l^Δ is the turning-point saturation for the

transition from the primary drainage curve to the first-order wetting scanning curve, and $S_{gr,max}$ is taken as a function of porosity ϕ from the /DOU 06/.

$$S_{gr,max} = -0.3136 * \ln(\phi) - 0.1334 \quad (4-25)$$

It is obvious from Equation (4-24) when $S_l^\Delta = S_{lr}$ (complete drainage of the medium before wetting begins), $S_{gr}^\Delta = S_{gr,max}$ and that when $S_l^\Delta \approx 1$ (only slight drainage before wetting begins), $S_{gr}^\Delta \approx 0$. Here the difference between drainage and imbibition should be indicated. The drainage is the displacement of the wetting phase by the non-wetting-phase. The imbibition on the other hand is the spontaneous presence of the wetting phase in the porous medium. The imbibition is also called as *suction* which is preferred in “repository” terminology.

4.2.2.11 Capillary Pressure

The relationship describing the capillary pressure required to obtain a given non-wetting phase saturation in a rock. Rocks have a distribution of pore throat sizes, so as more pressure is applied to the non-wetting phase, increasingly smaller pore openings are invaded. According to Kelvin’s law the capillary pressure necessary to desaturate a capillary of diameter b is given by:

$$p_c = \sigma \left[\frac{1}{r_1} + \frac{1}{r_2} \right] = \frac{2\sigma}{b} \quad (4-26)$$

where r_1 and r_2 are the radius of curvature of the wetting and non-wetting phases. The second member is obtained when $(1/r_1) = 0$ and $r_2 = b/2$ (assuming that the contact angle is 0).

The capillary pressure curve is important for understanding saturation distribution in the reservoir and affects imbibition and multiphase fluid flow through the rock. If gas and water (a liquid) are present in a porous medium the difference of the pressures of each phases is called capillary pressure and is given by the equation:

$$p_c = p_g - p_w \quad (4-27)$$

The gas and water saturations on the other hand, should be equal to unity.

In a conventional rigid porous medium, the capillary pressure arises from the pressure differences due to the wettability of each phase to the walls of the pathways. For a water wet system as the case for the most of the geologic media, the capillary pressure causes gas to tend to access larger –sized pores before smaller sized pores, so that the gas saturation increases and smaller sized pore spaces become gas filled, the capillary pressure increases. In terms of geologic repository terminology capillary pressure is often called as matrix suction.

In low-permeability water-saturated, water wet, compacted clay formations the pore sizes may be too small and hence the capillary pressures too high for gas to be able to enter the medium without dilation of the pore spaces. In some cases, the capacity to support gas flow may be dependent not only on the dilation of the flow channels by elevated gas pressures, but also on the creation of gas flow channels by micro-fracturing of the medium.

Figure 4-11 depicts capillary pressure curves for Boom, Opalinus formations and Serrata compacted bentonite. These curves are based on measured data /ZHA 04/. As concluded from the figure for the same degree of saturation the capillary pressure required for gas to enter is higher in the case of Opalinus Clay.

The primary drainage and wetting curves are based on the Van Genuchten capillary pressure function /GEN 80/

$$P_c = -\frac{1}{\alpha^\gamma} \left[\left(\frac{S_l - S_{l_{\min}}}{1 - S_{gr}^\Delta - S_{l_{\min}}} \right)^{\left(\frac{n^\gamma}{n^\gamma - 1} \right)} - 1 \right]^{\left(\frac{1}{n^\gamma} \right)} \quad (4-28)$$

Where γ denotes the branch (*d* for drainage and *w* for wetting) of the capillary pressure curve and $\alpha, S_{l_{\min}}, n$ are the fitting parameters. For both primary and drainage curves $S_{gr}^\Delta = 0$ is defined.

4.2.2.12 Gas Entry /Threshold Pressure

Threshold capillary pressure (or displacement pressure) is the pressure difference between gas and water at that critical point as gas pressure is increased when the gas phase is able to penetrate the pore space of an initially water-saturated porous rock. The gas entry pressure or threshold pressure which is one of the most important parameters of reservoir engineering can be explained Figure 4-12 presenting the general shapes of the two-phase flow constitutive relationships and taken from /CRO 06/. From the Figure the gas entry pressure can be defined as a threshold value at which the gas starts to form a continuous phase and becomes mobile. On an imbibition path it is the gas which remains trapped within the pore network.

The existence of a threshold pressure as gas entry criterion seems first to have been reported by Pusch and co-workers /PUS 85/ but has subsequently been observed by most other workers. Figure 4-13 shows the measured threshold pressures as function of the water permeability for a wide range of lithologies including shales, limestone and anhydrite. As expected, gas entry pressure increases as the permeability to water increases. Figure 4-13 also shows the obvious importance of the threshold capillary pressure for clay formations where the permeability to water can reach to very low values.

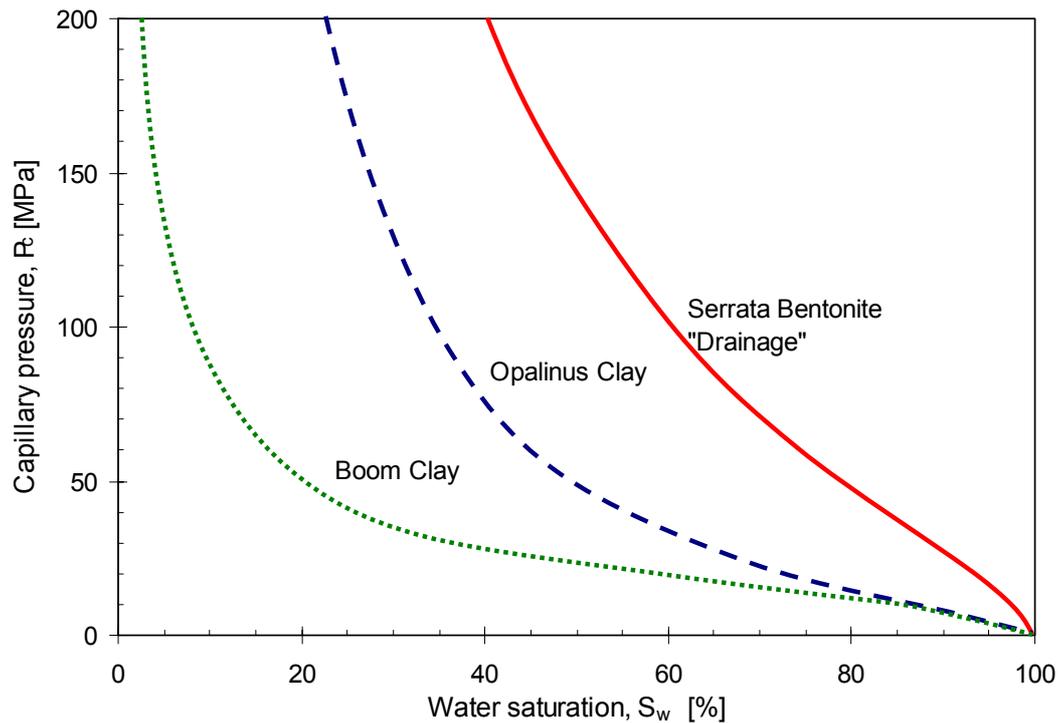


Figure 4-11: Capillary pressure curves for Boom Clay, Opalinus Clay and Serrata Bentonite (Van Genuchten Model) /ZHA 04/

The regression line in Figure 4-13 is represented by a power-law relationship relating the threshold capillary pressure, p_t to permeability, k :

$$p_t = 5,874 \times 10^{-6} \left[\frac{1}{k} \right]^{0,33} \quad (4-29)$$

where p_t is obtained in MPa when k is entered as m^2 . The introduction of the basic relationship between porosity and permeability (Kozeny-Carman) to the above given equation yields the following semi-empirical equation:

$$p_t = A \left[\frac{(1-\phi)}{k} \right]^{0,33} \quad (4-30)$$

in which A represents the internal specific surface. Many similar relationships exist in the literature; they have mainly empirical character, which suggest that a direct application of these equations to the specific cases is doubtful.

Under constant volume test conditions, breakthrough and peak gas pressures can significantly exceed the sum of porewater pressure and swelling pressure. Observed sensitivity of the breakthrough and peak gas pressures to the test boundary conditions suggests that gas entry is accompanied by dilation of the bentonite fabric. The experiments provide conclusive evidence that gas moves through a system of highly unstable pressure-induced pathways.

Gas entry and breakthrough under constant volume boundary conditions causes both the total stress and the porewater pressure to increase. It is possible to determine the point at which gas enters the clay by monitoring changes in these parameters. Abrupt drops in gas injection pressure, accompanied by similar increases in total stress, can be interpreted as pathway propagation events. The first pathways which form in the clay may not intersect the gas sinks. Additional gas pressure is often required to produce fully-conductive features which connect with the sinks /CRO 05/.

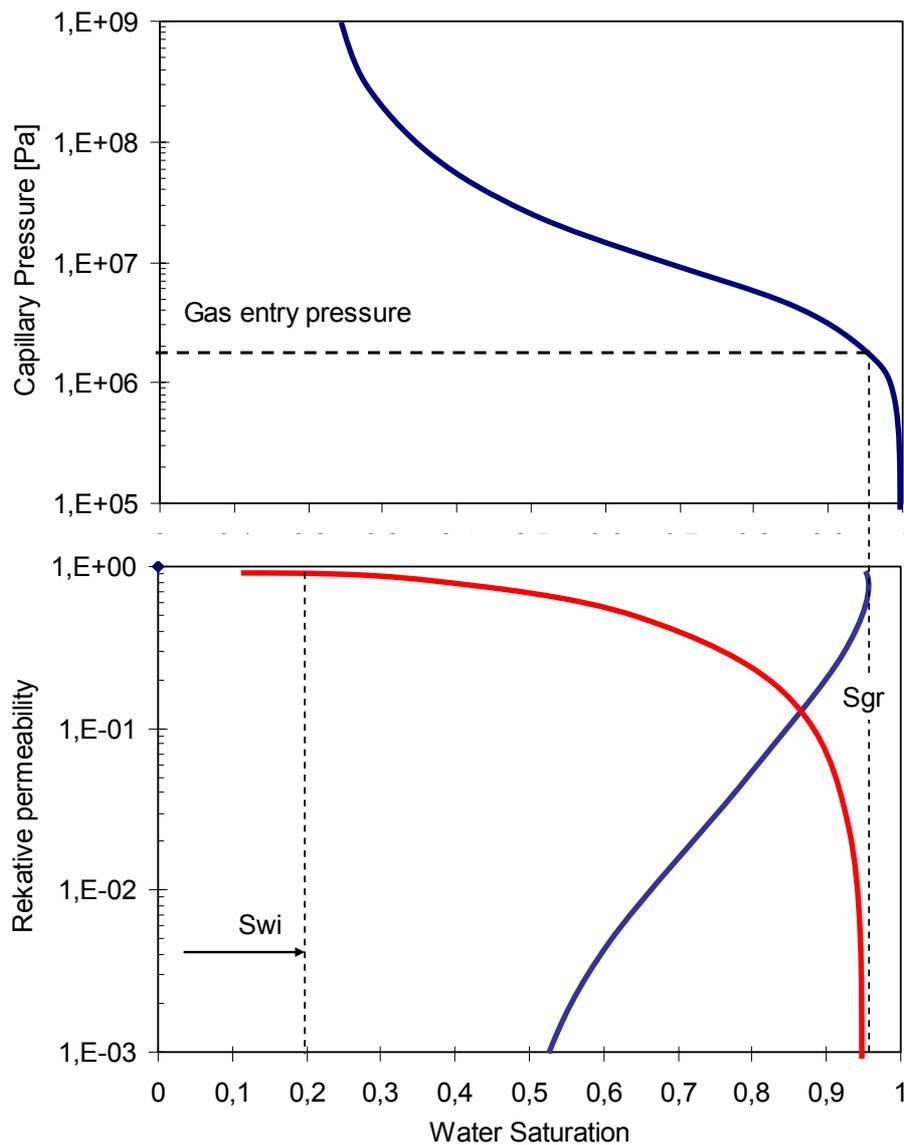


Figure 4-12: Capillary pressure and relative permeability curves for Opalinus Clay (calculated with van Genuchten-Mualem Eq.) /CRO 06/

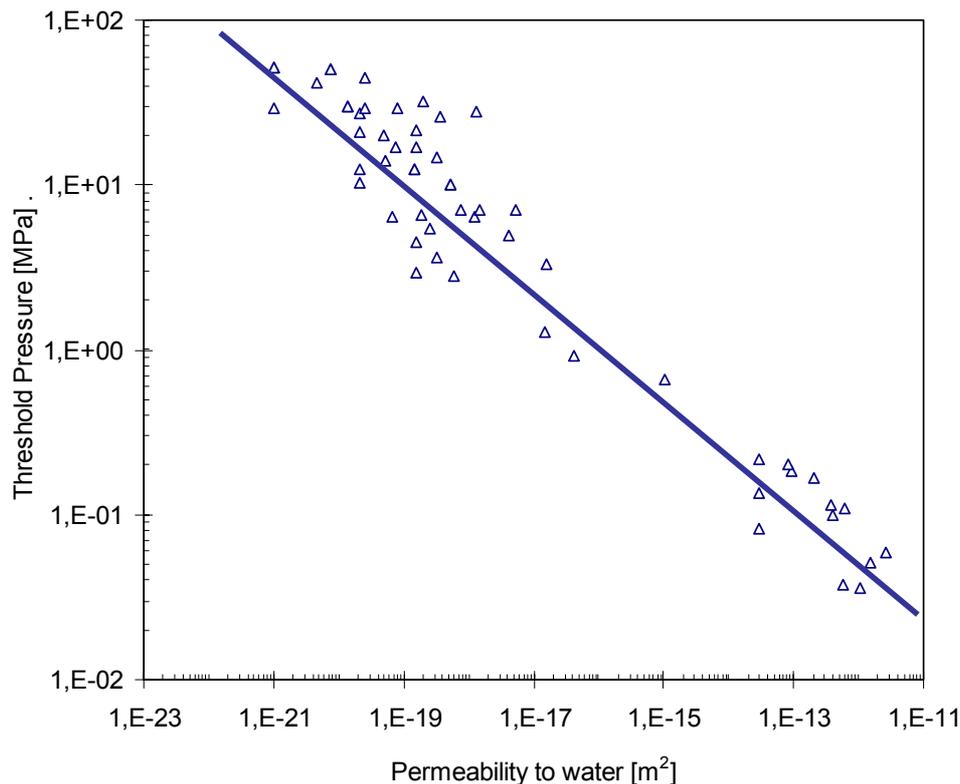


Figure 4-13: Relationship between threshold pressure and permeability for a range of measured data from various types of formations /ROD 99/

4.2.2.13 Diffusion Coefficient

Given the general importance of diffusion as a transport mechanism in the unfractured and generally more plastic clay rocks, the factors affecting the diffusion coefficients of various chemical species in the clay environment are of particular interest. In one dimensional form, Fick's first law can be written as

$$J_A = -D \left(\frac{dC}{dx} \right) \quad (4-31)$$

where J_A is the flux of solutes, D is the diffusion coefficient and dC/dx is the concentration gradient.

The diffusion of one chemical species at low chemical concentration into another is known as tracer diffusion. The limiting value of the tracer diffusion coefficient at infinite dilution can be predicted theoretically. The term self-diffusion is understood to mean the diffusion of a molecule or ion within a system comprising the same molecules or ions, where no distinction is made between isotopes (e.g. water in water, HT0 in water). Chemical species diffusing through the solution-filled pore spaces of a rock encounter along their path an irregular network of pore channels and frequently collide with the walls of these channels. Diffusion

through this porous space is slower than it would be in the absence of the mineral framework. Based on these simple concepts of the diffusion process, the physical characteristics of the rock responsible for slowing down molecular diffusion are generally considered to be the porosity itself, the pore size distribution (represented by a constrictivity term) and the tortuosity, τ , of the diffusion path. A number of different diffusion coefficients are quoted in the literature. These are not always clearly distinguished and there is a conspicuous need for standardization. The specification of a diffusion coefficient depends on the type of test (i.e. steady-state or transient method), the assumed cross-sectional area for diffusion (i.e. total area of porous medium or total area of pore channels normal to the transport direction), and whether or not the diffusant is sorbed during its passage through the porous medium. It is generally assumed that the sorption sites within the porous medium are totally saturated at steady-state, so retardation due to sorption does not occur during steady-state diffusion.

The effective diffusion coefficient D_e , also known as the intrinsic coefficient, of a non-retarded chemical species moving through the porous medium can then be related to the free-water coefficient D_0 by

$$D_e = \phi \left(\frac{\chi}{\tau^2} \right) D_0 \quad (4-32)$$

where ϕ is the porosity (appropriately defined), χ is the constrictivity and τ is the tortuosity. The porosity term is included because the cross-sectional area available for diffusion is reduced by the presence of the solid phase. If the medium is strongly anisotropic or the diffusion accessible porosity is substantially lower than the total porosity, it may not be appropriate to use total porosity when considering diffusion in clay systems.

The diffusion coefficient measured using a transient method on a diffusant which is retarded within the porous medium is usually known as the apparent coefficient, D_a . Based on conventional theory D_a can be formulated as:

$$D_a = \frac{D_e}{\phi R} = \left(\frac{\chi}{\tau^2} \right) \frac{D_0}{R} \quad (4-33)$$

where R is the retardation factor. The retardation factor is a standard parameter in the advection-dispersion model for solute transport. The retardation factor can be determined by independently measuring the quantities D_a and D_e . However, it should be noted that a variety of transient chemical effects will be lumped together in any R value which is derived in this way. The application of R values in transport calculations assumes that retardation is the result of fast, reversible, equilibrium reactions exhibiting a linear sorption isotherm.

A generic example of the diffusion from the outer boundary of a cylinder representing a canister of waste surrounded by a bentonite buffer is given in /ROD 99/. A number of measurements of the diffusion coefficients of clay formations have been reported. A compilation of obtained values is given in /MAZ 03/. The effective diffusion coefficients for HTO are in the range of $1-2 \times 10^{-11}$ m²/s perpendicular to bedding and $5-10 \times 10^{-11}$ m²/s parallel to it. Effective diffusion coefficients for Cl⁻, Br⁻ and I⁻ are smaller by factors of 10 and 3, respectively, than corresponding values of HTO.

The dependence of the diffusion coefficient on the effective stress is also experimentally investigated. This feature which can be very important for the modelling is shown in Figure 4-14 for N₂ and CH₄ for two different effective stresses namely 17 MPa and 47 MPa. As can be concluded the diffusion coefficients are clearly lower for the higher effective stress case.

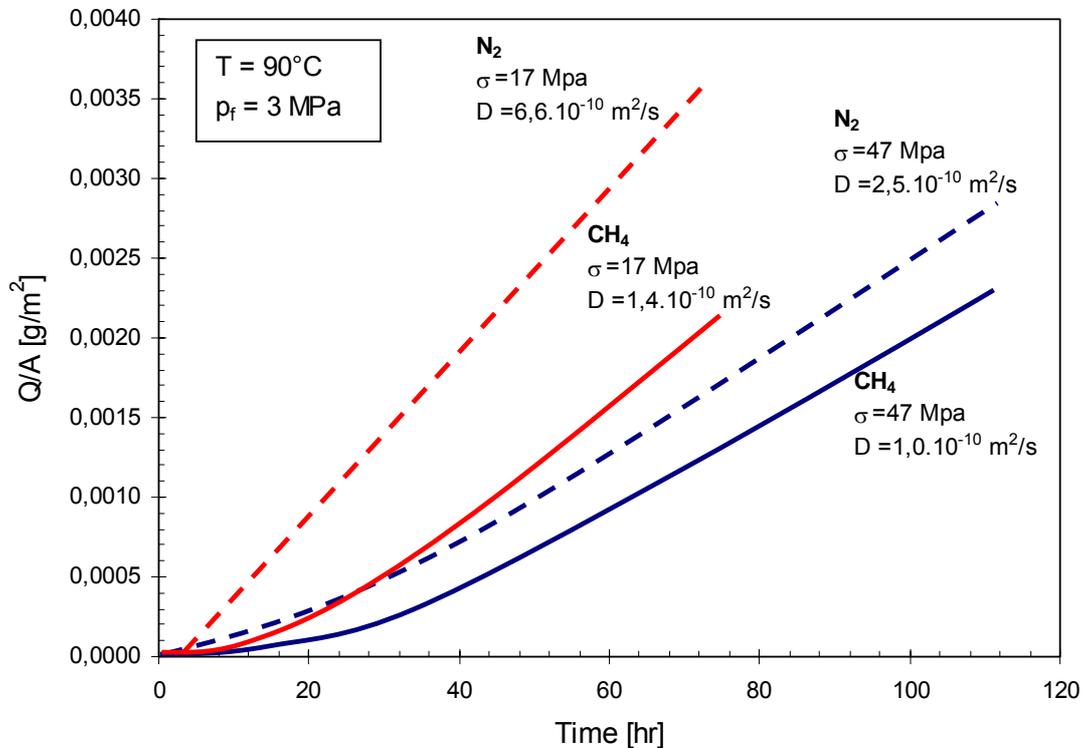


Figure 4-14: Influence of the effective stresses on diffusion behaviour /ROD 99/

4.2.3 Adsorption

Adsorption is a physico-chemical process that occurs when a gas or liquid or solute (called adsorbate) accumulates on the surface of a solid or more rarely a liquid (adsorbent), forming a molecular or atomic film (adsorbate). If a solvated ion does not form a complex with a charged surface functional group, but instead neutralizes surface charge only in a non-local sense, it is said to be adsorbed in the diffuse ion-swarm. The diffuse ion-swarm and the outer-sphere surface complex mechanism of adsorption involve almost exclusively electrostatic bonding, whereas inner-sphere complex mechanisms are likely to involve ionic as well as covalent bonding. Inner-sphere complexation is, therefore, termed specific adsorption and outer-sphere complexation, together with diffuse ion association are called non-specific adsorption.

The adsorption can be expressed as a linear function of the solute concentration. However, according to Yong et al. (1992) /HOR 96/, very few sorption isotherms actually exhibit linear behaviour. The most common relationships that are used to fit nonlinear isotherms are those

due to Langmuir and Freundlich. If k_1 and k_2 are constants, the Langmuir isotherm can be expressed in the form:

$$c = \frac{k_1 C}{1 + k_2 C} \quad (4-34)$$

where C is the concentration of solute. Adsorption is one of the main mechanisms contributing to the retardation of the species in mass transport in clay formations.

4.3 Gas Transport; Basic Transport Definitions

One of the difficulties in the quantitative treatment of gas-phase transport in clay formations is the very diverse range of approaches to this problem. The mathematical theories of *multi-phase flow* in porous media are based on the semi-empirical generalisation of Darcy's Law and are based on the concept of *relative permeability*. The theories deals largely with oil industry interest in the movement of gaseous and liquid hydrocarbons in geological media and are widely applied to the problems and rock types of concern to that industry. Early pioneering studies of the *capillary behaviour* of porous media and reservoir rocks are provided by Scheidegger (1974) and Dullien (1979) /SCH 74/,/DUL 79/. The works on capillarity and gas flow in low permeability rocks are helpful reporting on the observations on departures from Darcy's law at high flow-rates due to inertia and turbulence. More recent work on unstable displacement during two-phase flow is also of interest when the transport in these low permeability and often heterogeneous formations are examined.

Studies which have addressed the migration of repository gases in unfractured and initially water-saturated clays include the experimental work on natural clay samples and on MX-80 bentonite (smectite) buffer material. Pusch et al. have examined models for the movement of water and gas in a bentonite /PUS 87/. Given the propensity of the harder and more indurated clay rocks to exhibit fracturing, work on gas movement in discontinuous geological media is also relevant. Various aspects of gas movement in underground storage caverns in fractured rocks have been examined by various authors. Theoretical aspects of gas flow in fractures are discussed in /SCH 86/ and calculations of gas migration in discrete fractures and fracture networks have been reported by /THU 86/ /THU 90/. Gas generation and migration in radioactive waste repositories in hard rock have been discussed also by many researchers /MÜL 00/ /BRA 03/. The possible effects of gas overpressurization, including gas-water interactions, have been also a subject of the related studies.

Based on the published literature, it is generally accepted that initially water-saturated, compact clays do not behave as classic porous media and that the theories developed for other rock-types, is inadvisable when one attempt to quantify gas phase transport in such materials. Distinguishing features of compact clays include the complex interaction between the mineral phases, water and solutes, the sub-microscopic dimensions of the pore channels, the deformable matrix and the generally low tensile strength. These characteristics are of key importance to the problem of gas transport in compact clays. Although the transport of gas in solution is a very slow process in unfractured clay formations its general importance in geological repository systems is obvious. As the clays are chemically active, the importance of

chemical features and processes on the transport is higher for clay rocks than other host rocks. A study published by NEA provides a good categorized compilation of the features, events and processes which play or can play major/minor roles in all steps of waste disposal in clay formations whether indurated or plastic clays /MAZ 03/. Some important aspects of the transport in clay formations as well as in bentonite buffers are given based on this catalogue and also on related new publications.

4.3.1 Darcy Law

The basic of the fluid flow in a porous medium is formulized for water flow in sand packs by Darcy. Darcy law describes the laminar flow of an incompressible fluid which saturates an isotropic porous media:

$$q = \frac{k}{\mu} A \frac{dp}{dl} \quad (4-35)$$

where q is the flow rate as m^3/s , k is the permeability m^2 , μ is the fluid viscosity as $Pa \cdot s$, A is the flow area as m^2 , dp/dl is the pressure gradient across the flow media as Pa/m . This well-known equation is modified for the flow of the compressible fluids such gases as shown:

$$q = \frac{k}{\mu} A \frac{(p_2^2 - p_1^2)}{2p_2 L} \quad (4-36)$$

where the p_2 is the pressure at inlet and p_1 is the pressure at the outlet. However, the laminar flow of a gas through porous media is not only dependent on fluid properties but at the same time on the properties of the porous media. Especially at low permeability media and for low flow rates the permeability of the medium should be corrected taken the “slip” of the gas molecules on the walls of the pores. This effect is formulized by Klinkenberg with the following equation to describe the permeability to gas, k_g :

$$k_g = k \left(1 + \frac{b}{p_g} \right) \quad (4-37)$$

where b is the Klinkenberg parameter which is dependent on the composition of the gas as p_a and p_g is the gas flow pressure in p_a . In the equation k is the absolute permeability in other terms permeability to a liquid determined after Darcy law.

4.3.2 Non-Darcy Flow

In the analysis of experimental data three possible types of deviation from Darcy's law can be defined:

- a nonlinearity in the relationship between flux and hydraulic gradient,
- a threshold hydraulic gradient, below which the flux is zero,

- the occurrence of components of flux which cannot be attributed to the hydraulic gradient.

A number of important effects can occur at the boundaries of a compact clay or clay rock. One side of this boundary are the free water and dissolved salts (with an approximate ionic charge-balance). The other side is interparticle water films of molecular thickness containing a predominance of positively charged ions. This is evidently a description of many laboratory and field situations. Specific conditions must be met before an aqueous solution can be transported by *advection* across this boundary and into the clay-medium.

According to Darcy law the flux of groundwater in a porous medium is linearly proportional to the hydraulic potential gradient. Clay minerals exhibit exceedingly complex interactions with both water and solutes and there are good reasons to suspect anomalies in flow behaviour as aqueous solutions moves through the sub-microscopic flow channels of compact clays or mudrocks. Direct laboratory evidence for non-Darcy flow through clays has been widely reported, but is still fairly inconclusive.

4.3.3 Flow in Fractures

The presence of fractures in clay formations is a disturbing factor in performance analysis for repository concepts. Fluids such as groundwater or gas will always tend to follow the paths of least resistance in a formation therefore they create extraordinary problems on modelling of the gas/fluid transport. If such media are transacted by permeable faults or interconnected fractures flow would be focused along these discontinuities. Many publications in the literature report on the presence of natural fractures in clay formations. On the other hand, the formation and/or the opening of the cracks in the EDZ's are a well known aspect of the geologic repository systems /GER 96/, /NEA 96/. An evaluation of the occurrence of fluid flow through faults and fractures is thus of primary importance for assessment of radionuclide transport from radioactive waste repositories located in clay formations:

- Faults are generally weaker than the surrounding rock.
- Faults seldom occur as isolated features, but most frequently as parts of genetically related systems, so both must be considered in evaluating fluid flow.
- Faults can act as conduits or seals to fluid flow; they can be both at the same time in different parts of a fault or fault system and they may change in time.
- Not all faults enhance fluid migration not act a seals; some appear to have little effect on fluid migration.
- Fault geometry is complex both in strike and dip sections.
- Damage zones and fault rocks generally have widely different properties.

The fabric of fault rocks seldom is random and is often predictable which allows estimations of its contribution to fluid flow. Faults may often be anisotropic to fluid migration; flow parallel

to the fault trace is enhanced in the damage zone and along fractures within the fault rock, but inhibited at high angles to it.

Fault properties are not homogeneous along a fault nor are they static in time. The fabric may be altered by mechanical processes, chemical interaction of fluids and the rock or most likely some combination of two.

The flow of fluids through fractures in rocks is a process that has importance for many areas of the geosciences, ranging from ground-water hydrology to oil. Research on fluid flow in fractures and in fractured porous media has a history that spans nearly four decades. Several conceptual models have been developed for describing fluid flow in fractured porous media. Fundamentally, each method can be distinguished on the basis of the storage and flow capabilities of the porous medium and the fracture. The storage characteristics are associated with porosity, and the flow characteristics are associated with permeability. Four conceptual models have dominated the research:

1. explicit discrete fracture,
2. dual continuum,
3. discrete fracture network, and
4. single equivalent continuum.

In addition, multiple-interacting continua and multi-porosity/multi-permeability conceptual models have recently been introduced in the literature. Further distinctions can be drawn on the basis of the spatial and temporal scales of integration, or averaging, of the flow regime. Four scales are described of concern in fracture flow /BEA 91/:

1. the very near field, where flow occurs in a single fracture and porous medium exchange is possible;
2. the near field, where flow occurs in a fractured porous medium and each fracture is described in detail;
3. the far field, where flow occurs in two overlapping continua with mass exchanged through coupling parameters; and
4. the very far field, where fracture flow occurs, on average, in an equivalent porous medium.

4.3.3.1 Explicit Discrete Fracture Formulation

Several investigators have published numerical models incorporating explicit discrete representations of fractures. Most of the models incorporate fractures explicitly, but these models are restricted to fractures with vertical or horizontal orientation. The advantage of explicit discrete-fracture models is that they allow for explicit representation of fluid potential gradients and fluxes between fractures and porous media with minimal non-physical parameterization. But the fact that fractures may be very tortuous and may have significant impacts on the characterization of flow is often unaccounted for in these models. The numerical models developed in many studies are mainly attempts for allowing analysis of flow through fractures of any arbitrary orientation and shape.

4.3.3.2 Dual-Continuum Formulation

Dual-continuum approaches were introduced by Barenblatt et al. (1960) and later extended by Warren and Root /WAR 63/. Dual-continuum models are based on an idealized flow medium consisting of a primary porosity created by deposition and lithification and a secondary porosity created by fracturing, jointing, or dissolution. The basis of these models is the observation that unfractured rock masses account for much of the porosity (storage) of the medium, but little of the permeability (flow). Conversely, fractures may have negligible storage, but high permeability. The porous medium and the fractures are envisioned as two separate but overlapping continua. Fluid mass transfer between porous media and fractures occur at the fracture-porous medium interface. In some numerical approaches, the mass transfer is lumped at the nodes common to the fracture and porous medium grids. The transfer occurs according to a fluid-potential-dependent coupling parameter. This approach averages, or “smears,” the transient response between fracture and porous medium.

The basic equation of fluid flow through discrete fracture is derived from the Navier-Stokes Equation for a smooth walled planar fracture and is given as cubic law:

$$q = -\frac{b^3}{12\mu} \frac{dp}{dl} \quad (4-38)$$

From the "cubic law" for flow in a fracture of aperture b , the hydraulic conductivity can be derived. The effective hydraulic conductivity K of a rock containing N parallel microcracks (each of aperture b) per unit width across a plane normal to the flow is then given by the following equation

$$K = \frac{N\rho_w g b^3}{12\mu f} \quad (4-39)$$

where f is a surface characteristic factor which is introduced because real fractures do not have smooth surfaces.

4.3.3.3 Fracture Characterization

4.3.3.3.1 Discrete Fracture Network

Discrete fracture network (DFN) models describe a class of dual-continuum models in which the porous medium is not represented. Instead, all flow is restricted to the fractures. This idealization reduces computational resource requirements. Fracture “legs” are often represented as lines or planes in two or three dimensions /AET 04/.

4.3.3.3.2 Dual Porosity Model, Warren Concept

In dual porosity model, which is illustrated schematically in Figure 4-15 porosity is divided between a connected fracture porosity, through which flow throughout the rock can occur, and a matrix porosity, which is segregated into finite sized blocks which can exchange fluids

with the fracture matrix /WAR 63/. The latter exchange can be important for water; it is likely to be less important for gas migration through initially water saturated fractured rock, where capillary pressure may exclude gas from the water-saturated matrix and gas flow will occur through the fracture matrix alone.

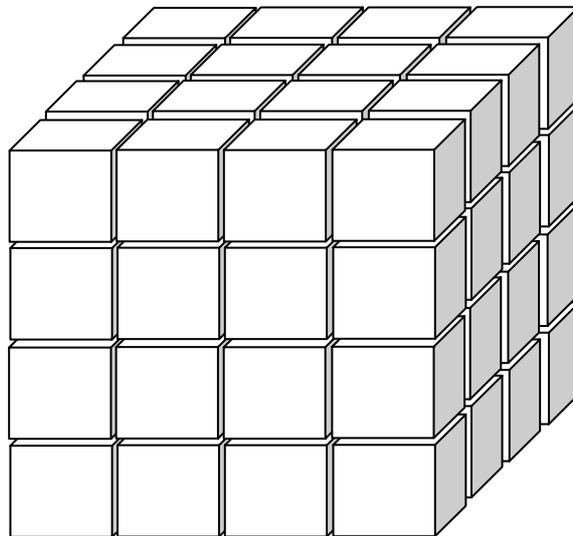


Figure 4-15: Schematic of the dual porosity fracture network model

Dual porosity models generally treat the flow characteristics of the fracture network in the same way as continuum porous medium flow models, and therefore do not address the limitations in that approach that have motivated the use of specific fracture flow models. In the dual porosity model, global flow may occur in both fracture and matrix continua, with exchange of fluids allowed also between the two continua.

4.3.3.3 Multiple Interacting Continua

The method of multiple interacting continua provides a further improvement on considering the fractures by portioning the matrix blocks into several continua on the basis of the distance of matrix material from the fractures /PRU 99/. The MINC approach can resolve gradients driving interporosity flow under conditions where the perturbations in the fracture system invade the matrix blocks slowly.

4.3.3.4 Statistical Models

In a series of papers, M. Oda and co-workers presented a statistical approach for describing and modelling the elastic deformation and fluid flow properties of fractured rocks /ODA 85/. The tensors for each physical property are derived by taking a volume average of the expected effect of each fracture in the population. The volume average contains functions of the fracture orientation, length, and aperture in such a way that long fracture or wide fractures contribute relatively more than their smaller cousins.

Envisioned that a general geometric property of cracked rock, termed the fabric, determines many mechanical properties of geological materials he developed a mathematical description, a fabric tensor, which considers the following elements of crack geometry:

1. position and density of cracks;
2. shape and dimension of cracks, and
3. orientation of rocks.

One of the primary simplifying assumptions in the derivation of the fabric tensor concerns the relative position of fractures. Fractures are assumed to have a random position in the network, and all fractures are distributed uniformly throughout the network, as is often described by a Poisson point process. For example, the exact position of any one fracture with respect to any other is not taken into account. Only the length, orientation, aperture, and stiffness of each fracture are retained in the calculation. Thus, highly conductive clusters of fractures will not affect the Oda analysis but may in reality have significant effects on fluid flow. In Oda's model, fractures in the network can be arranged in an infinite number of different ways and still have the same mechanical and fluid flow properties. He developed a tensor model for the fluid permeability of fractured rock. An assumption required for fluid flow in his derivation requires that the fractures be comprised of smooth parallel plates with a constant separation, or aperture h . In that case, fluid flow is described by the parallel plate model, where the volumetric flow rate is proportional to the aperture raised to the third power (h^3). Thus a small variation in aperture results in large variations in fluid permeability.

The parallel plate model for fluid flow can only be considered a qualitative description of flow through real fractures. Real fracture surfaces are not smooth parallel plates but are rough and contact each other at discrete points. Fluid will take a tortuous path when moving through a real fracture; thus deviations from the parallel plate model are expected. Simulating fluid flow and visualizing its motion affected by tortuosity and varying geometry have been the aim of the related studies. It is worth noting that further empirical studies showed a relationship between aspects of the crack tensor and the anisotropy of acoustic wave velocities in laboratory specimens. This result suggests the potential to develop an inverse method to derive important aspects of fracture geometry from geophysical methods. Hence the importance and future prospect of a simulation tool that would handle the details and complexities of a real fracture and model the flow of reservoir fluids through it is not trivial.

The mathematical fundamentals of reservoir simulators are based on the substitution of Darcy's equation into the mass balance equation for a system and obtaining expressions for pressure in discrete grid-blocks within that system. The pressure equations contain some terms that are related to the rock and fluid properties. One of the most important and probably the most uncertain among all is called the transmissibility – a lumped parameter that retains information about the property of the porous medium, the fluid flowing through the medium, the direction of flow, and the position in space.

Because of the tortuosity of the flow paths, the actual fluid velocity will vary from point to point within the rock. But the velocity used in Darcy's equation (often referred to as Darcy velocity) is actually an average velocity over the core, and hence the conventional simulators are limited in scope to analyze the flow at the microscopic (pore) scale. Because actual ve-

locities are difficult to measure, they are rarely used in reservoir-engineering calculations. However, in order to understand fluid flow in fractured media, the analysis of its motion and hence have a realization of the variation of its velocity at a pore scale is needed. Therefore, the equations used in most of the studies must be different than the conventional reservoir simulation equations.

Another problem with conventional reservoir simulation is how the rock permeability, to be used in the transmissibility term, is assigned to each grid-block. Simulators often use a-priori knowledge of the permeability and are rarely derived from the transmission or conductive capacity of actual flow paths in a particular grid block. The conventional methods sometimes cannot incorporate the proper anisotropy information in the flow model, which results into inaccurate flow simulation. For more accurate reservoir simulations, and particularly for identifying high potential production zones in fractured reservoirs, a conventional approach of assigning the permeability without having correlated with actual flow paths must be changed. Hence tools to visualize and improved models to analyze flow in complicated network of fractures to understand the pattern of flow are needed and thus step forward towards finding more accurate ways of tying permeability information to reservoir simulators. Clay formations that are cut by fractures and faults consists a very important part of the hydraulic and mechanical considerations of the transport. On the other hand, damaged and disturbed zones are due to the formation of network like fracture formation with the unbalance of the acting stresses on the corresponding zone. Therefore flow through fracture should also be examined in the framework of flow through fractures.

Pattern of flow in sedimentary basins are often controlled by the geometry, size population and spatial distribution of faults and fractures that link or compartmentalize permeable horizons. The microstructural properties of individual faults determine whether they act as conduits, or barriers to convective, diffusive and multiphase fluid transport.

4.3.4 Advection; Limitations of Darcy Law

Darcy law for flow in porous media is of empirical character and due to some assumptions. One of these assumptions is linear proportionality of the hydraulic potential gradient. The second is the chemically inert coupling of the fluid and rock. One basic requirement for the validity of this phenomenological law is that the fluid phase should be non-reactive with the porous medium. Another important assumption of Darcy Law is the isotropy of porous medium. However, flow in clay formations exhibits features that can make the validity of Darcy law questionable. Direct laboratory evidence for non-Darcy flow through clays has been widely reported, but is still fairly inconclusive. Since most laboratory experiments have been performed on samples that are far less compacted than many naturally-occurring clay formations, the possibility of non-Darcy behaviour in the more indurated rock-types should not be excluded. A number of the proposed mechanisms for non-Darcy flow are likely to become more important as the apertures of pore channels decrease to molecular dimensions during the process of compaction.

In the analysis of experimental data four possible types of deviation from Darcy's law are concluded:

1. a nonlinearity in the relationship between flux and hydraulic gradient,
2. a threshold hydraulic gradient, below which the flux is zero, and
3. the occurrence of components of flux which cannot be attributed to the hydraulic gradient

Coupled flow is also important in clay systems, therefore its effect on Darcy's law should also be considered. Chemical interactions and mechanical perturbations may cause in many cases important variations which in turn disturb the isotropy and linearity of the system. Although the occurrence of osmosis in compact clays is now well-substantiated, this should not lead us automatically to the conclusion that Darcy's law is invalid for these materials. The following sections give a discussion of the probable causes which leads to a deviation from the Darcy Law.

4.3.5 Interactions Fluid-Rock

When clay exposed to an aqueous solution which is more dilute than the "equilibrium solution" it will swell as water is drawn into interparticle spaces and the double-layers increase in thickness. Conversely, exposure to an excessively concentrated solution may lead to chemosmotic consolidation. Use of an unmatched solution chemistry is also likely to cause ion exchange reactions, which may also lead to changes in the both the double-layer thickness and the fabric of the clay /OLS 62/. The passage of an electrolyte solution through a clay membrane can also cause electrical streaming potentials to develop along the flow paths which can produce an electro-osmotic back-flow. These phenomena may at least partially explain the well-established sensitivity of the hydraulic properties of clays and clay-bearing rocks to the solute chemistry and the concentration of permeating electrolyte solutions.

4.3.6 Unrepresentative Flow Velocities

Unrepresentative flow velocities are one of the most difficult problems to address in testing the flow behaviour in clays. Because of the exceedingly low permeability of compact clays and the difficulty of measuring very small fluxes, most experimental techniques impose a hydraulic gradient on these materials which is many orders of magnitude greater than any naturally-occurring gradient. The velocity of the water in the narrow interparticle spaces of the clay during an experiment will be substantially larger than in the natural situation. The tiny particles of clay minerals move if the velocity of water is too high, leading to plugging and unplugging of the narrow pore channels. Such mechanisms are another potential source of apparent deviations from Darcy's law /OLS 62/.

The application of a very high hydraulic gradient can also have other disturbing effects on flow in clay. Since the total stress σ acting on the clay medium remains constant, the act of raising the pressure of the test fluid leads to a reduction in the effective stress σ_e . This produce a gradual increase in the pore volume of the clay as it attempts to re-equilibrate with a new level of effective stress by swelling.

4.3.7 Disjoining Pressure Threshold

There are close links between the chemico-osmotic threshold and the disjoining pressure threshold. Threshold phenomena are likely to be most important if the matrix flow in very compact clay rocks (e.g. oilfield shales) is examined, although it can be acknowledged that fractures in these materials might completely bypass matrix flow. It is important to remember that there is no threshold for the diffusion of water across the boundary of compact clay in chemical equilibrium with its surroundings.

4.3.8 Viscosity and Adsorption Effects in Compact Clays

Since the viscosity of water can be regarded as a key parameter in the theory of advective transport (viscous flow) in porous media, it is worth examining whether unusual viscosity effects might lead to departures from Darcy's law in compacted and soft clays. There is evidence to suggest that this might, indeed, be the case in very compact materials. The effect of a simple change in viscosity on Darcy's law would not be noticed and would be accommodated in the hydraulic conductivity term without any recognition of the effect. The important finding is the evidence for non-Newtonian water in compact clay systems. A non-Newtonian fluid might display a nonlinear relationship between shear stress and shear strain-rate and might also exhibit a plastic yield point (e.g. a Bingham fluid).

4.3.9 Evidence from Experiments on Thin Films

When two surfaces are farther apart than 10 molecular diameters (= 3 nm), a simple liquid (e.g. cyclohexane) in the gap retains its bulk Newtonian behaviour and the shear plane remains coincident with the physical solid-liquid interface (to within one molecular diameter) even at high shear rates. However, for thinner films the "effective viscosity" is found to rise dramatically. For example, when smooth mica sheets separated one or two molecular layers of cyclohexane slide past each other, the effective viscosity of the liquid is 5 to 7 orders of magnitude greater than that of the bulk liquid. More importantly, it is found that the whole concept of a Newtonian viscosity breaks down for such thin films; they exhibit a yield point and the shear stress no longer depends on the shear rate. This can lead to "stick-slip" behaviour. Even very small amounts of water present as a contaminant can suppress this intermittent response. It is noted that stick-slip is not observed when aqueous solutions are used in this type of experiment. Nevertheless, the experimental evidence for the non-Newtonian behaviour of liquids in very thin films is becoming more convincing /NEA 96/.

4.3.10 Shales as a Diffusive Barrier to Groundwater Movement

When the passage of water molecules through the matrix of a very compact clay rock (e.g. an oil-field shale), with interparticle spacings which may be less than a few nanometres is examined, it is very doubtful whether the concepts of normal viscous flow (advection) are applicable. The motion of water molecules in such a system is best characterized as a diffusion process, even although this motion may be driven by a pressure gradient. However, the

concept of diffusion down a pressure gradient seems a little obscure until recalling that chemical potential depends on pressure.

4.3.11 Dispersion

As a contaminant move through a porous medium it tends to spread out from the path predicted by considering advective hydraulics alone. This spreading phenomenon is known as hydrodynamic dispersion. The process occurs as a result of mechanical mixing and molecular diffusion. Mixing is a consequence of the essentially inhomogeneous nature of flow in a porous medium. Contributions arise from (a) flow velocity variations within individual pores due to the viscous drag exerted adjacent to the pore walls, (b) differences in the pore sizes along the flow paths and (c) the tortuosity, branching and interfingering of pore channels. Flow along paths of interconnected fractures results in very similar effects in fractured rocks.

4.3.12 Distribution Coefficient and Retardation Factor

The distribution coefficient K_d may be defined as the mass of the chemical species which is bound to the solid phase per unit mass of solids, divided by the mass of the chemical species remaining in solution per unit volume of the solution:

$$K_d = \frac{(m_{sm}/m_m)}{(m_{sw}/V_w)} = \frac{(m_{sm}/m_m)}{C} \quad (4-40)$$

where m_{sm} is the mass of the chemical species sorbed on mineral solids of mass of m_m , m_{sw} is the mass of chemical species in volume V , of groundwater solution and C is the groundwater concentration. The mass of radionuclides sorbed on mineral solids per unit volume of the porous medium can then be expressed in terms of C using the following equation:

$$m_{sm}/V_t = \rho_g(1-\phi)K_d C \quad (4-41)$$

where ρ_g is the *grain density* of the mineral solids, V is the volume of mineral solids and V_t is the total volume of the element of the porous medium. K_d is a valid representation of the partitioning between liquid and solids only if the reactions that cause the partitioning are fast and reversible and the sorption isotherm is linear. The *retardation factor* R is then related to the distribution coefficient by

$$R = \left[1 + \frac{(1-\phi)\rho_g K_d}{\phi} \right] = \left[1 + \frac{\rho_d K_d}{\phi} \right] \quad (4-42)$$

4.3.13 Retardation Mechanisms

Gas attenuation is the mechanism by which a flux of gas molecules in aqueous solution becomes depleted during its passage through a porous medium by chemical or biological processes occurring within the medium. The mechanism may prompt the introduction of a sink- or reaction-term in the transport model. Batch reaction experiments on slurries of Boom Clay

and hydrogen have been performed by SCK/CEN /HOR 96/. The reaction capacity for fresh (unoxidised) clay was found to be very small (1,2 mg H₂ per kg of clay) but was roughly an order of magnitude larger in slurries which were deliberately oxidised before exposure to hydrogen. The precise details of the reaction are not known.

The transient flow of gas in solution can also be modelled using a retardation factor, R , and a diffusion accessible porosity term, ϕ_d , in much the same way as other retarded solutes. Although it may be important to distinguish between the intrinsic and the apparent diffusion coefficients, this distinction has rarely been made in the studies reported in the general literature.

4.3.14 Reverse-Osmosis

Reverse-osmosis is the coupled-flow mechanism whereby a concentration difference is established across a semi-permeable membrane when a solution is passed through it. The mechanism may be regarded as the inverse of chemico-osmosis. The efficiency of the filtration process in the laboratory is observed to increase with increasing exchange capacity of the clay and with decreasing input solution concentration. The efficiency also increased with clay compaction pressure, but decreased slightly at higher temperatures. Field evidence for reverse-osmosis remains inconclusive. The mechanism has been proposed as a source of highly saline brines in sedimentary basins although there are some serious doubts on this matter. The membrane efficiency of a shale is greatest when the porosity, and hence the permeability, both approach zero. If the shale is fractured, the semi-permeable membrane may be bypassed.

4.3.15 Gas Transport in Solution

Provided that the solubility limit is not exceeded, gas molecules will move through the pores of an argillaceous medium in aqueous solution by the mechanisms of advection and dispersion, in much the same way as other soluble chemical species. If the average linear velocity of the pore water is very small, advection and hydrodynamic dispersion will be relatively unimportant and Fickian diffusion will be the primary transport mechanism.

4.3.16 Diffusion of Gas to Ground Surface

Fick's law represents the diffusion of dissolved gas due to concentration gradients in the porewater and Henry's law describes the solubility of gas in porewater. The transport of dissolved gas occurs even at low (total) gas pressures; the pressure-dependent dissolution of gas in porewater and the increased groundwater flux induce the specific flux of the dissolved gas to increase with an increase in the gas pressure. As described in previous chapters, the main parameters affecting the transport behaviour of dissolved gas are Henry's coefficient, the diffusion coefficient in water, the tortuosity, the accessible porosity and the hydraulic conductivity. The low hydraulic conductivity of argillaceous rock significantly restricts the efficiency of this transport mechanism. Nevertheless, the general importance of diffusion and advection as slow background processes in all types of cap rock formations is beyond ques-

tion and has been addressed in the context of many hydrocarbon exploration and reservoir engineering studies.

4.4 Thermal Effects

4.4.1 Thermal Effects on Mineral Stability and Pore-Water Composition

The equilibrium state of chemical reactions varies with temperature, as do reaction rates. Increasing temperatures increase the solubility of most solids, decrease the solubilities of most gases and increase most reaction rates. Results of changing temperature could be modification of the chemistry of pore-water and/or of formation mineralogy. Thermal effects on clay minerals and organic materials are most prominent in clay formations. This process is relevant to the region in which thermal anomalies from the repository extend, although it will be most relevant to the region of highest temperatures in the affected field.

In a study aiming at examining the thermal effects on Opalinus Clay, the development of the thermal pulse emanating from the heat-producing waste was quantified /NAG 02/. Over a period of maximal 1 000 year, temperature at the interface of bentonite and Opalinus Clay will exceed 80°C with a maximum of 95°C in the (worst) case. These temperatures are only slightly higher than the maximum temperature of ca. 85°C experienced by the formation during maximum burial. At the time when the thermal pulse will occur, the repository system will not be fully saturated, so that water is expected to flow from the formation into the engineered barrier system (and not vice versa). The following processes related to the thermal pulse were taken into account:

- thermal maturation of organic matter,
- illitisation of the illite/smectite mixed-layer phase,
- acceleration of oxidation reactions,
- changes in pore-water chemistry.

The first three processes involve kinetics; the fourth process can be described by equilibrium thermodynamics and is reversible. The processes by which changing thermal conditions will affect mineral and solution properties are well understood and can be evaluated by geochemical modelling. For such modelling to be reliable requires data on the temperature-dependence of mineral transformations and water-rock interactions. It also requires the assumption of equilibrium or data for modelling reaction kinetics. However, there are uncertainties in thermodynamic and kinetic data for many reactions. Chief among these reactions are those for transformations among clay minerals /MAZ 01/.

4.4.2 Thermal Rock Properties

The most important thermal rock properties include:

- Thermal conductivity K [$\text{W}\cdot\text{m}^{-1}\cdot\text{°C}^{-1}$]
- Heat capacity C [$\text{J}\cdot\text{kg}^{-1}\cdot\text{°C}^{-1}$]
- Specific heat C_p [$\text{W}\cdot\text{s}\cdot\text{kg}^{-1}\cdot\text{°C}^{-1}$]
- Coefficient of linear thermal expansion $\sum t$ [°C^{-1}]

Thermal conductivity and specific heat yields:

Thermal diffusivity $k = K / (\rho \cdot C_p)$ [m^2/s] with ρ = rock density

K , $\sum t$ and k may be anisotropic, predominantly depending on the rock-specific degree of bedding parameters measured \perp [normal] and \parallel [parallel] to bedding. A good review of experimentally determined thermal rock properties for some clay formations which are candidates of host rocks for repository systems is given in /MAZ 03/, /JOR 05/. Thermal conductivities of Boom and Opalinus Clays and Serrate Bentonite are given in /ZHA 04/ as function of water saturation. /JOB 05/ represents thermal conductivity measurements on 10 samples of Callovo-Oxfordien clay from the EST205 borehole of the M/HM underground laboratory in parallel and perpendicular directions to the bedding. The thermal conductivity measured in the perpendicular direction to the stratigraphic plane decreases from 1,84 to 1,16 $\text{Wm}^{-1}\text{K}^{-1}$ with increasing depth. In the horizontal direction, the thermal conductivity is relatively constant and it is about 2 $\text{W m}^{-1} \text{K}^{-1}$.

Modelling of heat transport in clay formations is based on the mechanism of conduction (application of heat transfer equations). Radiation and convection are neglected. Heat capacity and conductivity are used as input parameters for the calculation of the temperature evolution of a repository. The data have a direct implication on the layout of the repository. Within the conceptual model used for the Spanish performance assessment, it is assumed that the thermal properties of the engineered barrier system (bentonite backfill) depend on the water content. For the host rock, however, thermal properties are assumed to be constant in time and independent of the water content and temperature. SCK•CEN conclude that the impact of heat is rather limited as long as the container or overpack will prevent that ground water will come into contact with the waste during the thermal phase of the repository.

The scientific level of understanding of the thermal effect on clay formations is very good. The mechanism of heat transport relevant for argillaceous rock with very low hydraulic conductivity ($< 10^{-13}$ m/s) is predominantly conduction. Heat convection due to fluid flow and radiation are mechanisms of minor or no importance. In comparison with the mechanical and hydraulic properties of the rock, the natural scatter of the thermal rock properties is rather small.

4.4.3 Thermally Induced Consolidation of Host Rock

The term “thermally-induced consolidation” relates on one hand to a radioactive heat source which is located in the backfilled emplacement tunnel and, on the other hand, to a time-dependent solid-water interaction of cohesive materials. The time span over which the

waste-derived heat pulse will act is of the order of some 1.000 to 10.000 years. Subjecting a saturated cohesive material, such as a saturated clay formation, to a temperature increase leads to a consolidation process which is similar to conventional mechanical consolidation. Initial thermal loading leads to a significant, irreversible consolidation which is manifested in a decrease of the void ratio. Further temperature cycles yield comparatively minor, mostly reversible deformations as long as the maximal temperature of the first heat cycle is not exceeded. Thermal consolidation is a broadly measured phenomenon. Its effect is, however, more marked for reconstituted materials than for natural rocks.

The reduction of the strength of intact rock and the associated internal, irreversible deformation of the rock can lead to secondary consolidation effects. In case of a temperature decrease with its associated shrinkage of the intact rock and of the pore-water, suction will develop. This will lead to an adsorption of water without any significant non-elastic reverse deformations within the intact rock matrix.

4.5 Mechanical Effects

4.5.1 Geomechanical Stability

In geotechnical engineering, the term “stability” is associated with the absence of large-scale failures or of excessive deformations which are detrimental to the function and safety of the engineered structure. The term is associated mainly with the stability of the underground excavations of a repository and, to a minor degree, with the stability of boreholes in clay formations. The considerations on the stability of underground openings include the ground support system, if required. This is a very important system component for the design and the operational phase of a repository. The geomechanical stability of the excavated underground openings is explicitly considered within the engineering analysis. Potential stability problems of the galleries after the emplacement of the waste and backfilling are considered to be irrelevant and are not addressed by this process. Furthermore, this is neither associated with the global stability of the repository as a whole nor with the stability of geological host formation (e.g. the re-activation of a geological fault by increased pore-water pressures).

The geomechanical stability of the excavated underground openings is explicitly considered within the engineering analysis of the repository. The methodology is in line with established engineering tunnel design procedures. The design includes the selection and dimensioning of the tunnel support system, if required.

4.5.2 Effect of the EDZ

The EDZ includes not only the zone containing induced fractures (also termed “plastic zone”) but also the distal part, which is characterised by elastic deformations due to excavation-induced stress changes (also termed “elastic zone”). Both zones can have hydraulic properties that are different from those in the far field. These properties evolve with time in response to various processes that occur during the operational phase (e.g. stress redistribution, desiccation) and after backfilling (e.g. resaturation, swelling, self-sealing).

4.5.3 Dilatancy-Controlled Gas Flow

Dilatancy controlled gas flow (or “pathway dilation”; terminology after Horseman et al., 1996, /HOR 96/) is a transport mechanism of special importance for argillaceous media with low tensile strength. Clay-rich rock cannot withstand long-term gas pressures with a magnitude greater than the minimum principal stress acting on the rock mass. Due to the expected microscale variability of the geomechanical rock properties, it even seems plausible that microfractures will form before the level of minimum principal stress is reached. Gas flow along microfractures is anticipated in situations where the shear stress is large in comparison with peak strength or where the stress state favours extensile rock deformation. The process of gas-driven microfracturing leads to an increase of the pore space, which is accompanied by a detectable increase in intrinsic permeability and a change in the capillary pressure saturation relationship. In the terminology of multiphase flow concepts, gas flow is still controlled by visco-capillary forces (phase interference between wetting and non-wetting fluid) the main difference with respect to conventional two-phase flow is that the transport properties of the solid phase (rock permeability, relative permeability, capillary pressure relationship) can no longer be viewed as invariants since they depend on the state of deformation of the rock.

4.5.4 Gas Flow along Macroscopic Tensile Fractures

As a rule of thumb, a macroscopic tensile fracture (hydrofrac/gasfrac) develops when the gas pressure is larger than the sum of the minimum principal stress and the tensile strength of the rock /VAL 97/. The macroscopic fracture is initiated quasi-instantaneously and propagates at about the velocity of a shear wave. Gas flow in such a macroscopic tensile fracture can be seen as a single-phase flow process. The propagation comes to a halt when the gas pressure in the fracture becomes less than the value of the minimum principal stress (shut-in pressure). Successful hydrofracs are characterised by a fracture transmissibility which increases the bulk permeability of the treated rock by many orders of magnitude. In a rock with low tensile strength, a macroscopic frac develops only when the gas pressure build-up is rapid, *i.e.* when the combined effect of porewater displacement and formation of small-scale fractures (*i.e.* dilatancy) no longer counterbalances the gas production rate. The conceptual, theoretical and experimental framework for fracture propagation is well documented in standard hydrocarbon exploration literature.

4.6 Gas Transport in Bentonit Based Barriers

At various points during the course of the GAMBIT Club project, the experimental data available on gas migration through saturated bentonite has been reviewed /HOC 04/. 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:

1. Behaviour of the bentonite as a conventional porous medium, with the gas flow governed by conventional concepts of capillary pressure and relative permeability.
2. 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.
3. Macroscopic fracturing of the clay to provide fracture pathways for gas flow.

This differs from (2) 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. 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 threshold pressure for gas entry. This has been related by some to the bentonite swelling pressure.
- Apparently, the displacement of only small volumes of water.
- 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.
- Changes in pore-water pressure in response to the applied gas pressure.
- Evidence of macroscopic fracturing events with radial flow from a central source.

4.6.1 Bentonite Swelling

Bentonite-based backfill of waste emplacement tunnels is a fundamental component of the repository system in many designs. With the water resaturation process of the EDZ after closure of an emplacement tunnel, water will seep into the emplacement tunnel, and the bentonite backfill will start swelling. At full saturation, the effects of swelling of the bentonite on the rock will, amongst others, depend on the composition and density of the backfill and on the convergence of the emplacement tunnel, i.e. the radial displacement of the EDZ towards the backfilled tunnel. If the density is comparatively low, swelling will predominantly be in form of swelling strain which will tend to close any existing voids. In confined conditions such as those of a fully backfilled and tightly packed emplacement tunnel, swelling will be pre-

dominantly manifested by swelling pressures which may rise to considerable magnitudes. These pressures will act as radial stresses onto the boundary (i.e. the excavation surface) of the emplacement tunnel. This effect causes increased confining pressures within the EDZ and tends to contribute to more stable conditions with regard to failure conditions and convergence movements, as long as the radial stresses do not exceed the tangential stresses at the excavation boundary.

Increased confining pressures will change the material behaviour of the EDZ rock towards a more ductile behaviour. All these factors contribute to the effect of self-sealing of fractures within the EDZ. Swelling strain and swelling pressure are interconnected parameters. The higher the swelling strain, the lower the swelling pressure, and vice versa. At equilibrium, the swelling stress of the bentonite backfill is of equal magnitude as the radial stresses at the excavation boundary, and the rates of the swelling strain and of the convergence become zero.

4.6.2 Rock Properties

In a general sense, the term “geomechanical rock properties” relates to the mechanical characteristics of a rock. These characteristics include the generic mechanical behaviour (e.g. brittle or ductile) and the specific parameters that are commonly used to describe and specify the rock behaviour in mathematical terms.

In a narrow sense, the term is exclusively associated with the parameters which are used to specify the natural state of a rock (“state parameters”) and to determine its mechanical response to imposed loads and/or deformations in a model (“design parameters”; e.g. in a load test or a FE-model). Examples of “state parameters” are the density, the water content and the Atterberg Limits. Examples of “design parameters” are Young’s modulus E , the strength parameters c and ϕ and the hydraulic conductivity K . The “design parameters” are intrinsically related to the material (“constitutive”) law chosen in the model.

Geomechanics is the science of the mechanical behaviour of soil and rock. While clay formations predominantly have rock-like features, they behave like soil in certain geological and technical conditions. This, for instance, is evidenced in the occasional usage of the Atterberg limits which constitute typical soil mechanical state parameters.

Ventilation of shafts and tunnels may result in desaturation of EDZ fractures or the rock matrix, especially where there is no lining or where a lining of the sliding rib type is used. This process potentially affects the geochemical, geomechanical and thermal properties of the EDZ. Desiccation cracking is the result of shrinkage of an argillaceous material beyond the limits of a reversible material behaviour. Shrinkage is characterised by a volume decrease of the material. The physical reason for shrinkage is the lowering of the repulsion forces of the water bound to clay minerals (both “hydration water” and “double-layer water”) in connection with the evaporation of pore-water. As with the underlying process of shrinkage, desiccation cracking is a volumetric feature. This means that cracking must be in the form of a (quasi homogeneous) fracture pattern and not in the form of discrete single structures. This characteristic constitutes a major difference to hydraulic and pneumatic fracturing.

4.6.3 Visco-Capillary Two-Phase Flow

In its conventional form, visco-capillary two-phase flow is described as a transport process whereby porewater in the pore volume of a rock formation is displaced by gas under the influence of viscous and capillary forces /BEA 72/. In a geomechanical sense, the rock mass behaves like an elastic medium, characterised by the porosity and the rock compressibility. The controlling factor for the two-phase flow characteristics of a porous medium is the gas entry pressure p_{ae} , also known as the capillary threshold pressure, which represents the difference between gas pressure and water pressure needed to displace the pore water from the initially fully saturated medium. In porous media, Young's equation can be adopted to define an equivalent pore radius of the medium by measuring the entry pressure with a non-wetting fluid (e.g. mercury porosimetry). Once the gas entry pressure has been exceeded, the gas mobility is controlled mostly by the intrinsic permeability k of the formation, the permeability-saturation relationship (relative permeability), and the relationship between the capillary pressure and the water saturation (suction or water retention curve). The functional dependency between the pore space saturation and the relative permeability or the capillary pressure is commonly described with parametric models.

4.7 Chemical Processes

The possible chemical processes which can take place in a clay repository as well as in a bentonite based buffer system can be cited as follows:

4.7.1 Surface Complexation

Surface complexation is one of the processes underlying sorption, the other being ion exchange. Surface complexation is the reversible binding of dissolved species on surfaces with charges that vary with solution chemistry and crystal-chemical effects. Both chemical complexation (co-ordination) and electrostatic interaction with surfaces occur. Prominent substrates for surface complexation include metal oxides and hydroxides of Fe (ferrihydrite, goethite), Al (alumina) and Si (amorphous silica, quartz), broken bond sites on clay-mineral edges, and organic substances such as humic and fulvic acids and polysaccharides. Surface complexation models are widely applied in studying the movement of pollutants in surface waters and shallow ground waters. Surface complexation occurs in all types of argillaceous media and is relevant in the far field for site characterisation and nuclide transport properties for Performance Analysis.

The processes involved are well understood and can be adequately modelled for the non-clay mineral phases that provide the main sites for surface complexation, such as hydrous ferric oxide minerals manganese oxides and some silicates. However, surface complexation processes are less well understood on clay minerals and in complex media containing carbonates or organics. Ion (cation) exchange i.e. electrostatic attraction onto constant-charge surfaces may be a more important process than surface complexation for univalent, divalent and some trivalent cations for the basal planes of clay minerals.

4.7.2 Ion Exchange

Ion exchange is one of the processes underlying sorption, the other being surface complexation. It differs from surface complexation in that the charged sites on which it occurs represent charge imbalances in the solid lattice and do not change with external conditions. Prominent ion exchange media include zeolites, the permanent charge sites of clay minerals (predominantly on their layer surfaces, and certain artificial organic resins. Ion exchange equilibria are described by mass action equations that do not include consideration of variably-charged surfaces nor of electrostatic effects. Ion exchange among major cations is an important control on the chemistry of water in clay formations. The effects of cation exchange can also be observed in regional water chemistry changes in formations with clay-mineral contents of only a few percent. The sorption of solutes present in trace amounts in argillaceous formations can also be described by an ion exchange model. Ion exchange is relevant to the far field in connection with site characterisation and nuclide transport properties for PA as well as to the affected field.

4.7.3 Chemical Interaction between Gas and Pore Water

This process is concerned with gases dissolved in the pore and fracture water *in situ* and the dissolution of gases present during the operational phase of the repository and/or from degradation of parts of the engineered barrier system. It further addresses the chemical interactions that might occur between pore-water and gases. It is relevant to the affected field in connection with the EDZ. The solubility of a gas depends on the partial pressure of the gas and its temperature dependent Henry's Law or other gas law constants as discussed in previous sections. In a closed system (a system with a limited total gas volume) the dissolved concentration also depends on the volume ratio of solution to total gas. Henry's Law constants are commonly included in the thermodynamic data bases used for geochemical modelling. Other forms of gas solubility data (e.g. IUPAC or Van der Waals expressions) are summarised in handbooks. The identities and availability of the dissolved gases must be known for modelling purposes. This information will come from knowledge of the chemistry of pore-water *in situ*, and from consideration of repository construction and operation procedures and of the waste products and other materials present in the repository.

Gas dissolution and other equilibrium reactions and the diffusional transport of dissolved gases are well understood. They can be satisfactorily predicted if site-specific boundary conditions are known. The kinetics of gas reactions are, like those of all reactions, less well known. If the site is heated, by radioactive decay of waste or by a shifting geothermal regime, gas solubility will decrease and a separate gas phase may appear. The parameters governing gas transport are generally less well known.

While the processes are reasonably well understood, there are uncertainties in site-specific gas-concentration data and in knowledge of the identities and rates of production of gases within the repository.

4.7.4 Dissolution/Precipitation of the Solid Phases

The process refers to the process by which solids dissolve in and/or are precipitated from solutions. Dissolution/precipitation reactions occurring during diagenesis and metamorphism can change the fabric of porous media and fractures, and minerals found in the formation may reflect diagenetic and metamorphic events. The occurrence and extent of these reactions may affect and be affected by the pH and redox potential of the water-rock system. This is likely to be particularly important in the excavation-disturbed zone (EDZ) where oxidation is probable. Dissolution/precipitation in the context refers to pure phases. These processes are relevant to the far field in connection with site characterisation and nuclide transport properties for performance assessment, as well as for the affected field in connection with the excavation-disturbed zone.

Calcite is by far the most abundant fracture-filling mineral. There is a direct correlation between the degree of induration and the abundance of fracture infills. In weakly and moderately indurated formations (Boom Clay, Opalinus Clay, Toarcian-Domerian at Tournemire, Callovo-Oxfordian at Bure), they are volumetrically quite insignificant (less than 10% of the rock volume). In strongly indurated formations (e.g. Boda Clay Formation at Mecsek, Palfris Formation at Wellenberg), they become more abundant and may account for several percent of the rock volume.

The chemistry of dissolution/precipitation reactions of relatively simple pure phases such as carbonate and sulphate minerals is well understood and such reactions can be modelled with confidence if appropriate thermodynamic data are available. Reactions affecting the EDZ will be driven by oxidation processes. Redox modelling may be less definitive because of uncertainties in thermodynamic data and the need to consider reaction kinetics in some cases. Changes in clay-mineral assemblages in response to changing formation chemical and physical environments are known semi-quantitatively.

Solubilities of elements of concern in Performance Assessment (PA) may be controlled by the precipitation of solids. The properties and even the identities of possible controlling phases for many elements (e.g. the actinides) are not well known so that solubilities used in PA (or the thermodynamic data from which such solubilities are calculated) must be estimated.

From a generic point of view, the process of dissolution/precipitation is important as a control on the solubility of certain elements included in PA analyses. From a site-specific point of view, examination of existing minerals can illuminate the geologic history of the formation and site area and guide the regional description of the site used in performance assessment. Dissolution/precipitation as a result of repository excavation, construction and operation can affect the transport properties of the repository and adjacent host rock.

On the other hand, the co-precipitation is another chemical process by which two or more chemical components are simultaneously and permanently incorporated into a single solid during its precipitation from solution, either in amorphous or crystalline compounds. The term solid solution refers to a special type of co-precipitation in which a foreign component substitutes in regular lattice sites of crystalline compounds. This definition excludes processes of

surface complexation and ion exchange by which an ion can be released into solution without dissolution of the solid or replacement by another ion(s) of like charge.

The best-known, naturally-occurring solid solutions include carbonate minerals (e.g. substitution of Fe^{+2} for Mg^{+2} in dolomite forming ankerite, and the trace concentrations of alkaline earth elements, Fe^{+2} , Mn^{+2} and other ions of similar size and charge in the calcite or aragonite lattice). Clay mineral groups are sometimes treated as solid solutions, but the mechanisms of their precipitation and dissolution are too poorly understood to consider them in performance assessment. Elements of performance assessment interest can be immobilised or retarded by co-precipitation in solids such as ferrihydrite that may form during degradation of repository materials, and other solids that may form during interactions between pore waters and repository fluids, especially those of high pH that can issue from cement. This feature should be considered relevant for all far-field features containing carbonate and clay minerals. These include not only the matrix of argillaceous rocks but also surface coatings and infill of water-conducting fractures, which are commonly, enriched in carbonate and clay minerals.

4.7.5 Oxidation of Host Rock

During repository operation and following closure, transient oxidising conditions will be encountered from oxygen in air introduced during operations. They could have a large effect upon redox potential and pH and thus on solubility limitation of radionuclide concentrations and the corrosion of the inner steel overpack, and could cause mineralogical changes in the host rock. Radiolysis of water in the immediate environment of waste packages (especially for high-level waste) can also produce species such as free hydrogen and oxygen influencing the redox potential. Oxidation of host rock refers only to mineralogical changes in the host rock. It is particularly relevant to pyrite-bearing formations, but the process can also affect organic material and other Fe^{+2} -bearing minerals. This is relevant to the affected field in connection with the EDZ. Oxidation of pyrite may lead to the precipitation of new phases such as $\text{Fe}(\text{OH})_3$. The sorption capacity of this phase, when freshly-precipitated, may be high and it can act to retard the movement of radionuclides through the affected field into the host formation because all formations considered (except London Clay) contain carbonate, pH is buffered by calcite dissolution, and acidic conditions are not expected to develop at any time.

4.7.6 Redox Buffering Capacity of the Host Rock

The redox buffer capacity of a system is a measure of its ability to resist changes in the redox potential. To be fully analogous to the widely used pH buffer capacity, the redox capacity would be defined at a given Eh as the quantity of strong oxidant that, if added to 1 litre of sample, would raise the Eh by one volt. Redox capacity values defined this way are similar to the total acid or base consuming capacity of a system. The ability to resist oxidation depends on values of $[\text{Red}]_i$, the concentration of substances such as sulphide and elemental sulphur, ammonium, organic carbon, and ferrous iron and other reduced metals. The capacity to resist reduction depends values of $[\text{Ox}]_i$, the concentrations of substances such as dissolved oxygen, nitrate, sulphate, and ferric iron and other oxidised metals. Concentrations of spe-

cies that can be readily oxidised (reduced manganese, reduced iron, oxidizable organic carbon, reduced sulphur and reduced nitrogen).

Substances oxidise at different oxidation potentials, and some substances can be oxidised only slowly. Thus the concept of an *effective* rather than a *total* redox capacity may be more useful. The effective redox capacity would include only those substances that would oxidise within the range of redox potentials of interest and at a rate commensurate with the time periods of interest.

4.7.7 Chemical Osmosis

Chemical osmosis is the most studied off-diagonal Onsager process. It refers to the fluid pressures or fluxes that develop across a semi-permeable membrane in response to a chemical concentration gradient. The converse process, called hyperfiltration, is the process by which solute molecules are prevented by their size and/or charge from passing through a membrane. Hyperfiltration may increase the concentration of solutes within or on the upstream side of a membrane through which a solvent is flowing.

The solvent flux due to chemical osmosis, q , is commonly expressed by an equation analogous to Darcy's law (here written for flow in the x -direction):

$$q_{\Pi} = \sigma \frac{k}{\mu} \frac{\partial \Pi}{\partial x} \quad (4-43)$$

and the osmotic pressure, Π , given by

$$\Pi = - \left(\frac{RT}{V_w} \right) \ln a_w \quad (4-44)$$

In the first expression, k = permeability, μ = dynamic viscosity, σ = osmotic efficiency, and V_w and a_w are the molar volume and activity of water, respectively, R is the gas constant and T is absolute temperature

Scoping calculations, based on properties of the Opalinus Clay suggest that chemical osmosis is unlikely to affect the affected-field performance of a repository after resaturation. However, there are four aspects of site characterisation (far field) to which osmosis may be of potential importance:

- as a driving force for fluid flow;
- as a cause of hydraulic overpressures;
- as a cause of erroneous hydraulic pressure measurements due to concentration gradients between borehole and formation fluids;
- as a thermodynamic potential that affects the geomechanical rock properties (e.g. swelling, mechanical instability).

4.7.8 Organics from Waste

Organics from waste include different types of organic substances that are found in radioactive waste products and waste matrices. They may be leached or degraded both from material in which radioactive waste is embedded (e.g. compacted and cemented cellulose-based waste, resins, plastics, organic decontamination agents) as well as from waste encapsulating matrix material (e.g. bitumen in bituminised waste products, modifiers that influence the rheological properties of mortar used to produce cemented waste). Organics from waste are formed either as unaltered leaching products or as radiolytical, chemical and/or microbial degradation products that are generated according to waste- and repository-specific decomposition rates. Organics that originate from leaching or decomposition reactions, like those naturally present in the host rock and pore-water, may adsorb onto solid phases, precipitate, form complexes with radionuclides, and/or migrate in complexed or uncomplexed form in the affected and far field. Note that the use of organic materials in construction materials of the repository galleries (e.g. modifiers in the mortar for the concrete linings) will also result in the release of organics with properties and fates similar to those originating from the waste.

Potential effects of organics on transport through the host rock include

- Interactions with clay minerals (shrinkage, collapse, swelling), with resulting effects on hydraulic properties;
- Complexation of solutes on dissolved organic complexes or colloids, with effects on retention properties of the argillaceous formation.

4.8 Coupled Processes

The generation of heat that will dissipate into the backfill and the surrounding host rock is a well-known characteristic of high-level radioactive waste emplaced in the underground. The associated mechanical, hydraulic, thermal and chemical effects are of potential importance for the behaviour of the repository system, particularly in the disturbed/damaged field. In the far field, the effects are limited as long as possible pore-water pressure and effective stress variations remain within acceptable limits.

High-level radioactive waste constitutes a decaying heat source. For the surrounding host rock, this implies that, after the heating stage, which is initiated at the time of waste emplacement, there will also be a cooling phase with a convergence towards the re-establishment of the natural thermal conditions. The time span over which such a heat pulse is acting depends on the type of waste (less important for vitrified high-level waste and more important for spent fuel). Commonly it is of the order of some 1 000 to some 10 000 y. The thermal impact is negligible for all other types of waste. The heat pulse causes complex mechanical, hydraulic and chemical interactions in the host rock, and all phases (gas, liquid, solid) need to be considered. Coupled thermal-hydraulic-mechanical (THM) models are generally required to adequately describe the repository response to the heat pulse (Figure 4-16).

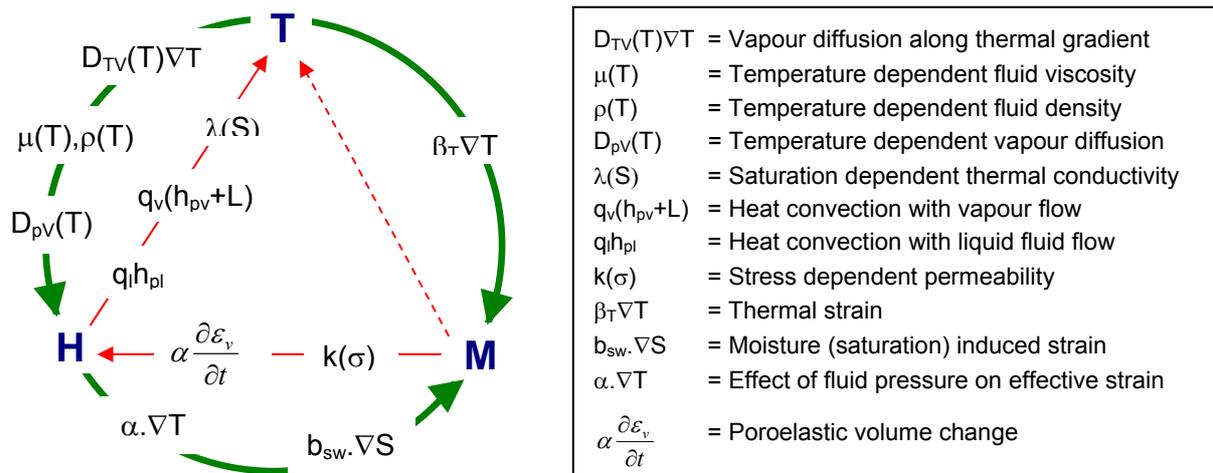


Figure 4-16: Schematic description of THM coupling processes /NOO 96/

Of particular importance are thermally triggered changes in the transport of the fluids (hydraulic conductivity, gradient) and a possible non-linear behaviour of the solids, e.g. in form of permanent deformations due to consolidation or due to cracking and fracturing (“heat cracks”; deterioration of the rock material under the influence of heat). The influence of heat on hydraulic conductivity is well known and is due to the decrease of viscosity of water with increasing temperature.

Due to the previous discussion it is clear that the chemical processes play a major role in clay formations. This means that the chemical coupling should be an obvious part of the modelling the transport processes in clay formations.

For a better understanding of coupled processes in clay formations, the general approach of /HOR 96/ can be repeated here. In general terms a coupled flow process is one in which flow of any kind (e.g., fluid, solute, heat, electrical current) is driven by the gradient of a potential not usually associated with that flow or, in mathematical terms, the flow depends on a non-conjugate force. Based on the principles of irreversible thermodynamics, the flows J_i are usually assumed to be linearly related to the gradients X_i with the following equation:

$$J_i = -\sum_k^n L_{ik} X_k \quad i = 1,2,3...n \tag{4-45}$$

where the subscripts i and k indicate the various types of flows and driving gradients, respectively, and L_{ik} are their phenomenological coefficients /BEA 72/. Onsager's reciprocal relation suggests that the coefficients are related as follows:

$$L_{ik} = L_{ki} \tag{4-46}$$

Table 4-4 illustrates direct (on diagonal) and coupled (off-diagonal) flow phenomena after /HOR 96/. The off-diagonal processes are often collectively known as Onsagerian coupled-

flow processes, after the famous thermodynamics scientist. There seems little doubt that most, if not all, of these processes operate in compact clays. Non-hydraulically driven fluid flow is given the general name osmosis. The term chemico-osmosis refers to flow driven by a chemical potential gradient, thermo-osmosis to flow driven by a temperature gradient and electro osmosis to flow driven by an electrical gradient (strictly flow is driven by the negative gradient of a potential).

The mechanical processes are necessary to be coupled in modelling the transport especially for near waste field as additional effect to the above discussion of coupled phenomena. In addition to thermally induced mechanical changes, swelling of the backfill material, mechanical changes occurring in excavated disturbed and damaged zones and the time effects are of primary importance for a realistic modelling of the transport processes.

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Table 4-4: Matrix of direct (on-diagonal) and coupled (off-diagonal) flow phenomena /HOR 96/

	Potential Gradient, X			
Flow, J	Hydraulic	Temperature	Electrical	Chemical
Fluid	Advection	Thermo-Osmosis	Electro-Osmosis	Chemico-Osmosis
Heat	Isothermal Heat Transfer	Thermal Conduction, Fourier's Law	Peltier Effect	Dufour Effect
Current	Streaming current	Thermo-electricity	Electrical conduction, Ohm's Law	Diffusion membrane potentials
Ion	Streaming current	Soret Effect (thermo-diffusion of electrolyte)	Electrophoresis	Diffusion Fick's Law

5 MODELLING OF GAS TRANSPORT IN CLAY FORMATIONS

As discussed previously the key considerations in safety analysis of clay formation are the same with other geological media as repository systems. Gas transport deals basically with two-phase flow considering the additional presence of liquid phase as brine in the cascade like barrier system of a repository. The transport of the gas as “unsaturated flow” from the waste to the biosphere is due to the various mechanisms and coupled effects. An overview of the transport processes taking in a repository place is given as function of system components in previous sections. Making this, the system components are generally classified as disturbed, undisturbed and external.

The external components of the transport consideration in a repository system are responsible mainly from the long-term geological effects. They can affect the transport mechanisms with a very complex way and they can be integrated to these mechanisms with time dependency. On the other hand, a subdivision of the features affecting the transport of the fluids/radionuclides as function of system components do not make a big sense taking the inconsistency on the definition of these components into account.

The modelling attempts for gas transport in clay formations are given in the following part of the study in four sections. The first one deals with the basic formulations of the transport and related phenomena in geologic media. These formulations constitute the background of the numerical applications of most of the physical concepts for gas transport. The second part provides the summaries of existing models describing gas transport in clay formations both in plastic and indurated clays. In the following part of the chapter the modelling effort of gas movement in EDZ's are given. The last part consists of a compilation of the transport models that are conceptualized especially for bentonite buffers.

5.1 Basic Formulations

The basic formulations of transport phenomena in geological media are given in the following section. These formulations establish a background for all of the modelling attempts of gas transport and coupled effects. They are also used to form the structure of the numerical codes developed for modelling the transport of the fluids in porous and/or fractured media.

5.1.1 Flow and Transport

The flow of one phase, gas or liquid and the immiscible displacement of one phase by another phase in porous or fractured media has been one of the basic subjects of petroleum and geothermal engineering. The flow velocity of a phase in a porous media, v , is given with Darcy Law as follows

$$v = -\frac{kk_{rf}(S_g)}{\mu_f}(\nabla p_f - \rho_f g) \quad (5-1)$$

Where k and k_{rf} are the absolute and relative permeability to fluid f , μ is the dynamic viscosity, p_f is the fluid pressure and the product $\rho_f g$ is the potential head of the fluid.

The gas, g and water, w pressures are related by

$$p_g - p_w = p_c(S_g) \quad (5-2)$$

the gas and water saturations are, by definition, related by

$$S_g + S_w = 1 \quad (5-3)$$

If any chemical and/or equilibrium dynamics results in dissolution or precipitation of the solid phases in pore volume, this should be taken in saturations calculations into account. In porous media, the capillary pressure respectively the wettability of the medium causes gas to tend to access larger-sized pores before smaller sized pores, so that as the gas saturation increases and smaller sized pore spaces become gas filled, the capillary pressure increases. In soil science, capillary pressure is often called matrix suction. For inert porous materials, the term are equivalent, but for active soils such as swelling clays, adsorption of the water at the particle surfaces may provide an additional component to the matrix suction, This is relevant for the transport in clay formations.

For porous media in which the interactions between the pore fluid and the solid matrix are considerable, the theories of soil-water potentials provide a framework in which the parameters determining the nature and effect of this interaction can be discussed.

In low-permeability clay formations, the pore geometry may be very important causing to very high capillary pressures. This means that gas can in many cases not enter to the pores without the dilation of the pores. The capacity of the pores to support gas flow may be dependent not only on the dilation of flow channels by elevated gas pressures but also on the creation of gas flow channels by micro-fracturing of the medium.

The solution of the gases in the water (local or injected) introduces the potential for advection and diffusion of dissolved gas to contribute to the transport of the gases from and within the repository.

Taking into account of the transport by advection and dispersion-diffusion, the mass flux of a dissolved gas component in the aqueous phase can be given by:

$$q_{cw} = c_{cw}Q_w + D_{cw}\nabla c_{cw} \quad (5-4)$$

where q_{cw} is the mass flux of the component c in the aqueous phase w ($\text{kg m}^{-2}\text{s}^{-1}$) and D_{cw} is the diffusion –dispersion tensor for component c in the aqueous phase w (m^2s^{-1}). In practice the dispersion is the other factor that changes the concentration profile at the advection front; however the flux will not be differed from the dispersion. The following equation is the generally assumed dispersion tensor for an isotropic porous medium fully saturated with phase f :

$$D_{cf} = (d_{cf} + \alpha_{fT}Q_f)I + (\alpha_{fL} - \alpha_{fT})\frac{Q_f Q_f^I}{Q_d} \quad (5-5)$$

where d_{cf} is the molecular diffusion coefficient for component c in phase f within the porous medium (m^2s^{-1}) and α_{fL} , α_{fT} are longitudinal and transversal dispersion coefficient, respectively, for phase f and I is the unit tensor.

5.1.2 Heat Flow

As discussed in previous sections also heat effects are especially important on the transport phenomena in clay formations. Heat transfer in clay formations occurs by conduction and convection due to the advection of water and gas and by means of vapour/gas diffusion driven by vapour/gas pressure gradients. Soil sciences studies have demonstrated that vapour diffusion in porous media can be considerably enhanced compared to diffusion of non-condensable gases due to pore level phase change effects.

The heat flux consisting of conductive and convective components is given by:

$$Q = -\lambda \nabla T + \sum_f h_f q_f \quad (5-6)$$

where Q is the heat flux [$\text{J m}^{-2}\text{s}^{-1}$], λ is the thermal conductivity of the rock-fluid system [$\text{Js}^{-1}\text{m}^{-1}\text{K}^{-1}$], T is the temperature [K], h_f is the specific enthalpy in the phase f [J kg^{-1}] and q_f is the mass flux of the phase f [$\text{kg m}^{-1}\text{s}^{-1}$].

The dependence of the thermodynamical (solubility of the species, densities, chemical-kinetic constants, diffusion properties) thermophysical (viscosities, heat capacities, heat transport parameters, etc) and geomechanical (swelling-compaction properties, mechanical constants, creeping, etc) on the temperature should be taken into account by applying the corresponding formulations.

5.1.3 Conservation Laws

The basic law of conservation can be applied for describing the mass and energy transfer in clay formations. This is based on making a balance between the inputs and outputs of the system elements.

The mass balance can be formulized as follows:

$$\frac{\partial}{\partial t} \left[\phi \sum_f S_f c_{cf} \right] = - \sum_f \nabla q_{cf} + x_c \quad (5-7)$$

where ϕ is the porosity and x_c is the rate of production or lost of component c [$\text{kg m}^{-3}\text{s}^{-1}$].

The corresponding equation for energy conservation is:

$$\frac{\partial}{\partial t} [(1 - \phi) \rho_R c_R T + \phi \sum_f S_f \rho_f u_f] = \nabla \cdot G + \zeta \quad (5-8)$$

where ρ_c is the grain density of the rock [kg m^{-3}], c_R is the specific heat of the rock [$\text{J kg}^{-1} \text{K}^{-1}$], u_f is the specific internal energy of the phase f [J kg^{-1}] and ζ is the rate of heat production or loss per unit volume [$\text{J m}^{-3}\text{s}^{-1}$].

5.1.4 Chemical Balance

The reactive transport and physico-chemistry makes an obvious part of modelling of gas movement in clay formations. For representing a geochemical system, the mostly preferred way is to select a number of aqueous species as basis species (or component or primary species). All other species are called secondary species that include aqueous complexes, precipitated (mineral) and gaseous species. The number of secondary species must be equal to the number of independent reactions. Any of the secondary species can be represented as a linear combination of the set of basis species such as

$$S_i = \sum_{j=1}^{N_C} v_{ij} S_j \quad i = 1, \dots, N_R \quad (5-9)$$

where S represent chemical species, j is the basis species index, i is the secondary species index, N_R is the number of reactions (or secondary species), and v_{ij} is the stoichiometric coefficient of j^{th} basis species in the i^{th} reaction. Chemical processes to be considered in modelling of chemical processes in a clay repository can be cited as follows:

Aqueous complexation: These reactions are assumed to be at local equilibrium. By making use of the mass action equation to the dissociation of the i^{th} aqueous complex concentrations of aqueous complexes can be expressed as functions of the concentrations of basis species:

$$c_i = K_i^{-1} \gamma_i^{-1} \prod_{j=1}^{N_C} c_j^{\gamma_j} \gamma_j^{\gamma_j} \quad (5-10)$$

where c_i is molal concentration of the i^{th} aqueous complex, and c_j is molal concentration of the j^{th} basis species, γ_i and γ_j are thermodynamic activity coefficients and K_i is the equilibrium constant.

Equilibrium mineral dissolution/precipitation: The mineral saturation ratio can be expressed as

$$\Omega_m = X_m^{-1} \lambda_m^{-1} K_m^{-1} \prod_{j=1}^{N_C} c_j^{v_m} \lambda_j^{v_{mj}} \quad m = 1, \dots, N_p \quad (5-11)$$

where m is the equilibrium mineral index, X_m is the mole fraction of the m^{th} mineral phase, λ_m is its thermodynamic activity coefficient (for pure mineral phases X_m and λ_m are taken equal to one), and K_m is the corresponding equilibrium constant. At equilibrium:

$$SI_m = \log_{10} \Omega_m = 0 \quad (5-12)$$

where SI_m is called the mineral saturation index.

Kinetic mineral dissolution/precipitation: Kinetic rates could be functions of non-basis species as well. Usually the species appearing in rate laws happen to be basis species. In this model, we use a rate expression given by /LAS 04/:

$$r_n = f(c_1, c_2, \dots, c_{N_c}) = \pm k_n A_n |1 - \Omega_n^\theta|^n \quad n = 1, \dots, N_q \quad (5-13)$$

where positive values of r_n indicate dissolution, and negative values precipitation, k_n is the rate constant (moles per unit mineral surface area and unit time) which is temperature dependent, A_n is the specific reactive surface area per kg H₂O.

Effect of the dissolution/precipitation on the petrophysical properties: Porosity changes in matrix and fractures are directly tied to the volume changes as a result of mineral precipitation and dissolution. The molar volumes of minerals created by hydrolysis reactions (i.e., anhydrous phases, such as feldspars, reacting with aqueous fluids to form hydrous minerals such as zeolites or clays) are often larger than those of the primary reactant minerals; therefore, constant molar dissolution-precipitation reactions may lead to porosity reductions. The porosity of the medium (fracture or matrix) is given by:

$$\phi = 1 - \sum_{\mu=1}^{v_\mu} \phi \rho_\mu - \phi \rho_v \quad (5-14)$$

where v_μ is the number of minerals, $\phi \rho_\mu$ is the volume fraction of mineral μ in the rock ($V_{\text{mineral}}/V_{\text{medium}}$, including porosity), and $\phi \rho_v$ is the volume fraction of non-reactive rock. As the $\phi \rho_\mu$ of each mineral changes, the porosity has to be recalculated at each time step. The change in porosity can be converted to the change in other petrophysical properties namely permeability and capillary pressure and for this purposes numerical correlations found in the literature (Kozeny-Karman, cubic law, etc) can be applied.

Gas dissolution/exsolution Reactions involving aqueous and gaseous phases are usually assumed to be at equilibrium. According to the Mass-Action Law, the following equation is given:

$$p_f \phi_f K_f = \prod_{j=1}^{N_c} c_j^{v_j} \gamma_j^{v_j} \quad (5-15)$$

where subscript f is gas index, p is the partial pressure (in bar), ϕ is the gas fugacity coefficient. The gaseous phase for low pressures (in the range of atmospheric pressure), is assumed to behave like an ideal mixture, and the fugacity coefficient ϕ is assumed equal to one. At higher temperatures and pressures the assumption of ideal gas and ideal mixing behaviour is not valid, and the fugacity coefficients should be corrected according to temperatures and pressures. For example, for the H₂O-CO₂ mixtures in boiling conditions, it is mostly assumed that H₂O and CO₂ are real gases, but their mixing is ideal. The fugacity coefficient as well as the ionic activity coefficient of CO₂ can be calculated with the aid of semi empirical correlations.

Cation exchange: Cation exchange takes place when free cations in solution exchange with interlayer cations. This process can be described as an equilibrium reaction between an exchangeable cation and an exchange site. The equilibrium constant is usually known as the exchange coefficient because its value depends on the ionic strength of the solution. A general expression for cation exchange reactions according to the Gaines-Thomas convention is /XUT 06/:



where v_i and v_j are the stoichiometric coefficients (equal to their charges) of dissolved and interlayer cations, respectively; S_i and S_j denote dissolved cationic species and $(x_{vj}-S_j)$ and $(x_{vi}-S_i)$ represent exchange sites or exchange interlayer cations. The detailed description of the modelling of chemical processes are given in related literature /XUT 06/.

5.1.5 Recapitulation of the Basics

The basic formulations used for modelling gas transport in clay formations and its coupling with potential creating thermal and chemical processes as discussed in Chapter 4 and 5 are summarized in Table 5-1 with corresponding Equations. In many of the cases considered in this Table there exists one than more modelling attempts that are acceptable for various cases. If one than more formulation exists which is mostly for determining the petrophysical parameters, only one of them –the mostly applied- is introduced, some others are only cited.

Table 5-1: Recapitulation of the basic modelling formulations of gas transport in clay formations

Process, Method	Equation	Comment
Advection		
Fluid flow velocity, one phase,	$\vec{v} = -\frac{k}{\mu} (\text{grad } p - \rho \vec{g})$	Darcy Law, with SI units k is m^2 , v is $\text{m}^3 \text{s}^{-1}$, μ Pa•s and p Pa. <i>Valid only under Darcy assumptions</i>
Fluid flow velocity, multi-phase	$\vec{v}_i = -\frac{k k_{ri}}{\mu} (\text{grad } p - \rho_i \vec{g})$	For the phase i , k_{ri} relative permeability to the phase i
Fluid flow rate, flow through fractures	$q = -\frac{b^3}{12\mu} \frac{dp}{dl}$	Hagen-Poiseuille Eq. b is the aperture of the fracture <i>Equations exist in the literature depending on the geometry and configuration of the fractures and cracks</i>
Continuity Eq.	$\text{div}(\rho \vec{v}) + \phi \frac{\partial p}{\partial t} = 0$	Porous medium rigid, isothermal

Process, Method	Equation	Comment
Conservation Eq.	$\frac{\partial}{\partial t} \left[\phi \sum_f S_f c_{cf} \right] = - \sum_f \nabla \cdot q_{cf} + x_c$	x_c is the sink/source term
Retardation Factor	$R = \left[1 + \frac{(1-\phi)\rho_g K_d}{\phi} \right] = \left[1 + \frac{\rho_d K_d}{\phi} \right]$	K_d is the distribution coefficient
Petrophysical, Phase properties		
Porosity, Absolute permeability, Fracture permeability	$\phi = \frac{V_p}{V}$ $k = \frac{q \cdot \mu}{A dp}$ $k = \frac{N g b^3}{12f} \text{ (for N fractures)}$	Permeability definition after Darcy Equation, for flow through fractures or heterogeneous formation structure (layered, cross-linked) the permeability is calculated taken the geometry into consideration
Porosity-permeability relationships	$K = \left[\frac{\phi^3}{(1-\phi)^2} \right] \left[\frac{\rho_w g}{\tau^2 (\rho_s S)^2 C_s \mu_w} \right]$	Kozeny-Karman based Many correlations exists in the literature such as cubic law
Relative Permeability to water (liquid) and to gas	$k_{rw} = (S_w^*)^{\frac{2+3\lambda}{\lambda}}$ $k_{rg} = (1 - S_w^*)^2 \left(1 - (S_w^*)^{\frac{2+\lambda}{\lambda}} \right)$ $k_{rl} = \sqrt{\bar{S}_l} \left[1 - \left(1 - \frac{S_{gr}}{1 - \bar{S}_l^\Delta} \right) \left(1 - (\bar{S}_l + \bar{S}_{gr})^{\frac{1}{m}} \right)^m \right]^2$ $- \left(\frac{\bar{S}_{gr}}{1 - \bar{S}_l^\Delta} \right) \left(1 - (\bar{S}_l^\Delta)^{\frac{1}{m}} \right)^m$ $k_{rg} = (1 - \bar{S}_l - \bar{S}_{gr})^{\frac{1}{3}} \left(1 - (\bar{S}_l + \bar{S}_{gr})^{\frac{1}{m}} \right)^m$	Corey-Brook correlation Parker-Lenhard correlation <i>There exists many other correlations for gas-water relative permeability curves such as Core, Grant et al.</i>
Entry pressure, threshold pressure	$p_t = 5,874 \times 10^{-6} \left[\frac{1}{k} \right]^{0,33}$	Empirical or semi-empirical correlations as function of permeability
Capillary pressure	$p_c = - \frac{1}{\alpha^\gamma} \left[\left(\frac{S_l - S_{lmin}}{1 - S_{gr}^\Delta - S_{lmin}} \right)^{\left(\frac{n^\gamma}{n^\gamma - 1} \right)} - 1 \right]^{\left(\frac{1}{n^\gamma} \right)}$	Van Genuchten Eq. <i>Many other semi empirical correlations exist in the literature such as Leverett, Corey-Brooks, Pickens et al.</i>
Gas phase behaviour	$p = \frac{ZnRT}{V}$ $p = \frac{RT}{v-b} - \frac{a(T)}{v^2 + 2bv - b^2}$	Real gas law, Peng-Robinson EOS <i>There exists many other empirical and semi-empirical relationships such as Redlich-Kwong, Zudkevich-Joff</i>
Gas-liquid equilibrium,	$p_a = K_h x_h, \quad p_g = p_a + p_v$	Fugacity concept, Partial pressure and Henry Law for the dissolution of gases in liquid

Process, Method	Equation	Comment
Gas solubility in water, brine	$K_a = \frac{p_a M_a}{H M_w}$ $\frac{1}{K_a} = 110^{-10} + \frac{N_m}{5} \left[\frac{1}{410^{10}} - 10^{-10} \right]$	Air solubility in brine, K as function of partial pressure, p_a , molecular weights, $M_{a,w}$ or mixture molarity, N_m after Henry's Law /ZAH 04/ /PRU 99/. Various semi empirical formulations exist in the literature
Solution and gas properties density, viscosity, enthalpy	$\rho_w = 62,368 + 0,4386 S + 1,6 \cdot 10^{-3} S^2$	Density of brine with NaCl equivalent salinity, S , as weight percent /CAI 90/. Many correlation exist in the literature
Dispersion-Diffusion		
Mass flux of a dissolved gas	$q_{cw} = c_{cw} Q_w + D_{cw} \nabla c_{cw}$	
Dispersion	$D_{cf} = (d_{cf} + \alpha_{fT} Q_f) I + (\alpha_{fL} - \alpha_{fT}) \frac{Q_f Q_f^I}{Q_d}$	Dispersion tensor for an isotropic porous medium
Diffusion coefficient	$D_g(p, T) = D_c(p_0, T_0) \frac{p_0}{p} \left[\frac{T + 273,15}{273,15} \right]^\theta$	Diffusion coefficients for gases depending on pressure and temperature
Thermal Processes		
Heat Flux	$Q = -\lambda \nabla T + \sum_f h_f q_f$	Conductive and convective heat flux for the phase f
Energy conservation	$\frac{\partial}{\partial t} \left[(1 - \phi) \rho_R c_R T + \phi \sum_f S_f \rho_f u_f \right] = -\nabla Q + x$	For rock of density, ρ , specific heat of c
Thermal properties	$\lambda = -0,6 + 0,6 \rho_b + 0,004 w \rho_b^3 + 0,01 \sqrt{T}$	Empirical heat conductivity [W/mK] for a bentonite buffer as function of bulk density, ρ_b [kg/m ³], water content, w [%] and temperature, T [°C]. Empirical relationships for Rock heat capacity, specific heat conductivity.
Chemical processes		
Chemical balance	$S_i = \sum_{j=1}^{N_C} v_{ij} S_j \quad i = 1, \dots, N_R$	For the species S
Aqueous complexation	$c_i = K_i^{-1} \gamma_i^{-1} \prod_{j=1}^{N_C} c_j^{\gamma_j} \gamma_j^{\gamma_j}$	where c_i is molal concentration of the i^{th} aqueous complex, and c_j is molal concentration of the j^{th} basis species, γ_i and γ_j are thermodynamic activity coefficients and K_i is the equilibrium constant.
Dissolution/Precipitation	$\Omega_m = X_m^{-1} \lambda_m^{-1} K_m^{-1} \prod_{j=1}^{N_C} c_j^{\nu_m} \lambda_j^{\nu_m} \quad m = 1, \dots, N_p$	where m is the equilibrium mineral index, X_m is the mole fraction of the m^{th} mineral phase, λ_m is its thermodynamic

Process, Method	Equation	Comment
		activity coefficient and K_m is the corresponding equilibrium constant.
Porosity-permeability-capillary pressure change	$\phi = 1 - \sum_{\mu=1}^{v\mu} \phi \rho_{\mu} - \phi \rho_v$	The change in porosity is calculated based on the change in mineral volume, the relationship between porosity and other petrophysical properties are calculated with corresponding correlations.
Advection-Dispersion Eq. (One dim.)	$\frac{\partial C}{\partial t} = D_h \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} - G$	To account the effect of chemical reactions on advection-dispersion in a homogeneous porous media with G source-sink term and D_h as hydrodynamic dispersion
Adsorption	$c = \frac{k_1 C}{1 + k_2 C}$	Langmuir isotherm with coefficients k Freundlich or other semi empirical isotherms can be used

The basic formulations given in Table 5-1 are validated and applied approaches of the transport modelling in geologic media. As indicated before, this table does not and could not include all of the models presented in the corresponding literature for calculating the phase behaviour of the existing fluids or petrophysical properties of the transport media. The equations on these features are given exemplarily based on the mostly applied ones. The mechanical processes and properties are not included in this Table because a coupling of the geomechanics to the thermo-hydro-chemical coupling is not a priori and includes more difficulties and varieties consisting of formulation and validation. The primary and obvious effects in terms of geomechanics in clay formations are compaction and swelling. The mechanical disturbance of EDZ's, on the other hand is one of the most investigated problems in the framework of safety analysis. It is affirmed that the mechanically influenced and increased permeability of the near repository zone may change the transport considerations significantly for all host rock types. The possible induced permeability changes in EDZ of clay formations are experimentally and theoretically investigated.

The following chapters deal with the efforts on the physical modelling of the gas transport in clay formations and their numerical applications. Performing this, a principal classification due to clay formation types is avoided while the affirmed approaches are not always case specific. The modelling attempts are reported under the representative title, they can be applied for both plastic and indurated clays. The modelling attempts of EDZ's are examined in an individual chapter. The last section covers the modelling attempts for bentonite buffers. The so presented section ranking does not match with the natural analogy of gas transport beginning from waste to surrounding buffer material. A significance based ranking has been applied. It should also be noted that the reported modelling attempts includes only the key features and their up-to date applications. The completed formulations are found in the cited references.

5.2 Transport in Clay Formations

As discussed previously, several mechanisms can contribute to gas transport in clay formations. The relative importance of the mechanisms for any given situation depends on several factors, including the pore water pressure, which determines the solubility of the gas, the confining stresses, the microstructure and texture of the rock, the intrinsic permeability of the rock, and the rate of increase of gas pressure with time. The phenomenological description of the transport mechanisms for clay formations are made by NAGRA on the basis of Opalinus Clay and illustrated as given in Figure 5-1 coupled with geomechanical and transport considerations /MAR 05/. The background provided in this project supports this conceptualization. Therefore it seems to be a rational way of generalizing these mechanisms for all types of clay formations. These include:

Advection and diffusion of dissolved gas: At gas production rates likely to occur in a repository in Opalinus Clay, neither advection nor diffusion are capable of transporting dissolved gas away from emplacement tunnels sufficiently rapidly that a gas phase is prevented from forming. The validity of this assumption is supported with modelling studies of gas generation and transport for other repository systems /ALK 06/. As explained in previous sections the transport of the dissolved is characterised by three fundamental laws. The advective groundwater flow is governed by Darcy's law. Fick's law represents the diffusion of dissolved gas due to concentration gradients in the porewater and Henry's law describes the solubility of gas in porewater. The transport of dissolved gas occurs even at low (total) gas pressures; the pressure-dependent dissolution of gas in porewater and the increased groundwater flux causes the specific flux of the dissolved gas to increase with an increase in the gas pressure. The main parameters affecting the transport behaviour of dissolved gas are Henry's coefficient, the diffusion coefficient in water, the tortuosity, the accessible porosity and the hydraulic conductivity. The low hydraulic conductivity of clay rock significantly restricts the efficiency of this transport mechanism.

Two-phase flow: When the gas pressure exceeds the threshold for two-phase flow (pore pressure of 6,5 MPa plus gas entry pressure), leakage of gas into the Opalinus Clay takes place. This process is non-dilatant, i.e. the intrinsic properties of the rock are not affected by the gas transport process. In a geomechanical sense, the rock mass behaves like an elastic medium, characterised by the porosity and the rock compressibility. The controlling factor for the two-phase flow characteristics of a porous medium is the gas entry pressure. Once the gas entry pressure has been exceeded, the gas mobility is controlled mostly by the intrinsic permeability k of the formation, the permeability-saturation relationship (relative permeability), and the relationship between the capillary pressure and the water saturation (suction or water retention curve). Another possibility for two-phase flow is the exceeding of the saturation pressure of the solution in which gas is dissolved. Regarding thermodynamical considerations (Chapter 4.2), the decreasing solubility of the gases in the solutions with higher ionic strength should be reminded.

Pathway dilation: If gas pressure increase further because two-phase flow cannot transport gas quickly enough, then microscopic gas pathways may form. Clay-rich rock cannot withstand long-term gas pressures with a magnitude greater than the minimum principal stress acting on the rock mass. Due to the expected microscale variability of the geomechanical

rock properties, it even seems plausible that microfractures will form before the level of minimum principal stress is reached. This is a dilatant and slow process, in which the gas generation rate is compensated by the creation of new pore space. As discussed in /NAG 02a/, this may occur simultaneously with two-phase flow, as both these transport mechanisms are sensitive to microstructural and textural characteristics of the rock.

Formation of macroscopic gas fracs (tensile mode): Tensile gas fracs are to be expected when the pressure build-up in the rock is rapid, in which case microscopic pathway dilation cannot keep up with the gas production rate. The macroscopic fracture is initiated quasi-instantaneously and propagates at about the velocity of a shear wave. Gas flow in such a macroscopic tensile fracture can be seen as a single-phase flow process. The propagation comes to a halt when the gas pressure in the fracture becomes less than the value of the minimum principal stress (shut-in pressure). Successful hydrofracs are characterised by a fracture transmissivity which increases the bulk permeability of the treated rock by many orders of magnitude. Macroscopic gas fracs require gas pressures in the order of the minimum tensile strength. At Benken, the frac pressure is 17,5 MPa /NAG 02a/. Macroscopic gas fracs cannot occur in the case of gas build-up in the repository, due to the slow increase in gas pressure, the effectiveness of other gas transport mechanisms and the low creep rate involved in pathway dilation.

Gas transport through low-permeability rock formations is controlled not only by the hydraulic and mechanical properties of the rock mass (intrinsic permeability, porosity, rock strength), but also by the gas pressure at the generation locus and the hydromechanical state of the rock (*i.e.* water saturation, pore water pressure, stress state). The complex hydromechanical processes are decomposed into a problem of transport of immiscible fluids and a geomechanical problem. The effect of gas transport on the hydraulic barrier function of the rock is highlighted for each of the transport mechanisms.

For a low-permeability, deformable medium, such as a clay, the large pressure gradients that may be required to sustain a particular flow may lead to significant deformation of the medium and hence the permeability that is dependent on the fluid pressure, p_g . This dependence may sometimes be most naturally expressed through one of the effective stress, σ_e . This is because of the pore pressure relative to the confining stress that is expected to be the major determinant of the dilation of the fluid flow channels.

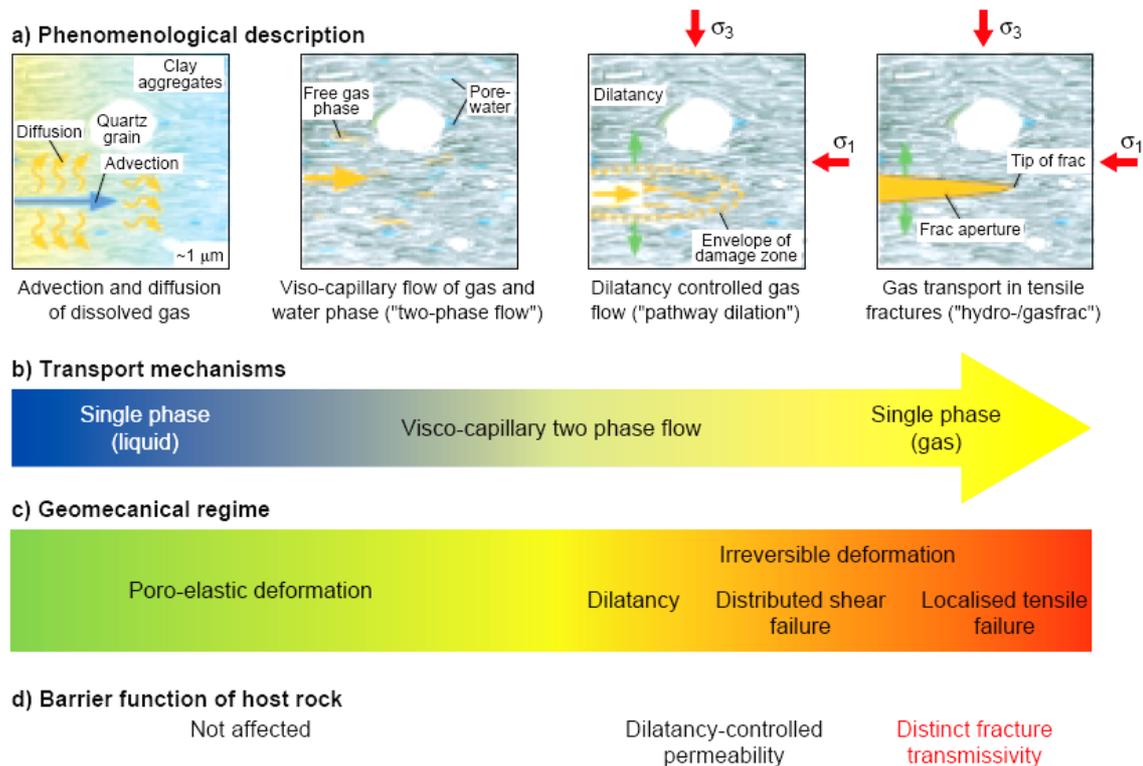


Figure 5-1: Analysis of the gas transport in Opalinus Clay /MAR 05/

5.2.1 Empirical Attempts

Experimental studies were conducted to investigate the gas transport properties of Boom Clay /ROD 99/. Gas flow measurements conducted in various equipments (uniaxial, triaxial permeameters, oedometers) were reported to make clear the migration processes through Boom and Pontida plastic clays under the effects of temperature and gas saturation. In a series of test, the gas breakthrough was investigated using a cell submitted to a uniaxial compaction up to a predetermined vertical (axial) stress (0,4 to 2,5 MPa). Various initial saturations were allowed. For saturated Pontida clay it was observed that the breakthrough pressure was proportional to the vertical stress. For saturated Boom Clay, the measured breakthrough pressure varied over a range (0,8 to 1,8 MPa) due to heterogeneity of the material. It was observed that once a gas pathway was created, increase in the vertical load had no influence anymore on the breakthrough pressure. For unsaturated clays (S_w up to 0,91 for Boom Clay and S_w up to 0,81 for Pontida Clay) gas flow was observed immediately at a gas overpressure of 10 kPa. The gas specific discharge was shown to be dependent on the inlet pressure, on the saturation and on the vertical stress. The following relationship was found for Pontida Clay:

$$q = (3,984 + 9,01 \times 10^{-4} \sigma_v) p_g^{(1,2348 - 4,29 \times 10^{-5} \sigma_v)} 17,663 \left[\frac{(S_t - S)}{S} \right] \quad (5-17)$$

where q is the gas discharge, $\mu\text{l s}^{-1}$, p_g the excess gas pressure, σ_v the vertical stress, Pa, S the saturation in the sample and S_t is the saturation limit below which the threshold pressure needed for the gas to penetrate the medium is equal to zero.

The effect of the temperature on gas transport behaviour in saturated and in unsaturated clay samples was determined in a series of experiments, performed in a triaxial cell. The saturation values were chosen as follows: 0,83 and 0,88 for Boom Clay and 0,91 for Pontida Clay (above the saturation limit). The global trend for saturated samples is that breakthrough pressure increases with increasing temperatures: for unsaturated samples, the gas specific discharge was found to be a function of the temperature and of the breakthrough pressure.

The influence of the stress and stress history on gas transport in Pontida Clay was also studied with the aid of a special designed centrifuge. The following observations were made:

- In a normally consolidated saturated soil, the breakthrough pressure increases linearly with the vertical effective stress.
- The soil stress history influences the breakthrough pressure since it modifies the state of effective stress (particularly the horizontal effective stress) and the strength of the soil. Overall, the breakthrough pressure increases for increasing overconsolidation ratios.

In quantitative hydrogeological studies it is implicitly assumed that rocks behave as linear elastic porous media. This means that the decrease in pore volume at fixed total stress is directly proportional to the decrease in pore pressure and is fully-recoverable if the pore pressure subsequently increases. Until quite recently this assumption was unchallenged, even when the theory was applied to rocks which are known to exhibit pronounced nonlinear, inelastic, non-recoverable, shear-dilatant or time-dependent responses (e.g. chalks, clays and most mudrocks). Although departures from the idealized responses of the linear elastic medium may have significant implications in transient flow modelling, the role of the interparticle physicochemical forces in determining the volumetric responses of compact clays is of fundamental importance in understanding and predicting the movement of the fluids. Water is the obvious part of modelling of gas transport in clay formations and therefore the thermo-chemo coupling is necessary to be able to construct a representative modelling study. The disjoining pressure, for example, determined by the difference in chemical potential between the molecularly-thin interparticle water films of a compact clay and the chemical potential of water in an external free solution plays an important role by determining the transport potentials /HOR 96/. The implications of the physicochemical forces to fluid flow is summarized in /HOR 96/. The introduction of the poroelastic theory (Biot's theory) on the models of the colloidal interaction between clay mineral particles, water and solutes is a key aspect for mass transport in compact clays.

5.2.2 Consolidation after Terzaghi

Terzaghi's theory is commonly used for the description of consolidation and compaction processes in saturated low-permeability soils (e.g. clay) due to extended load acting on such

a medium. The deformation of a finite volume of porous medium involves the compressible behaviour of both the solid matrix and the pores. Changes in the volume can be induced by changes in the internal fluid pressure p or an externally imposed stress σ . In /KOS 04/ a horizontal plane of area A embedded within a saturated porous media is considered. Any changes in the load on A should be essentially one-dimensional and vertical. The total load on A consists of the weight W of rock, soil, water, and atmosphere overlying this plane. The total stress on σ on A is therefore equal to W/A . The plane A intersects both the solid matrix and the pores. In a static case the total stress must be balanced by interparticle stresses and fluid pressure. Terzaghi uses the term effective stress to describe the stress that is only transmitted in the solid phase as opposed to the pressure p of the fluid that is filling the pores/TER 48/. The total stress σ is therefore composed of the effective stress σ_e and the fluid pressure: $\sigma = \sigma_e + p$. Then, changes in the effective stress, which lead to changes in porosity, can be induced by altering either the total stress or the fluid pressure, or both. The phenomenon of consolidation is associated with the outflow of interstitial water contained in the medium (soil, rock, clay). The load applied to the medium, which in case of glaciation is the additional load of an ice sheet, is absorbed by the solid phase (increase in effective stress) and partly by the interstitial water (increase in fluid pressure). During consolidation the external load, as well as the resulting total stress remains constant. At the beginning of the loading the excess load is completely absorbed by the pressure p . The increase in pressure starts a transient outflow of interstitial water and the load is gradually transformed into increased effective stress σ_e until the system is equilibrated again. The loss of fluid allows the consolidation. Terzaghi's theory of consolidation assumes that:

$$\nabla^2 p = \frac{(1-\phi)\alpha\rho_f g}{K} \frac{\partial p}{\partial t} \quad (5-18)$$

In this Equation α is the compressibility coefficient [$L T^2 M^{-1}$], p is the pressure [$M L T^{-1}$], ϕ is the total porosity [-], ρ_f is the fluid density [$M L^{-3}$], g is the gravitational acceleration [$L T^{-2}$], K is the hydraulic conductivity [$L T^{-1}$], and t is the time [T]

The coefficient C_v is called consolidation coefficient [$L^2 T$] and given by:

$$C_v = \frac{(1-\phi)\alpha\rho_f g}{K} \quad (5-19)$$

The factor $(1-\phi)$ can be neglected if it is close to 1.

Terzaghi and Peck (1948) give a one-dimensional analytical solution (equal to the standard solution for a diffusion/conduction problem) for the evolution of the pressure field $p(z,t)$ with the depth z and over the time t , /TER 48/. The pressure change is described by a step function $\Delta p(z,t)$. At $t=0$ the initial pore pressure p_0 applies onto the whole domain; for $t>0$ the pressure at the boundaries ($z=0$ and $z=2H$) equals zero. H is introduced as the half thickness of the clay layer.

$$p(z,t) = \frac{4p_0}{\pi} \sum_{n=0}^{\infty} \frac{1}{2m+1} \sin \frac{(2m+1)\pi z}{2H} \exp \frac{-(2m+1)\pi z}{2H} \exp \frac{-(2m+1)^2 \pi^2 T_v}{4} \quad (5-20)$$

A solution for the Darcy flux $v_D(z,t)$ in a medium with a hydraulic conductivity K_z in z direction is derived from this equation and is presented in /KOS 04/. The presented model is also coupled with mathematical formulations of the flow in fractures within the code FRAC3DS and tested for one-dimensional modelling of transport through Opalinus Clay. The diffusion dominated transport is modelled under various initial and boundary conditions. The main disadvantage of the model is the consideration of one-phase flow in which only the dissolved gas can be modelled.

5.2.3 Transient Flow in a Deforming Poroelastic Medium

The mathematical framework for the analysis of transient flow in a saturated, linear elastic, porous medium is provided by Biot's theory of three-dimensional consolidation /BIO 41/. A formulation of the theory for clay formations is made in /HOR 96/. Assuming that a porous medium is mechanically isotropic, relatively incompressible, and its volumetric strain ε_V , can be described by the linear thermoelastic constitutive equation:

$$\varepsilon_V = -\frac{\Delta V}{V_0} = \frac{1}{K}(\sigma_m - \frac{K}{H}p_w) - \alpha_b(T - T_0) \quad (5-21)$$

The introduction of this Eq. into the Darcy Equation leads to

$$\frac{1}{Q} \frac{\partial p_w}{\partial t} = \frac{\nabla(K\nabla\Psi_t)}{g} + \xi \frac{\partial \varepsilon_V}{\partial t} + (\xi\alpha_b + \alpha_m) \frac{\partial T}{\partial t} \quad (5-22)$$

where K is the drained bulk modulus, H , Q and ξ = Biot's poroelastic constants, α_b and α_m , are thermal expansion coefficients, p , is pore pressure, σ_m is the mean normal total stress ε_V is the volumetric strain, and T is temperature. The term $(\nabla(K\nabla\Psi_t))$ is the volumetric flux of water written in terms of Darcy's law for compressible flow where K is the hydraulic conductivity tensor and Ψ is the total potential defined by Darcy Equation. With some assumptions and simplifications (the compressibility of the rock β is the inverse of the drained bulk modulus ($\beta = 1/K$), β_w , is the compressibility of the pore water, the compressibility of the rock is substantially greater than that of the mineral solids) transient formulation of the flow equation reduces to:

$$\nabla^2 h + \frac{\beta \partial \sigma_m}{\partial t} = \frac{\rho_w g (\beta + n\beta)}{K} \frac{\partial h}{\partial t} \quad (5-23)$$

Assuming that the stress does not change with time (stable boundary conditions)

$$\nabla^2 h = \frac{\rho_w g (\beta + n\beta)}{K} \frac{\partial h}{\partial t} = \frac{S_s}{\partial t} \frac{\partial h}{\partial t} \quad (5-24)$$

where S_s , is the specific storage. This is then Jacob's equation. In the absence of any temporal changes in hydraulic head, this further reduces to $\nabla^2 h = 0$, which is known as the Laplace equation. This simple form is used in the calculation of the steady-state, gravitational component of regional groundwater flow. This modelling attempts, although addresses to one-

phase, liquid flow gives a theoretical overview on the modelling of transient and steady-state advection in poro-elastic medium as the case of clays. However, by adopting a poro-elastic model for the hydraulic responses of an argillaceous medium, the possibility that changes in shear stress might cause changes in porosity and consequential effects on local pore pressures is neglected.

5.2.4 A Thermo-Hydro-Plastic Coupling /LAL 02/

In a coupled model of the thermo-hydro-plastic behaviour of clay formation model, a saturated soil as a porous medium with two phases is considered: solid (assemblage of grains) and fluid (water). In the model external disturbances may be mechanical, hydraulic and/or thermal (three fields). Starting from a *microscopic level* where each phase is considered separately as a continuum, and using the homogenisation theory, a mathematical formulation for an equivalent continuum at a *macroscopic level* is derived /LAL 02/. The coupled equations obtained govern the evolution of pore pressure, solid displacement and heat flow under mechanical, hydraulic and/or thermal loading. The momentum conservation is given as the homogenized equilibrium equation as follows:

$$\nabla \sigma + \rho_{sat} g = 0 \quad (5-25)$$

Where σ is the total (Cauchy) stress tensor with tensile stresses taken as positive, ρ_{sat} the total average mass density ($= \phi \rho_f + (1-\phi) \rho_s$), with ρ_s , ρ_f the mass density of the solid and the fluid phase, respectively; ϕ is the porosity, g is the gravity vector. The divergence operator is defined as:

$$\nabla \sigma_{ij} = \sum_{ij} \partial_j \sigma_{ij} \quad i, j = 1,3 \quad (5-26)$$

The behaviour of the solid matrix is assumed to be governed by Terzaghi concept of effective stress. The stress tensor may be expressed in terms of the total strain tensor ε and the elasto-thermoplastic constitutive tensor D , thus the momentum conservation equation takes the form:

$$\nabla \{D : \varepsilon(u_s, T)\} - grad p + \rho_{sat} g = 0 \quad (5-27)$$

where u_s is the displacement vector of the total matrix and T the temperature, assumed to remain the same in both phases. The mass and energy conservation are expressed in the conventional way. The constitutive stress-strain relationship is assumed to be governed by a thermo-plastic model, the LTVP model is used. The LTVP model is a generalisation to non-isothermal conditions of the cyclic orthotropic elasto-plastic multi-mechanism model with kinematical hardening. It is known that contrary to the classical dilative behaviour of cohesionless porous media subjected to heating, clay behaviour shows an irreversible contraction response in some cases. This phenomenon is believed to be caused by a new arrangement of the internal structure of the clay and is more pronounced for higher initial void ratios. Based on numerous experimental results, it is possible to consider that temperature variation has three major effects on clays /LAL 02/:

- a reversible strain (dilation), a so-called “thermo-elasticity”, which is dominant in the case of a small overconsolidation ratio and can be assumed independent from the stress state,
- an irreversible strain (contraction), a so-called “thermo-plasticity”, a modification of mechanical behaviour; quantitatively, this corresponds to a continuous,
- variations of mechanical characteristics (e.g. stiffness, strength) with heat, and, qualitatively, it represents a transition to a more ductile behaviour.

When the free water cannot be drained out from the sample, the behaviour of the soil subjected to thermal loading is strongly affected. A consolidated, undrained sample submitted to heat shows a very small volume variation and an increase in pore pressure. This pore pressure increase results in an effective stress decrease under constant external forces. To represent these physical concept the thermo-elastic and thermo-plastic formulations of LTVP model is given in /LAL 02/. To illustrate the capacity of the LTVP model and to predict the major aspects of clay behaviour, the model is implemented in a finite element code. Two numerical simulations are performed for two plastic clay formations; Boom and Pontida. The main handicap of the model is the consideration of one-phase flow (saturated conditions).

5.2.5 Intermittent or Episodic Flow

The development of fractures and fissures during stress relief is well known in overconsolidated clay formations. Such fractures develop when the magnitude of one of the principal stresses becomes substantially less than the other components. These fractures often tend to be planer and are generally oriented so that the axis of the minor principal stress is normal to the fracture plane. They are probably associated with rupture of the fabric under extensile strain. It is important to note that extensile failure can occur even when all three of the principal stresses are compressive. The erosion and exhumation of a clay rock often leads to the development of natural sub-horizontal stress-relief fractures. Similar fractures are developed during tunnelling operations in fairly indurated clay rocks, where they tend to be oriented sub parallel to the tunnel walls. Because of the low stress acting normal to these discontinuities, extensile fracture are likely to act as conductive preferential pathways for the movement of groundwater and gases.

Fissures are small non-systematic joints that occur in most overconsolidated clays. The absence of shearing is though to be indicative of brittle (extensile) fracturing, suggesting that stress-relief due to erosion is important. How a fluid moves through a clay rock at a depth greater than the critical depth for pathway sealing is the situation of “forced-advection” alluded to the above discussions. The conceptual model of /HOR 96/ suggest that the pressure in the source reservoir will rise until the sealing criterion is no longer met and the incident flow pathways dilates (Figure 5-2, Figure 5-3). The flow rate along this pathway will then exhibit a highly nonlinear dependency on effective stress, with the flow rate increasing dramatically as the source pressure continues to rise. The flow to the sink will then drop off dramatically and it is possible that the source reservoir may become totally depressurized.

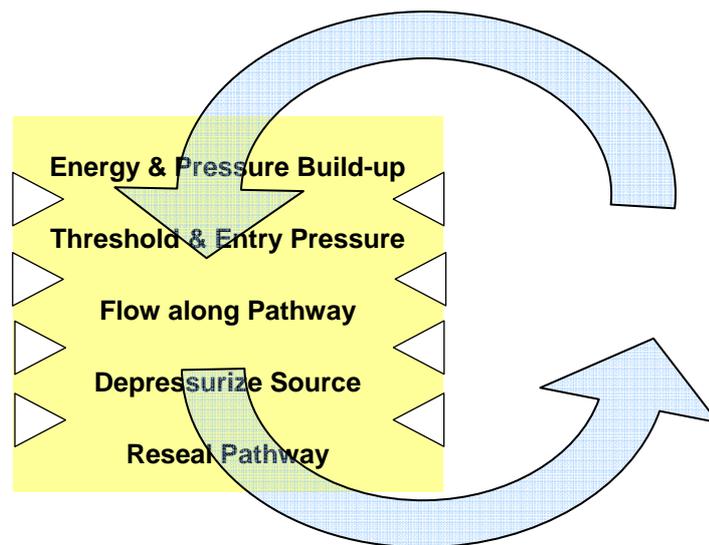


Figure 5-2: Schematic of intermittent flow processes

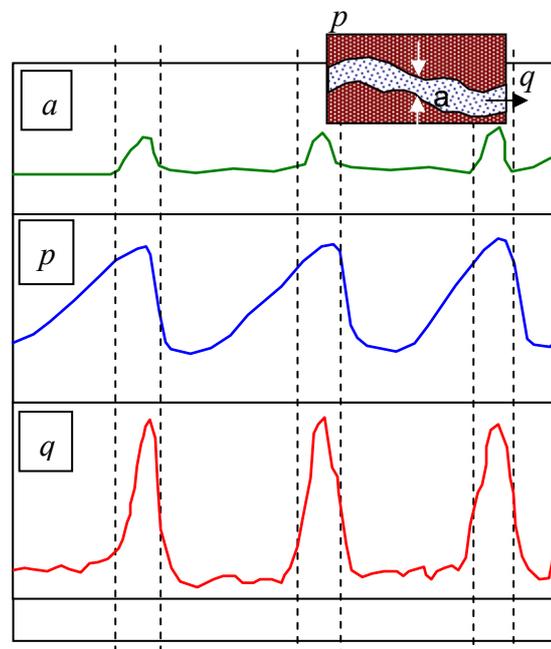


Figure 5-3: The changes of pressure (p), flow rate (q) and fracture geometry (a) during the intermittent flow processes

A simple modelling approach to pathway flow is given also by /HOR 96/ using the cubic law for determining the flow rate through a planar fracture (Eq. 4-39). The schematic of the considered model is given in Figure 5-4 in which the source and sink terms are determined with pressures p_1 and p_2 . It is assumed that the aperture of the pathway (fracture) is a function of the applied overburden (confining) stress (σ) and pore pressure (p_g):

$$b = f(\sigma - p_g) \quad (5-28)$$

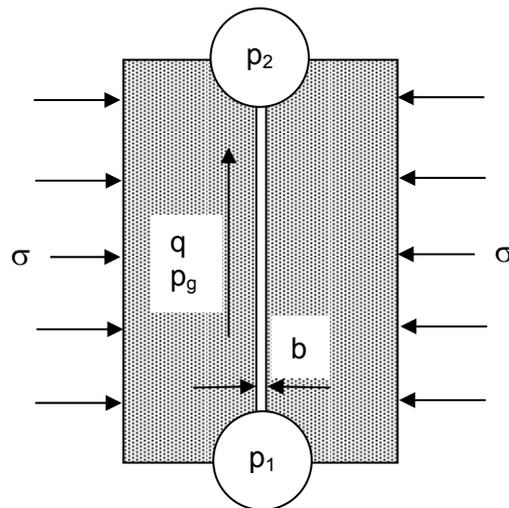


Figure 5-4: Simple conceptual model of pathway flow in clay formation
/HOR 96/

Following this concept a critical value of $(\sigma - p_g)$ is supposed which leads to total closure of the flow pathway with $b=0$. This is called as sealing criterion is written as:

$$q = 0 \quad \text{for} \quad (\sigma - p_g) > (\sigma - p_g)_{crit} \quad (5-29)$$

As fluid pressure gradually build up in the source reservoir, there will come a point at which the sealing criterion is no longer met and fluid starts to flow towards the sink. The introduction of the pathway aperture relationship into the cubic law makes the effective permeability of the pathway a highly nonlinear function of the local fluid pressure and stress distribution. The resulting flow law therefore exhibits both a threshold and nonlinearity. An increase in fluid (gas) pressure above the critical pressure leads to dilation of the flow pathway and a substantial increase ineffective permeability. This critical pressure is physically comparable with the threshold or entry pressure. The numerical application of the stress dependent pathway is easy if the flow through fracture is modelled by using a model depending on the geometry of the fractures.

However the modelling of the transport phenomena in clay formations only with formulation of flow in an idealized fracture is an obvious oversimplification. Some potential deficits of this assumption can be cited as follows:

1. Plastic yielding of stress-supporting asperities
2. Compaction of a clay-rich fault aperture under high effective stress
3. Swelling of the rock
4. Precipitation of minerals from in-situ or flowing liquid

The majority of these mechanisms are stress-dependent and mostly investigated as sealing capacity of the cap rocks. In petroleum reservoir engineering the sealing property of the shale caprocks are examined as pressure and capillary seals. In pressure sealing, the very

high pressure gradients acting on the caprocks inhibit the passage of the fluids totally. In the capillary sealing on the other hand, the seal is considered to be effective because the very fine pores of the shale lead to very high capillary pressures blocking the flow of the fluids totally. The recent investigations of the petroleum industry on the subject may allow therefore the development of the above given modelling concepts /BAZ 05/, /MAR 00/.

5.2.6 Capillary Bundle Model /ORT 96/

In capillary bundle model the porous media is assumed to compose from a series of non intersecting capillaries (Figure 5-5). The capillaries have a uniform radius of r , and the number of capillaries per unit cross sectional area of core. With radius in the range $[r, r+dr]$ is $N(r)dr$. The length of each capillary is τL where τ is known as the tortuosity factor. If it assumed that the portion of the capillaries filled with water is $R(r,t)$, with the assumption of the slow flow of water in the capillaries and introducing the capillary pressure concept, the position of the water $R(r,t)$ is calculated based on Navier-Stokes equation as follows:

$$R^2(r,t) = \tau^2 L^2 - \frac{t}{4\mu_w} (r^2 (P_g - P_w) - r\sqrt{2}\sigma) \quad (5-30)$$

This equation is valid in the region $0 \leq R(r,t) \leq \tau L$.

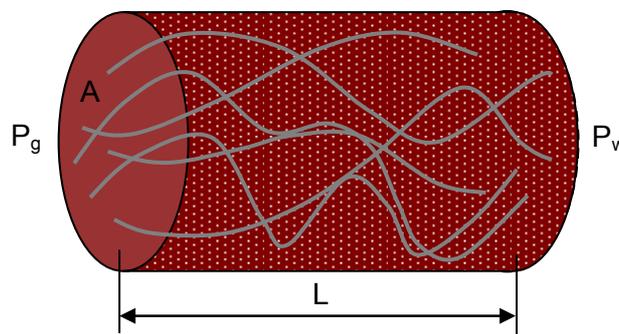


Figure 5-5: Capillary bundle model /ORT 96/

The gas pressure must exceed the water and capillary pressure combined in order for a capillary to start desaturation. The smallest capillary radius, r_s , which starts desaturation at given gas and water pressure, is given by

$$r_s = \frac{\sigma\sqrt{2}}{(P_g - P_w)} \quad (5-31)$$

Capillaries with radius smaller than r_s will remain totally saturated. At fixed gas and water pressure each capillary with radius greater than r_s will desaturate until gas breakthrough, which is when the length of the water filled part is zero. Hence at time t the largest capillary which contributes to the total flux of water from the capillaries has radius.

$$r_l(t) = \frac{\sigma + \sqrt{\sigma^2 + \frac{8\mu_w \tau^2 L^2 (P_g - P_w)}{t}}}{\sqrt{2}(P_g - P_w)} \quad (5-32)$$

Hence the total flux of water from the core is given by:

$$\Phi_w(t) = \int_{r_s}^{r_l} \Phi_w(r,t) N(r) A dr \quad (5-33)$$

After breakthrough in a capillary of radius r at time $t_b(r)$, the gas pressure distribution along the capillary reaches equilibrium at a rate controlled by conservation of mass and Darcy's law. The saturation profile of the core can be calculated at any point by summing the contribution of each capillary. At a point x along the core, the capillaries which contribute, must have $R(r_i, t) \geq \tau x$. Larger capillaries will be emptied beyond this limit. Hence at time t the largest capillary which contributes at the distance x along the core is

$$r_u(x,t) = \frac{\sigma + \sqrt{\sigma^2 + \frac{8\mu_w \tau^2 (L^2 - x^2)(P_g - P_w)}{t}}}{\sqrt{2}(P_g - P_w)} \quad (5-34)$$

The saturation $s(x,t)$ along the core is given by:

$$s(x,t) = \int_0^{r_u(x,t)} g(r) dr \left[\int_0^\infty g(r) dr \right]^{-1} \quad (5-35)$$

The numerical model, TOPAZ based on the above given formulation for two-phase flow through clay formations is used to simulate the experiments performed with Boom Clay core samples. It is affirmed that the comparison of the numerical results with the experimental data give good agreements. This provides support for the hypothesis that preferential pathways play a significant role in gas migration through Boom Clay. In reality, the method of gas transport may be combination of two processes, that is two phase flow and interfacial evolution within preferential pathways, but it is also significant that by using simple but realistic models for the pore radii distribution, one may produce results which show both qualitative and quantitative features of the experimental results.

Consideration of the geological and structural evidence suggests that the most appropriate model for the groundwater flow and solute transport for Boda claystone is a dual porosity model. The basic concept for this model is advection of groundwater and transport of solutes through a low permeability discrete fracture network coupled with diffusion of solutes into matrix. Thus the required parameters for advection include the hydraulic conductivities and porosities of both fractures and matrix. Parameters for diffusion and retardation of solutes within the claystone matrix include the effective diffusion coefficients, D_{eff} and distribution coefficients K_d for radionuclides that give significant release in PA. The efficacy of matrix diffusion in retarding radionuclide transport would depend on the extent to which diffusion-

accessible porosity is restricted by induration and the growth of secondary pore-filling minerals.

Key parameters that describe the geochemical environment within a clay rock matrix are the salinity, pH and Eh (or redox parameters) of pore waters. Other species that may influence the potential of the claystone pore water system to transport of radionuclides are the carbonate alkalinity or total inorganic carbon, dissolved organic carbon, microbial populations and the colloid concentration. Diffusion coefficients in indurated and cemented clay rock pore water system to transport of radionuclides are the carbonate alkalinity or total inorganic carbon dissolved organic carbon, microbial populations and colloid /BAT 05/.

5.2.7 Capillary Bundle Model with Geomechanical Effects

In some argillaceous media it could be argued that it is in fact geomechanical effects that are dominant because they control the form of the pathways. The gas may have to overcome the local effective stress to open or widen a micro-fracture. This opening will then be dynamically propagated through the medium, to form a preferential pathway held open by the gas pressure against the local effective stress along the pathway. Finally, when gas breakthrough occurs the gas pressure will drop and the pathway will close under the action of the effective stress. It may also be the case that in some media the gas migration is controlled by a mixture of capillary bundle model, which is called gas pathway generation model. The following discussion describes the mathematical formulation of the generic GPG model for a single pathway and discusses some initial results on simple material-specific formulation.

The model is based on generic formulation of gas pathway generation (GPG). It is assumed that the gas moves in the positive direction and that the gas pathway is radially symmetric. The GPG model is formulated by considering the forces acting at the interface between the pathway (assumed to be filled with gas) and the transport medium, which includes granular material (for example clay particles) and free or bonded pore water. The position of the gas-medium interface is given by $y=s(x,t)$, Figure 5-6)

For this model the balance of the forces that need to be overcome if the gas-medium interface is to move, whilst the drag term controls the rate at which the gas-medium interface propagation occurs. In this balance the forces acting normal to the gas –medium interface that need to be overcome if the gas-medium interface is lumped as σ_t , threshold tensor. These are for example capillary pressure and effective stress. The magnitude of the surface tension acting tangentially to the surface is also taken into account as force per unit length of interface F_t :

$$F(r,t) = P_g(x,t).n_N - \sigma(r,t).n_N + \frac{d(F_t.n_T)}{dx} \sqrt{1 + \left(\frac{\partial s}{\partial x}\right)^2} \quad (5-36)$$

Where n_T and n_N are the tangential and normal unit vectors to the gas-medium interface.

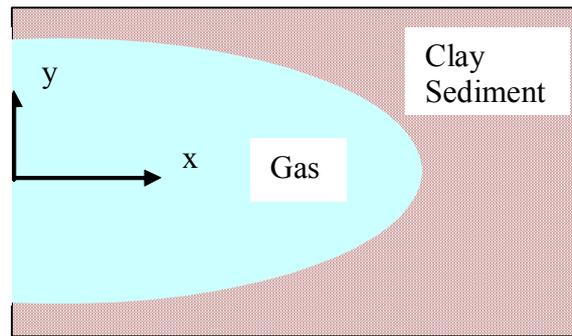


Figure 5-6: Propagation of gas in an idealized clay formation

Departing from this basic momentum conservation approach, with the assumption of constant surface tension and simple diagonal forms for the drag and generalized threshold tensor, the equation of motion for the infinitesimal section at position r can be written as function of time. In a further step the equation of motion of gas flow in the pathway itself which are derived from the mass conservation, gas flow and the gas equation of state. The gas velocity v is assumed to be governed by Stokes law for slow flow and the ideal gas law is used as an equation of state /IMP 96/.

$$\frac{\partial}{\partial t}(\rho s^2) = -\frac{\partial}{\partial x}(\rho s^2 v) \quad (5-37)$$

$$v = -\frac{\rho_g g s^2}{8\mu_g} \frac{\partial P_g}{\partial x} \quad (5-38)$$

where μ_g and ρ_g are the viscosity and density of the gas. The GPG model is tested and validated for some cases by considering the material specific parameters needed for the mass and momentum conservation equations. Two specific cases are studied:

1. Capillary pressure dominated pathways: In material such as sand or sand-bentonite mixtures it is likely that the action of capillary forces displacing pore water along pre-existing pathways will dominate the propagation of the gas-medium interface. In formulating the material-specific GPG model in this case, advantage can be taken of the fact that the pathways are existing pre-existing. The term s thus represents the pathway radius, which is constant in time vary along its length ($s=s(x)$)
2. Effective Stress Dominated Pathways: In an argillaceous medium, such as Boom Clay, it is apparent that the migration of gas is controlled by the effective stress. A simple approximation to this is to assume that the terms β^x and β^y are constant and the terms σ_x and σ_y in the generalized threshold tensor s can be approximated by:

These equations lead to the propagation of a gas pathway whose maximum width is given by:

$$s_{\max} = \frac{P_g(x,t) - \Sigma^y}{\lambda(x)} \quad (5-39)$$

For a given gas pressure the tip of the pathway will also move at a constant velocity. Preliminary numerical results showing the propagation of the gas-medium interface under constant pressure conditions are shown in Figure 5-7.

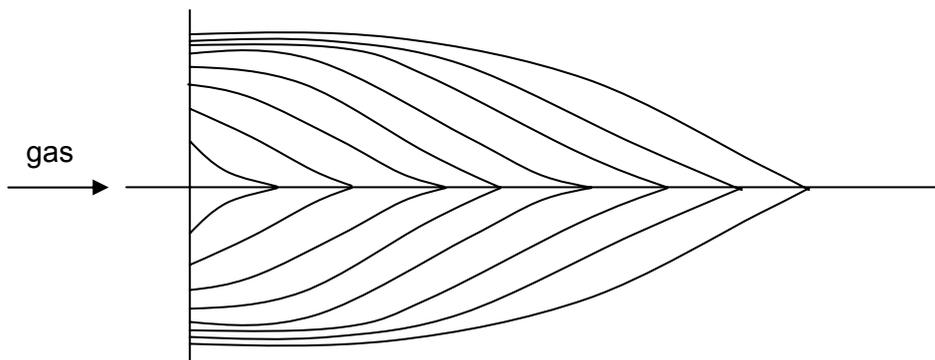


Figure 5-7: Propagation of a gas-medium interface overcoming effective stress, showing the interface at constant time intervals

The GPG formulation is extended to consider the displacement of free pore water. If the furthest point of the gas-medium interface $X(t)$ then the volume of the pathway is

$$\pi \int_0^{X(t)} s^2(x,t) dx \quad (5-40)$$

If the solid particles in the medium are assumed to be not compressed by water the volume of water displaced will equal the volume of the gas pathway, so the water flux will be:

$$\pi \frac{dX}{dt} s^2 + \pi \int_0^{X(t)} s \frac{\partial s}{\partial t} dx \quad (5-41)$$

Thus the fact that the gas-medium interface propagates at a constant speed means that water will be displaced at a constant rate before gas breakthrough, which is consistent with experimental observations. Further studies focusing on gaining greater understanding of the effective stress and drag terms, and validation of the model by reference to measurements of gas breakthrough times, expelled water volume before gas breakthrough and water saturation at breakthrough are however needed if further progress is to be made.

5.2.8 Crack Dilation Model /DUP 91/

A modelling approach was proposed to primary gas-oil migration in shales which can also be used especially the EDZ's in clay formations. The model takes the linear elastic fracture mechanics as the theoretical basis. Figure shows the layout of a crack dilation model for one-dimensional flow of gas through a core plug. The cracks are represented by ellipsoidal cavities with dimensions defined by semi-axes a, b and c . These parameters are regarded as suction-dependent variables. The cracks are arranged in a regular pattern. The scale is defined by a fixed characteristic distance, L . As a uniaxial case, an increase in suction can be represented by an equivalent radial tensile stress, σ , applied to the boundaries of the plug. The strain energy, W of the plug can be expressed as:

$$W = \frac{V}{E_c} \int_0^{\sigma} \sigma d\sigma = \frac{V}{E_c} \frac{\sigma^2}{2} \quad (5-42)$$

where E_c is the effective bulk modulus of the rock containing cracks and V is the volume of the core plug. This result can be derived from the Griffith theory of crack propagation which affirms that a crack propagates when the decrease in strain energy of the body containing the crack exactly balances the increase in the surface energy. If E_c is expressed as function of Young's modulus E of the intact rock as:

$$\frac{1}{E_c} = \frac{1}{E} + \frac{2\pi c^2}{hwE} \quad (5-43)$$

where h and w are the length of the rock and width of the crack successively. If the Eq. (5-43) is introduced to Eq. (5-42) the following equation is obtained:

$$W = \frac{V\sigma^2}{2E} + \frac{\pi c^2 \sigma^2 t}{E} \quad (5-44)$$

If the strain energy, W is expressed in terms of internal energy terms with the aid of adhesion theory, it can be affirmed that the maximum theoretical strength of an uncemented clay formation is equal to the cohesive strength of the interparticle water films. If the distance between water molecules is expressed as d_w , the crack propagation criterion can be relied to the gas entry phenomenon with the following expression:

$$\sigma = \frac{2\gamma_w}{\delta_w} \left(\frac{a}{c} \right) \quad (5-45)$$

affirming that gas can enter to the rock if the above given stress is reached. Note that in this equation γ_w can be taken as the interfacial tension of water-gas binary system. Analysis of the three-dimensional problem is quite complex and demands that the strain energy and the surface energy terms be expressed as functions of the semi-axes of the cracks. A possible relation of the effective gas permeability to the spatial density and dimensions of the cracks in the plane normal to gas flow is of primary importance.

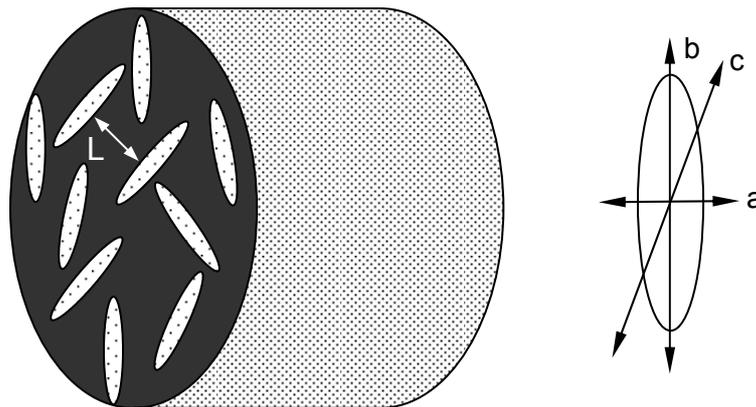


Figure 5-8: Schematic description of the crack dilatation model /DUP 91/

5.2.9 Multiple Front Propagation Model /NEA 96/

It is reported that due to the Project MEGAS experiments, gas flows in Boom Clay through a very limited number of preferential pathways and the saturation is always less than 5%. Moreover the influence exerted by the effective stress field or the presence of heterogeneities (anisotropy) seem to predominate in gas pathway formation and propagation. These paths are unstable and undergo successive opening and closure cycles depending on the local stress and gas pressure evolution.

It seems that the formation of a preferential pathway depends strongly on local discontinuities at the microscopic scale. Understanding the microscopic nature of clay particles is also very helpful in explaining the three modes of gas migration in clay that is diffusion or advection in solution, two-phase flow or flow through the formation of preferential ways.

As in the case of the implementation of the capillary bundle model described in the previous section, the multiple front propagation model has been designed to simulate laboratory gas migration experiments on cylindrical clay cores. This model is again based on the solution of mass conservation and Poiseuille flow equations for both fluids (wetting and non-wetting) and on the following equation for the advance through the clay of the tip of the propagating gas flow channel. The gas-filled pathways are assumed to dilate elastically for small displacements.

Each path i is constructed stochastically from a series of channel segments j . The number of paths is set by an input channel density $\Psi_{channel}$ and the area A of the core end face. Propagation of gas fronts along channels is allowed when the inlet gas pressure p_i exceeds the input threshold p_{start} and the front velocity v is positive. The front velocity along path i and channel j is modelled as:

$$v_{i,j}(t_n) = \left(\frac{1}{\beta} \right) \left[p_i(t_n) - p_{out} - p_{tension} \frac{r_{0,max}}{r_{0,i,j}} \right] \quad (5-46)$$

where β is the drag coefficient, $p_{tension}$ is a measure of the gas-gel surface tension. At any time t_n , a path with $v_{i,j}(t_n) < 0$ is assumed to have stopped. Fronts are propagated during each time step. During propagation, they may emerge at the outlet core face (breakthrough) or stop because they encounter a channel that is too narrow for propagation at the current inlet and outlet pressures. As the pressure change, stopped fronts may resume propagation. The radius of gas-filled channels behind it is all assumed to be at pressure p_i . However after breakthrough, the pressure throughout the open path is implicitly a function of the position along the clay core.

Also relevant to gas migration in plastic clays may be the preliminary development of a gas migration model for compacted bentonite in which pathway propagation and dilation is represented and an attempt is made to link the modelling approach to the development of understanding of the physical processes occurring.

5.2.10 Fluid Flow in Fractured System in Clay Rocks

As previously indicated tensile gas fracs are to be expected when the pressure build-up in the clay rock is rapid. The pathway dilation occurs with increasing pressure and a pathway network is created by the onset of the heterogeneities in the clay formations. The fracture network being created by this process as well as the damage induced permeability increase necessitates the application of the fracture mechanics and hydraulics in modelling the transport especially in indurated clay formations.

5.2.10.1 A Model for Crack Opening /ALO 02/

The basic idea of the model consists in the appropriate representation of single fractures embedded in a continuous finite element. Figure 5-9 shows a finite element composed by a rock matrix and a series of n fractures. The number of fractures in an element depends on the width associated with each fracture, a , which is a characteristic size of the material, and the element size s .

Hydraulic and mechanical effects have to be included because gas flow depends critically on the mechanical interactions because they control fracture aperture or porosity changes.

The flow phenomenon through a single fracture is considered first. Liquid and gas flow is calculated using Darcy's law. The most important parameter in this law is the intrinsic permeability which can be calculated, assuming laminar flow with Eq. (4-39). In finite element applications the element size becomes a limitation for fracture modelling, because it is not convenient to use very thin elements. Alternatively, there is the possibility of considering explicit joint elements. In this formulation, it is preferred to use homogenized properties because practical applications are an objective of this work. In fact, the introduction of a set of discrete fractures tends to complicate the analysis in a significant manner.

When a set of n fractures is included in a finite element (Figure 5-9), the equivalent intrinsic permeability of the element can be calculated as:

$$\begin{aligned}
 k &= k_{matrix} \left[\frac{s - nb}{s} \right] + \sum_{i=1}^n \left[k_{fracture} \frac{b}{a} \frac{a}{a} \right] \\
 &= k_{matrix} \left[\frac{s - nb}{s} \right] + \sum_{i=1}^n \left[k_{fracture} \frac{b}{a} \frac{1}{n} \right] \cong k_{matrix} + \frac{b^3}{12a}
 \end{aligned}
 \tag{5-47}$$

where k_{matrix} is the reference intrinsic permeability of the matrix. In the case of gas propagation through rock the matrix refers to the rock without fractures. s is the element size (width normal to flow direction), a is the width associated with each fracture, and $n = s / a$ is the number of fractures in the element. Permeability of the matrix will be important only for very low apertures; otherwise fracture permeability will dominate the total permeability and matrix permeability will be negligible. Eq. (5-47) shows that the element permeability does not depend on the size of the element but depends on the width associated with each fracture a , which can be considered a characteristic parameter for a specific medium.

The second hydraulic process that is included in the fracture is the variation of capillary pressure caused by changes in the aperture.

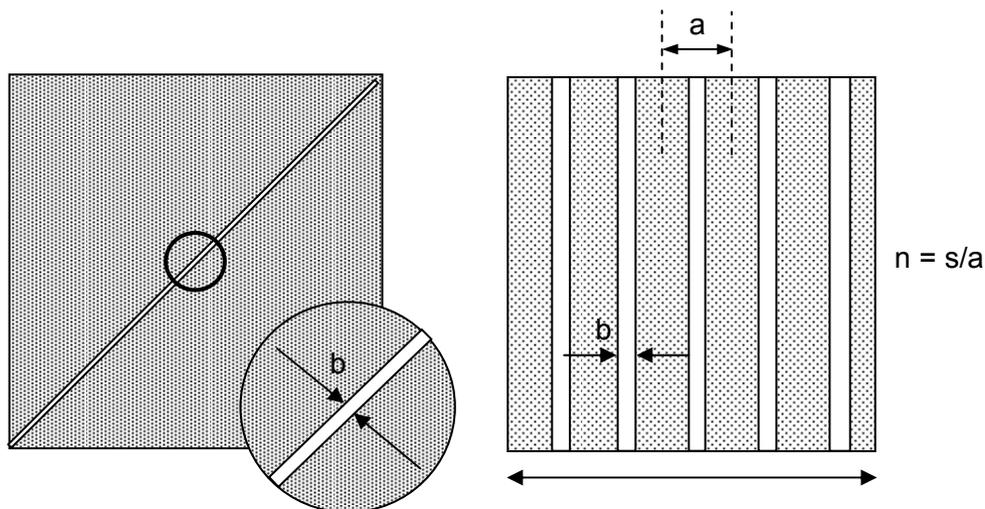


Figure 5-9: Rock with a single idealized fracture and a series of parallel fractures uniformly separated

The basic Equation (4-26) representing the capillary pressure in a fracture of width b can be used directly to calculate the air entry value of the element. If (5-47) is combined with the definition of capillary pressure to start desaturation is obtained as:

$$P = P_o \frac{\sqrt[3]{k_{fracture_o}}}{\sqrt[3]{k_{fracture}}}
 \tag{5-48}$$

where subscript o refers to a reference (initial) aperture.

From the mechanical point of view, the process of fracture formation and aperture is more interesting. The aperture of the fracture can be estimated as a function of deformation, ε , in the following way:

$$b = b_o + \Delta b$$

$$\Delta b = a\Delta\varepsilon = a(\varepsilon - \varepsilon_o) = (s/n)(\varepsilon - \varepsilon_o) \quad (5-49)$$

Here, it has been assumed that deformation is localized and results in changes in aperture. A threshold value (ε_o) is considered. Therefore the changes in aperture start when deformation reaches this value. Deformation perpendicular to the fracture plane is used when aperture changes have to be obtained. The threshold value (ε_o) is associated with fracture initiation. This parameter will be set to zero if the fractures already exist and have an initial aperture b_o . In practice, the initial aperture can be essentially zero when the fractures exist but are closed.

The stress-strain behaviour of the medium (clay barrier or rock), including fracture formation, is a crucial component of the aperture changes. As mentioned before the deformation normal to the fracture is considered in Eq. (5-49) in order to obtain aperture changes. If an elasto-plastic model is considered for the mass behaviour, fracture initiation can be associated with tension stresses or with dilatancy. On the other hand, fracture orientation is sensitive to the stress tensor orientation so the plane where the minimum principal stress (compression positive) occurs defines the plane of fracture formation. Eq. (5-49) is introduced in Eq. (5-47) to calculate the element permeability in the following way:

$$k = k_{matrix} + \frac{b^3}{12a} = k_{matrix} + \frac{(b_o + a(\varepsilon - \varepsilon_o))^3}{12a} \quad (5-50)$$

From this relationship it is clear that the element permeability depends on the fracture spacing (a), which is a characteristic parameter of the material, but is independent on the element size (s).

Normally, it is of interest to consider $s \geq a$ (i.e. $n \geq 1$, one or more fractures in each element) because in this way, some of the elements in the finite element mesh will develop higher permeability due to opening of the fractures contained in these elements. Other elements, will maintain the properties of the intact medium. Consequently, preferential paths can be simulated. On the contrary, if $s < a$ (i.e. $n < 1$, less than one fracture in each element), a single fracture would be homogenized into various elements and a suitable smoothing of the preferential flow path would take place.

In a general stress-strain behaviour coupled to aperture changes in the case of tension taking place in the medium, a threshold strain (ε_o) defines the initiation of fracture aperture, as mentioned before. A strain corresponding to failure is also considered (ε_f). In this case, failure is achieved when the normal stress reaches the tensile strength (σ_t). ε_o , ε_f , and σ_t are model parameters.

From this general model the following cases can be established:

a. Existing fracture initially closed:

$$\sigma_t = 0, \varepsilon_o \approx 0$$

b. Non existing fracture:

$$\sigma_t \neq 0 \text{ and } \varepsilon_o = \varepsilon_f \neq 0$$

The first case (a) corresponds to a fracture, that due to compression stresses, is almost closed or has an initial aperture b_o . Normal extension will induce aperture opening right from the beginning of stressing. As the normal stress reaches a zero value, deformation will increase under constant stress (irreversible deformations). Unloading will imply fracture closure but a residual aperture is expected due to irreversible deformations. An appropriate elastic modulus could be used if complete closure had to be achieved.

The second case (b) implies that a tensile strength exists and, therefore, aperture cannot be initiated before failure by tension occurs. For this reason the threshold strain (ε_o) is set equal to the strain corresponding to failure (ε_f). This latter value depends on the tensile strength. Normally, failure would have to be associated with softening because the material is damaged.

Another situation takes place in case of dilatancy induced by shearing. In this case, the formation of fractures is due to extension which is a consequence of dilatancy. Again the threshold strain is convenient to define the initiation of fracture opening.

Fractures induced by tension and fractures induced by dilatancy, even though they are processes physically different are jointly considered in elastoplastic models. For instance, in critical state models extension induced by tension or extension induced by dilatancy depend essentially on the stress path followed.

Some examples to show the capabilities of the formulation are presented in /ALO 02/ /DEL 02/ /OLI 05/. Modelling attempts of the tests conducted to study gas flow through compacted clays and rocks were presented /ALO 02/. The analyses showed the sensitivity of results to a number of factors controlling the tests usually performed. It is shown that the model reproduces in a natural way the peak discharge phenomena and peak gas pressure often reported in experiments. In Delahaye and Alonso (2002) a procedure to simulate the material heterogeneity effects on gas migration process is described. /DEL 02/ by using the above described modelling concept. Soil heterogeneity is defined by means of random fields of the key soil properties for gas migration. They generated two-dimensional stationary random permeability fields, described by a constant mean and a covariance function that depended only on the relative distance vector between two arbitrary points. They studied several cases in order to perform a sensitivity analysis due to the lack of reliable data on soil heterogeneity. In the cases in which preferential paths were simulated satisfactorily, once the random permeability field was generated, the intrinsic permeability value was linked to the element porosity through Kozeny's law. In addition, they related the air entry value from the retention curve, P_o , to soil porosity. The effect of local heterogeneities in gas flow is also examined. The approach was to simulate the behaviour of a randomly heterogeneous transmission zone /OLI 05/. The geometry, material properties and boundary conditions are inspired in a recent large scale experiment (GMT) conducted in the Grimsel Rock Mechanics

Laboratory. The variability of soil properties introduced in the simulation performed is rather weak. Nevertheless, their effect on gas migration is very relevant. All the soil elements were characterized by an embedded discontinuity in the sense described in the paper. The analysis has provided an additional insight on the mechanisms of gas transport in clay barriers. It was concluded that the formation of preferential paths requires some initial heterogeneity. It was also shown that paths may develop and close as a response to the changing stress state in the transmission zone. The existence of discharge peaks is a natural consequence of the formulation. The results are encouraging and may lead to more realistic computational procedures for the complex problem of gas migration through buffers.

Barcelona Basic Model (BBM) In the above represented concept the Barcelona Basic Model (BBM) is used to calculate the dilatancy induced by shearing. Barcelona Basic Model is first introduced by /ALO 90/ and widely used as constitutive model to represent the mechanical features of unsaturated soils respectively of the clay formations. This an elasto-plastic model calculating the elastic volumetric strain, elastic deviatoric strain, yield locus and hardening phenomena with corresponding formulations summarized in /ZHA 04/.

5.2.10.2 Dual-Continua Model

The DP model for simulating preferential movement of water and solutes in structured porous media is developed by Gerke and van Genuchten /GER 93/, /DUY 06/. The model is combined with two systems: a macropore or fracture pore system at the macroscopic level by fracture continuum (FC) and a less permeable matrix pore system by matrix continuum (MC). Transfer of water and solutes between the two pore regions is simulated by means of first-order rate equation. Two non-linear partial differential equations associating with the transfer and specific storage term are used to describe the model. That the weighted average pressure head of two different continua is given as that of the whole system is disputable, moreover that the fracture is treated as a continuum is still suspicious. Meanwhile the model has widely practical application in the simulations of unsaturated flow.

In DP model, the transfer value between these two continua plays an important role to model accuracy, and much attention is focused on it. One treatment is given by Zimmerman et. al /ZIM 96/ which is the MC is treated in a lumped parameter manner, with a single average pressure used for each matrix block, rather than assuming that fracture or matrix flux is proportional to the difference between the fracture pressure and matrix pressure at each point. The geometry-dependent coefficient β in first-order transfer formula is calculated by matching analytical solutions, thus allowing the dual-porosity approach to be applied to media with complex and mixed types of structural geometry. Though several kinds of transfer equations are put forward, the transfer coefficients are also difficult to measure in the nature soil system. Besides of the coefficients of transfer term, the specific coefficient is also the new parameter in the Richards equations, and the physical meanings of this term are also indistinct. As for the single equations, it does not exist basic on the mass conservation, and it is difficult to understand.

Based on the dual-porosity model of Gerke and van Genuchten (1993), the pressure-based Richards equations are given as

$$C_m \frac{\partial p_m^l}{\partial t} - \Delta(K_m(\Delta p_m^l - \rho^l g)) = \frac{Q}{\rho^l} + \frac{\Gamma^l}{w_m} \quad (5-51)$$

$$C_f \frac{\partial p_f^l}{\partial t} - \Delta(K_f(\Delta p_f^l - \rho^l g)) = \frac{Q}{\rho^l} + \frac{\Gamma^l}{w_f} \quad (5-52)$$

where t is time, the subscripts m and f denote the soil MC and FC respectively. Γ^l is water transfer term (s^{-1}), which is defined as the volume of fluid moving from the FC to the MC per unit volume of the bulk soil per unit of time; it is the space and time dependent exchange term. Q is the source term in the domain. The terms w_m and w_f denote volume fractions of the MC and the FC per unit volume of the bulk soil respectively. The relationship of these two variables is $w_m + w_f = 1$

C (Pa^{-1}) is the specific soil water capacity given by

$$C = S^l c_s^l + \phi \frac{\partial S^l}{\partial p} \quad (5-53)$$

in which, ϕ is porosity, c_s^l is the specific storage coefficient (Pa^{-1}), and the composite saturation of soil is

$$S^l = S_m^l w_m + S_f^l w_f \quad (5-54)$$

The first-order approximation of the transfer term by /GER 93/ is:

$$\Gamma^l = \alpha^* K_a(p_f^l - p_m^l) \quad (5-55)$$

in which α^* denotes first-order transfer coefficient, and K_a is unsaturated hydraulic conductivity (m/s). α^* is proportional to β/α^2 , where β is the geometry factor related to the shape of aggregates, α is the average soil aggregate radius.

The coupled system increases the non-linear of partial differential equations, and there are two primary variables to be solved. The numerical model for a Richards flow problem uses finite element method (FEM), and lumped mass modification with quadrature of the standard Galerkin method using piecewise linear approximating functions, and Picard iteration scheme. The principle in solving the equations lies in the linearization procedure and the method for dealing with the coupling between the equations. The pressure of MC is treated as the coupling variable.

5.2.10.3 Matrix Diffusion in Fractured Clay Rock, Brush Model

Figure 5-10 shows the dominant transport mechanisms in porous media and in fractured media. The dissolved contaminant (gas or salt) is transported advectively with the present liquid phase in the fractures. During this flow process diffusion takes places from the fracture

to the matrix saturated with a stagnant liquid phase. The porosity and the tortuosity of the matrix reduce the molecular diffusion coefficient D to a value of effective diffusion coefficient D_e . The relation between D_e and D is given by Berner taking the porosity ϕ and the tortuosity τ into account as follows:

$$D_e = D \frac{\phi}{\tau^2} \quad (5-56)$$

Consequently D_e is always smaller than D . The effective diffusion coefficient of the porous matrix can be determined based on the diffusion coefficients and the measured properties of the porous medium and/or with tracer techniques in-situ.

To better consider the matrix diffusion a model called brush model is proposed /LEG 96/. In this approach, gravitational effects are neglected and thus the schematization of nature yields a system of sub-horizontal fractures with an attached rock matrix. If it assumed that the dissolved substances are transported with the same velocity over the entire rock column, a model of one horizontal fracture is representative for the entire system. Due to the symmetry considerations, only one half of the system is modelled. The fracture plane is discretized by 2-D quadrilateral finite elements in the x, y plane with Cartesian coordinates. Advective-dispersive transport without and retardation is assumed. The transport of a substance that is not sorbed through a fracture is modelled using the following 2-D advection-dispersion equation:

$$\frac{\partial c}{\partial t} = D_L \frac{\partial^2 c}{\partial x^2} + D_T \frac{\partial^2 c}{\partial y^2} - \frac{v_D}{\phi_{eF}} \frac{\partial c}{\partial x}, \quad (5-57)$$

where C is solute concentration [mg/l]. In the processes described in this paper, the tracer velocity, v_D/ϕ_e , is sufficiently high that the term D_m does not contribute significantly to the total dispersion coefficient D_L and D_T .

Darcy law is applied for the flow velocity in the fracture. The rock matrix of the clay formation is discretized using 1-D elements. The elements are positioned parallel to the z -axis and coupled to the z -axis and coupled to the 2-D elements of the fracture through common nodes. A chain of 1-D elements is attached to every node of the 2-D mesh. The cross-sectional area of the 1-D elements is equivalent to the area surrounding the nodes of the corresponding 2-D mesh. Concentration in the rock matrix satisfies the 1-D diffusion equation:

$$\frac{\partial c}{\partial t} = D_e \frac{\partial^2 c}{\partial z^2}, \quad (5-58)$$

where D_e is the effective diffusion coefficient. This schematization uses the combination of elements with different dimensions that is implemented in the applied computer code ROCK-FLOW.

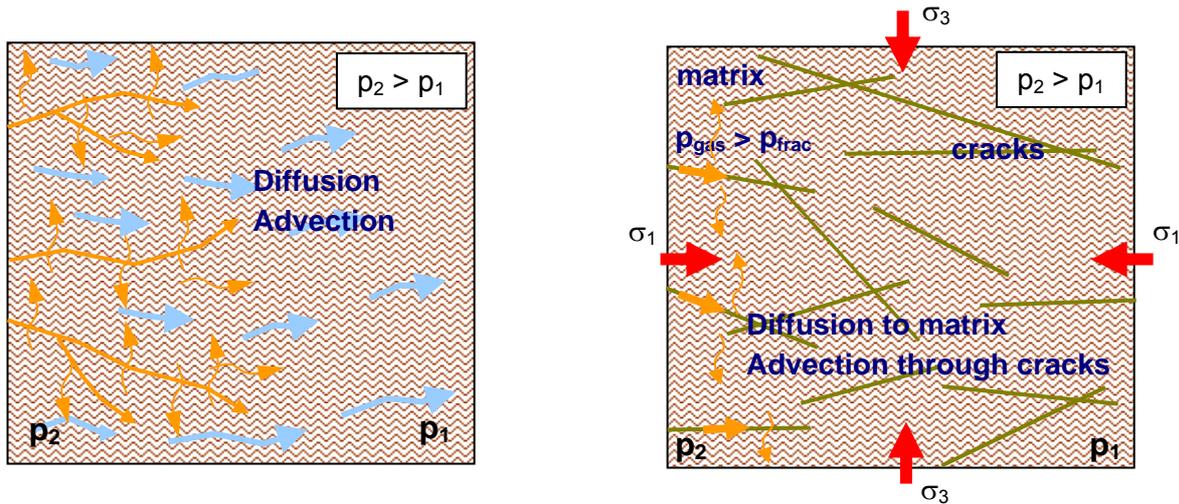


Figure 5-10: Transport mechanisms in porous and fractured geological media

5.2.11 A Thermo-Hydro-Mechanical Coupling /KOH 04/

A coupled thermo-hydro-mechanical solution is given by /KOH 04/ for modelling of partially saturated clay systems. Essentially the theory of porous media is based on certain axioms of continuum mechanics. Additionally constitutive equations are required for each constituent. It can be treated within the classical phenomenological approach by Biot using the effective stress concept of Terzaghi /BIO 41/. Furthermore, modern mixture theories combined with the concept of volume fractions are applied. In this context, a coupled initial boundary value problem (IBVP) of a geometrically linear porous solid is given. Thereby, the set of equations is conceptionally split into a solid and a fluid problem. These sub-problems are essentially the consequences of the balance of linear momentum and the balance of mass.

Deformations of the solid skeleton are described by the displacement field u . The buoyant density of the mixture is denoted by ρ_m and distributed body forces per unit mass are given by the vector field g . The symmetric tensor field of effective stresses is introduced as σ . Finally p_w defines the excess pore fluid pressure in the water phase while S_w is its saturation. The balance of linear momentum for the solid is given by:

$$\text{div}(\sigma[u] - \alpha S_w p_w) = \rho_m g \quad \text{where} \quad \rho_m = \rho_b + \rho_w n \tag{5-59}$$

α is the Biot coefficient defined with bulk modulus K of the solid grains, s and solid skeleton, T

$$\alpha = 1 - \frac{K_T}{K_s} \tag{5-60}$$

The effective stresses are obtained from the constitutive equations for generalized Hooke's law as a linear stress-strain relationship. In order to complete the IBVP for the solid a set of Dirichlet boundary conditions $u = u_p$ on $\partial_u B$ where B denote the configuration occupied by a

porous solid with placements consisting of a solid phase and a fluid-gas mixture, Neumann boundary conditions $(\sigma - S_w p_w)n = t_p$ on $\partial_u B$ and initial conditions $u = u_0$ in B at $t = t_0$ are prescribed.

With a gaseous phase that remains approximately at atmospheric pressure an unsaturated two phases system consisting of a compressible solid that is filled with a compressible fluid is modelled. With these assumptions, the mass balance equation is reduced to:

$$\operatorname{div}(\rho_w w_f [p_w]) = -\rho_w S_w \alpha \operatorname{div} u - \rho_w \left(n \frac{\partial S_w}{\partial p_w} + S_w S \right) p_w \quad (5-61)$$

The relative pore fluid velocity w_f as well as the saturation S_w is obtained from the constitutive equations. In order to complete the IBVP for the fluid a set of Dirichlet boundary conditions $p_w = p_p^w$ on $\partial_u B$, Neumann boundary conditions $w_f n = f_p$ on $\partial_u B$ and the initial conditions $p_w = p_p^w$ in B at $t=t_0$ are assumed. The flux terms σ and w_f are determined by solid and fluid sub-problems. The multiphase problematic is simplified by employing the Richards approximation assuming that the air pressure is constant in the whole domain.

Two case studies are presented as saturated and unsaturated single phase flows. In unsaturated case it is assumed that the desaturation takes place due to gravitational effects. The capillary pressure and relative permeability curves are taken from the experimental studies.

5.3 Modelling of EDZ's in Clay Formations

As explained in previous chapters the EDZ's is the one of the main focus of the modelling of the transport phenomena in repository systems. The permeability changes induced by the dilatancy are determined to be important for the transport phenomena taking place in the near field of the repositories. From a modelling point of view, the permeability increase should be coupled to the dilatancy which in turns should be coupled with the deviatoric stress changes around the excavation. This explains the importance of correct understanding and modelling of the mechanical features of EDZ's /GEE 03/, /MAR 03/. A good review of the short and long term mechanical behaviour of clay formations is given in MODEX-REP project based on Callovo-Oxfordian formation /SUK 03a/, /SUK 03b/. The typical stress-strain curve of the clay formations is examined in four successive phases as discussed in Chapter 3.2 of this report. These are the elasticity, damage before the failure, softening after failure and the residual phases. The hydromechanical constitutive approaches modelling this behaviour are investigated in terms of matching the behaviour of Callovo-Oxfordian clay. The strength-strain behaviours reproduced by various models are similar, but the strains at the failure point and their evolution after the failure are different. That difference is mainly due to the different laws chosen for simulating irreversible strain flow during pre- and post- failure phases. Indeed, the approaches to simulate damage, failure and associated irreversible strains used by the different research teams are different: classical plasticity theory, damage mechanics theory, and discrete model. Table 5-2 gives an overview of the constitutive models proposed by the project MODEX-REP. A large variety in model application is observed. They may be considered as complementary in the sense that they reproduce different

mechanisms acting in different situations: plasticity, damage, discrete model. For the time being, it is impossible to assess the performance of those models to simulate the in-situ behaviour of the rock without in-situ observations.

Table 5-2: Overview of the constitutive models for short and long term behaviour of clay formations /SUK 03a/

Research Team	Short-term Behaviour			Long-term Behaviour
	Type of model	Criterion of damage and damage approach	Failure of criterion	Time-dependent behaviour
CGES	Continuum model	-	Mohr-Coulomb	Lemaitre viscoplastic
G3S	Continuum-steady state	Von-Mises model plasticity	-	Lemaitre viscoplastic
ITASCA	Discrete-continuum	Bond strength Bond damage	Bond strength	Differed bond-failure
CIMNE/ ENRESA	Continuum bonded model	Ellipse in P-Q plan Damage model	Hoek-Brown	Visco-scalar damage
NAGRA	Continuum model	Mohr-Coulomb	Mohr-Coulomb	-
ANDRA	Continuum model	Hoek-Brown Damage simulated with plasticity	Hoek-Brown	Lemaitre viscoplastic
LML	Continuum model	P-Q function Damage simulated with plasticity	P-Q function	Differed damage
COYNE-BELLIER	Continuum model	Mohr-Coulomb Plasticity	Mohr-Coulomb	Lemaitre viscoplastic
SCK-CEN	Continuum model	Hoek-Brown Damage simulated with plasticity	Hoek-Brown	Lemaitre viscoplastic

The modelling example of the damaged zones around disposal tunnels is presented by means of modelling of two in situ tests in /MUN 03/: The HE (heating) experiment and the EB (Engineered Barrier) experiment, both currently in operation at the Mont Terri Rock Laboratory. In the first part, the mechanical constitutive law is outlined. It models the rock as a bonded material and distinguishes the response of the clay matrix, represented by an elastoplastic constitutive law and the response of the brittle bonds, represented by a damage model. In a second part, results from the simulation are discussed with a special emphasis given to the understanding of the mechanisms taking place in the disturbed zone. In the case of HE experiment, the different stages of the experiment – excavations of HE niche and borehole, hydration of bentonite buffer, heating and cooling stages – are simulated and their effect on the immediate rock is analysed. In the case of the EB experiment the excavation of

the gallery, pellet fill emplacement and subsequent hydration are simulated, with special attention to the behaviour of the rock. The computed distribution of damaged zones in this case seems to agree with field determinations /MUN 03/.

The implication of EDZ's on the transport processes is the dilatancy which is controlled by the mechanical disturbance and damage. The permeability induced by the dilatancy is the principal parameter representing the EDZ's in transport equations. The coupling of the permeability to the modelled dilatancy is investigated for various host rock types intensively. For crystalline and salt rocks as repository host rock, the dilatancy induced permeability, the geometry and the extent of the EDZ's are well studied /TSA 05/. For relating permeability to the dilatancy in crystalline rocks the relationship of Serrata and Fuenkajorn is widely used /SER 93/:

$$k = A \sigma_3^\lambda \cdot (\varepsilon_{ir}^N)^s \quad s = 1 - e^{-n\sigma_3/P} \quad (5-62)$$

with k , permeability, A , constant (m^2Pa), σ_3 minimum stress component (Pa), ε_{ir} non-elastic stress component, λ stress exponent und s porosity exponent. The geometry and structure of the structural changes occurring in EDZ's are widely discussed in related literature. A percolation like sudden permeability is a physical concept of the recent theoretical and experimental studies /PEA 91/, /PUS 02/. A geometrical model to account the fractures with "penny-shaped" crack geometry is given for example by Gueguen and Dienes as function of the structural parameters /GUE 89/:

$$k = (2/15)\theta\alpha\Delta\omega^2 p^* = (2/15)\theta\alpha\Delta\omega^2 \left[\frac{1 - 4((8A\alpha/\pi D) - 3/4)^{1/2} - 1/2}{+ 3((8A\alpha/\pi D) - 3/4)^{1/2} - 1/2} \right]^3 \quad (5-63)$$

The most important parameter in setting the percolative behaviour is to define the dilatancy boundary where the crack initiation begins. This threshold value is given experimentally for the host rocks studied mostly due to the experimental studies /ALK 07/.

In clay formations, the EDZ is also commented as a dilatancy related fracture opening and development phenomena /TSA 05/. Principally, the concepts originated from crystalline host rocks can be applied to plastic and indurated clays too. However the EDZ studies for clay formations are not advanced enough to set a universal solution of coupling the changes on stress equilibrium on to the hydraulic properties. In the following the existing physical and numerical modelling attempts of EDZ models for clay formations are cited.

5.3.1 Compression-Dilatancy Mechanism in Clay Formations

The porosity decreases due to shear-induced compaction or porosity increases associated with shear-induced microfracturing (dilatancy) is one of the typical mechanical responses of the clay formations. As discussed in previous sections the magnitude of the mean-normal effective stress, σ_e , is a primary factor governing these mechanisms. In a tectonized clay rock, dilatancy might cause underpressures and compaction might give rise to overpressures. One approach to quantifying these effects makes use of the empirical pore pressure parameters a and b , which represent a modification of the parameters first proposed by

Skempton /SKE 54/. The change in pore pressure, Δp_w , resulting from a general change in the stress acting on compact clay under undrained conditions can be written as

$$\Delta p_w = b\Delta\sigma_m + 3a\Delta\sigma_o \quad (5-64)$$

where $\Delta\sigma_m$ and $\Delta\sigma_o$, are the incremental changes in the mean-normal (total) stress and the octahedral shear stress, respectively, defined by

$$\Delta\sigma_m = \frac{1}{3}[\Delta\sigma_{11} + \Delta\sigma_{22} + \Delta\sigma_{33}] \quad (5-65)$$

and

$$\Delta\sigma_o = \frac{1}{3}\left[(\Delta\sigma_{11} - \Delta\sigma_{22})^2 + (\Delta\sigma_{22} - \Delta\sigma_{33})^2 + (\Delta\sigma_{33} - \Delta\sigma_{11})^2\right]^{0.5} \quad (5-66)$$

A complicating factor is that parameter a is not a constant, varying quite significantly with the level of the shear stress acting on the clay. At low shear stresses a is approximately zero in most materials. In soft clays which tends to compact during shear deformation, a is positive as the failure condition is approached. In overconsolidated clays and mudrocks which often tend to dilate at higher levels of shear stress, a may be negative as the failure condition is approached. Provided that the nonlinear functional dependence of this parameter on stress can be quantified, it is possible to incorporate an additional term in (5-64) to represent shear-induced dilatancy in compact clays and clay rocks. Given this background, transient flow in geological media is almost invariably quantified using theory based on the assumption of linear elastic volumetric behaviour. Although this is often perfectly acceptable in aquifer and water-resource calculations, the application of linear elastic theory to the long-term problem of fluid flow in clays and mudrocks is questionable. Specific areas of concern are possibility of visco-elastic (time dependent) and visco-plastic volumetric behaviour, stress-dependency, nonlinearity and hysteretic effects associated with the compressibility and specific storage terms, and the whole issue of the role of shear stresses in the volumetric responses of clay. In plastic clays, the values for the "elastic constants" are known to be very dependent on effective stress. It is shown that drained bulk modulus of elasticity K is actually proportional to the mean-normal effective stress. When K is substituted in the definition of specific storage, it can be found that this quantity must also be stress-sensitive. In poroelastic descriptions of transient flow it should therefore be very careful to select specific storage values which are representative of the in situ state of stress. Alternatively, in numerical modelling it is a relatively simple matter to make the storage term a function of the effective stress, should the need arise. In mudrocks which are undergoing active tectonic deformation it is important to consider the possible role of shear stress, as well as mean-normal stress, in determining the hydrogeological responses of the formation. Outside of geomechanics, this is a much neglected subject of investigation. Laboratory experiments have clearly demonstrated that the volumetric responses (changes in porosity) of mudrocks and overconsolidated clays are sensitive, not only to changes in mean-normal effective stress, but also to changes in the octahedral shear stress. At low levels of mean-normal stress and moderately high shear stresses, a mudrock has a tendency to dilate and newly-formed microcracks contribute to the total porosity. Since fluid flow is restricted by low permeability, the pore pressure falls during dilatancy. If shear deformation is inhomogeneous, this can lead to a region of sub-normal pressuring. Conversely, when both the mean-normal effective stress and the shear stresses are high, deformation can lead to enhanced compaction, leading to a drop in

total porosity. In this case, inhomogeneous deformation would tend to produce supra-normal pressuring. This complex hydro-mechanical coupling in strongly-deformed mudrocks could lead to internal flows in a formation which are solely driven by tectonic forces. This effect is not accommodated in any of the poroelastic models of transient flow, but is an intrinsic feature of elastoplastic models, based on the concepts of critical state soil mechanics. The possible hydrogeological applications of this type of model are virtually unexplored.

5.3.2 Hydro-Mechanical Coupling in Boom Clay (Mol URL, Belgium)/BAR 03/

The classical thermo-poromechanical framework of continuous media has been used successfully in reproducing and predicting the behaviour of the saturated Boom Clay /LAB 98/. At the Mol site, the Boom Clay is characterised by a high porosity ($\phi = 0,39$), and Biot's coefficient equal to unit ($\beta=1$) which is responsible for a strong hydro-mechanical coupling. Thus, under the assumption of elastic and plastic effective stresses, rate-form relations are defined for the poro-plastic isothermal, isotropic behaviour for the Boom Clay:

$$\sigma' = \sigma + p_w I = C': (\varepsilon - \varepsilon^p) \quad (5-67)$$

$$p_w = \frac{K_w}{\phi} \left[-tr(\varepsilon) + \frac{m}{\rho_w} - \phi^p \right] \quad (5-68)$$

where σ' is the effective stress tensor, σ the total stress tensor, p_w the pore pressure, I the unit tensor, C' the effective elastic matrix, ε the strain tensor, K_w the water bulk modulus, m the fluid mass content, ϕ the porosity and superscript p standing for 'plastic part'. For the Boom Clay at the Mol site, C' is computed from the effective elastic parameters $E' = 300$ MPa, $\nu' = 0.125$. From these relations, the hydro-mechanical coupling can be seen clearly: the pore pressure enters the effective stress formulation which represents the HM coupling, and the volumetric strain and plastic porosity enter the pore pressure formulation which represents the MH coupling.

The solution presented corresponds to the instantaneous solution, i.e. without any fluid flow. The evolution in time of this solution is mainly controlled by the fluid flow that will occur, which depends on the hydraulic boundary conditions, on the flow parameter and on the time considered. A first idea of these effects is obtained by estimating the characteristic time for hydraulic diffusion k_h in the present case. Given the problem geometry, t_h is given by:

$$t_h = \frac{r_i^2}{k_h}, \quad (5-69)$$

where r_i is the excavation radius and k_h the hydraulic diffusivity defined by

$$k_h = \frac{k}{\rho_w g} M \frac{3K' + 4G}{3K + 4G} \quad (5-70)$$

Using the typical mechanical parameters of Boom Clay, the value $k_h = 1,21 \cdot 10^{-7}$ m²/s is obtained. Then, considering $r_i = 4$ m (excavated radius), the characteristic time for hydraulic

diffusion can be found as $t_h = 4,2$ year, which is much larger than the times observed in-situ measurements /BAR 03/. Thus, the hydraulic diffusion should not allow explaining the discrepancy between observations and predictions. This can be confirmed by a HM calculation considering the case of a permeable boundary condition at the gallery wall (relevant as the lining permeability is several orders higher than the Boom Clay one). This boundary condition is then approximated by an imposed pressure $p_w = 0$, though in reality it is the relative humidity that is imposed. Using the Boom Clay hydraulic conductivity of $4 \cdot 10^{-12}$ m/s, the obtained pore pressure profile after one year is reported on Figure 5-11 (thick line). Clearly, the drainage effect over a one year period does modify only slightly the pore pressure profile with respect to the instantaneous solution (dashed line on Figure 5-11). The fluid drainage towards the shaft does not reduce the observed discrepancy at radii of 60-70 m, thus other phenomena must be invoked.

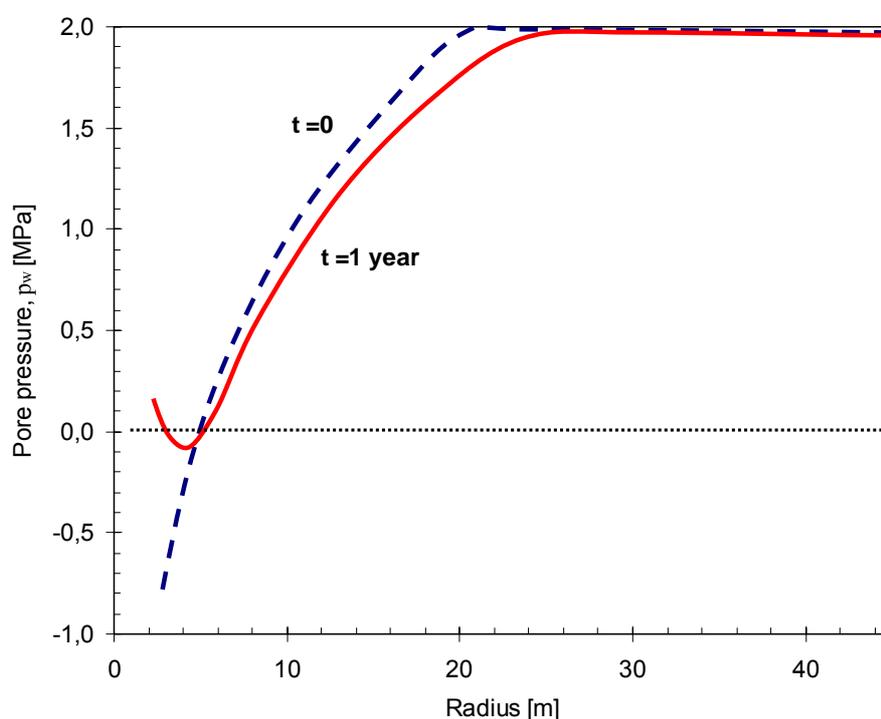


Figure 5-11: Evolution of the pore pressure profile from zero to one year (excavated radius = 4 m) /BAR 03/

5.3.3 Coupling between Damage and Permeability /DES 05/

The model provides a typical example of accounting the notions of crack damage and double porosity. The formulation is first obtained by simulation of a circular crack distribution system inside a REV (Representative Elementary Volume) and homogenisation at the macroscopic scale. The hydraulic behaviour of the rock is drawn from the classical Darcy law for the matrix permeability and Poiseuille law for the cracks. Percolation threshold phenomenon is observed by increasing the crack density. The anisotropic permeability tensor, before and after the percolation threshold appears to fit to a non-linear law with the crack damage tensor.

Extensive measurements on clay samples have allowed to valid the following power law between the trace of the permeability tensor and the trace of the crack damage tensor.

$$T(k) = \alpha T(D_c)^b \quad (5-71)$$

with $\alpha \approx 10^{-14}$ and $\beta \approx 3$

The above given crack damage law is derived from the mechanical damage law by projection onto the deviatoric plane. The model has been successfully implemented in Code_ASTER and Cesar for numerical modelling of the storage concepts.

5.3.4 A Numerical Model of Shear Banding Around an Excavation /COL 05/

A benchmark has been proposed concerning the numerical prediction of the extent and evolution of the Excavation Damaged Zones around the nuclear waste deep geological disposals. The final objective is the evaluation of the relevance of the numerical codes used by the participants to model the different tests of the benchmark with the same constitutive equation. In the proposed benchmark efforts, thermal aspects and creep effects are ignored. The modelling focuses on the coupling between mechanical behaviour of the host formation and the hydraulic diffusion (in saturated conditions) during the excavation process. The proposed constitutive laws should model two in-situ observations: the degradation of the rock mechanical properties and the induced increase of medium permeability. The mechanical constitutive model is an associated Drucker Prager elastoplastic model with a softening due to the degradation of the cohesion related with the deviatoric plastic strain:

$$F = \sqrt{\frac{3}{2}} II_\sigma + m \left[I_\sigma - \frac{3c_o f(\gamma^p)}{\tan \phi} \right] \quad (5-72)$$

where $II_\sigma = \sqrt{\sigma_{ij}\sigma_{ij}}$ is the second deviatoric stress invariant ($\sigma_{ij} = \sigma_{ij} - \frac{I_\sigma}{3}\delta_{ij}$),

$I_\sigma = \sigma_{ij}\delta_{ij}$ is the first stress invariant $m = \frac{2 \sin \phi}{3 - \sin \phi}$, ϕ is the friction angle and c_o is the initial value of the cohesion. The softening relation $f(\gamma^p)$ reproduces the degradation of the material strength as a function of the equivalent deviatoric plastic strain $\gamma^p = \sqrt{\varepsilon_{ij}^p \varepsilon_{ij}^p}$.

In the benchmark, the permeability evolution is described as a function of the porosity:

$$k = k_0$$

$$\frac{k}{k_0} = 1 + 2.10^{12} (\phi - \phi_0) \quad \text{if} \quad 0 < \phi - \phi_0 < 10^{-2} \quad (5-73)$$

$$\frac{k}{k_0} = 1 + 2.10^6 \quad \text{if} \quad \phi - \phi_0 > 10^{-2}$$

It is indicated that the softening models which have been extensively used in the past are now known to generate numerical problems especially when localized ruptures modes (like shear bands) appear in a computation. Numerical modelling of such kind of localized shear

zones suffers by a pathological sensitivity to the finite element discretization. Around a tunnel, this latter mesh sensitivity leads to undefined position and number of shear bands. In a coupled hydro-mechanical simulation, this renders more difficult the modelling of the increase of the permeability in the damage zone (EDZ) and more specifically in the localized bands.

The first attempts of the numerical computations obtained with the proposed model and the proposed boundary conditions are presented. In this classical computation, the patterning and the width of the shear bands are found to be the function of the mesh used. This is the confirmation of the well known properties of the classical constitutive equations. They are able to predict the occurrence of localization but unable to properly model the post localized failure of materials. This is illustrated by the result of the computations proposed in the benchmark. It is seen also that the directions of the band of coupled computations are in accordance with the classical Rice analysis made for the proposed constitutive equation without coupling.

To provide an objective description of post localized paths a non-local approach was first proposed for damage concrete mechanics and extended later to other materials. Models involving gradient of internal variables or with non-local internal variables are also been used in the framework of elasto-plasticity. Other modelling possibilities were also tested and discussed in the framework of this benchmark.

5.3.5 A Visualization Model for EDZ's /SAF 04/

The SAFETI project has produced a state of the art code (AC/DC) and visualization package (ACDCvis) that allows models of field-scale experiments in brittle materials (such as rock or concrete) to be performed /SAF 04/. The code makes use of parallel computing technology, and has been successfully tested on 40 nodes of the Networked Earth Science Super Computer (NESSC) at Liverpool University, and a smaller computer cluster in France. The models can contain excavations and an in-situ 3D stress field can be applied. Microcracking is interpreted at the regions in the model where bond breakages occur between the model particles. The microcracks can be viewed and analyzed in terms of their location, orientation, and basic failure mechanism (shear or tensile). Further algorithms have been developed for spatially and temporally interpreting the microcracks in terms of acoustic emission/ microseismic (AE/MS) parameters including magnitude and the moment tensor source mechanism. Methods for measuring the static and dynamic stiffness tensor at specific locations within a 3D AC/DC model have been developed, which allows the damage and anisotropy to be quantified. Algorithms have been produced for predicting time dependent behaviour in the AC/DC model, calibrated to laboratory measurements. Methods have also been developed for interpreting and visualizing (using 3FLO) the hydraulic fracture network, and calculating the corresponding hydraulic parameters. The basic building block for AC/DC is the periodic cell, known as the 'p-cell' or 'pbrick'.

The pbrick concept allows large models to be quickly built up, as well as allowing the model to be easily divided between parallelised processors. There are three types of pbrick:

- Particle Pbrick: A densely packed assembly of PFC3D particles at equilibrium.
- Matrix Pbrick: A particle pbrick in which the particles are replaced with a matrix. The matrix is essentially a network of masses and springs (i.e. no rotation can occur and no formation or loss of contacts).
- Degenerate Matrix Pbrick: A particle pbrick in which the particles are replaced by a continuum FLAC3D zone. This is a simpler version of the matrix pbrick.

The matrix pbrick is proposed as a reasonable assumption in regions where microcracking is not expected, and also makes the model much more computationally efficient. Degenerate matrix pbricks are even more computationally efficient than matrix pbricks, and are useful to use on the outer portions of large models to gain the correct boundary and stress conditions. Adaptive logic has been written to convert matrix pbricks to particle pbricks as required near regions of new bond-breakages (microcracking). Following the creation of new microcracks the model is seen to convert a number of the matrix pbricks into particle pbricks.

The strength and deformation test results from the Mont Terri site have been used to validate the constitutive model (failure criterion, crack initiation envelope and final failure envelope). Both short-term and long-term models have been calibrated by using experimental data from the Mont-Terri site. Model runs simulating the Mont-Terri experiment were performed with AC/DC. The following steps were followed to construct the numerical model: (a) construct a pbrick for Opalinus clay in periodic space, (b) apply the Mont Terri in-situ stress field into this AC/DC model, (c) use this pbrick to produce an AC/DC model of the region of rock surrounding the Mont Terri tunnel excavation, and (d) simulate the excavation by removing the particles in the tunnel region, and subsequently monitor the deformation and damage.

The excavation phase was simulated by removing particles in the tunnel region. The forces previously applied by the removed particles were first added at the tunnel boundary, and then slowly reduced, in order to mimic the excavation procedure, and avoid crack artefacts around the tunnel. When a steady-state stress was reached, the long term model was run for a period of 2 years. During the first two years, the model indicates crack propagation up to 25 cm from the tunnel perimeter. The number of connected cracks increases rapidly during the first 6 months, then remains virtually constant after one year. The computed evolution of the displacement field with the proposed model is presented in Figure 5-12.

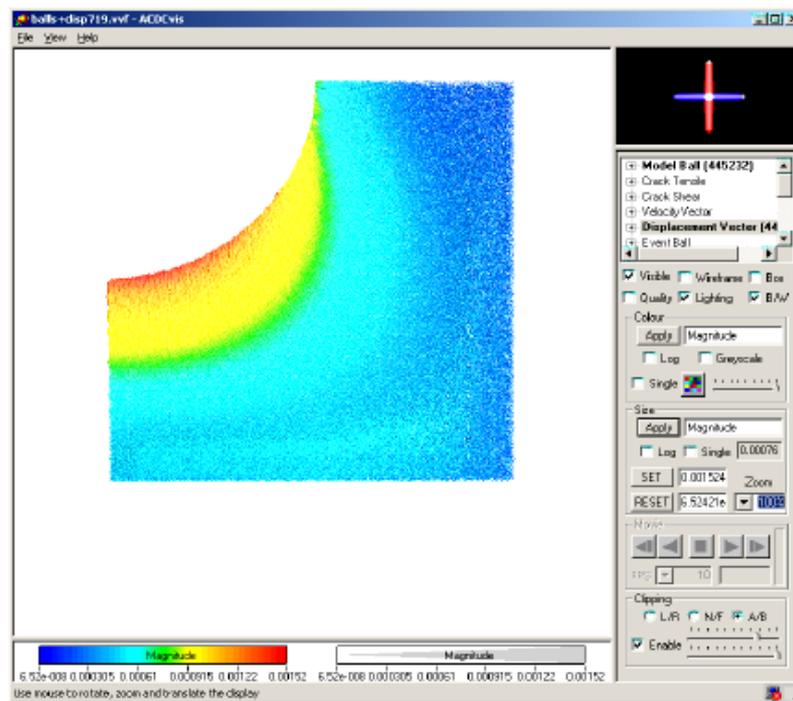


Figure 5-12: The displacement field around the Mont Terri excavation after two years /SAF 04/

5.3.6 Numerical Modelling of EDZ in Unsaturated Clay Formation /DUV 03/

A numerical modelling of hydromechanical responses in an unsaturated rock around a shaft submitted to excavation and drying is presented in /DUV 03/. In order to study influences of constitutive models, two representative models are used. The first one is an elastoplastic damage model (named IdepLML) developed for poromechanical behaviour of semi-brittle materials. In this model, a quadratic yield function is used to better describe pressure sensitivity of the material. The plastic flow rule is non-associated to describe the transition from plastic volumetric compaction to dilation. The plastic hardening law is defined as a function of equivalent plastic shear strain. Damage state is assumed to be isotropic and described by a scalar internal variable d . The damage evolution depends on plastic deformation. The elastic stiffness tensor is affected by the damage through a reduction of the elastic modulus. This model is extended to unsaturated materials. Therefore, the clay formation is considered as a porous medium saturated by a liquid phase and gas mixture (vapour and dry air). In order to take into account influences of capillary effects and material damage on plastic deformation, a generalized effective stress tensor is defined:

$$\hat{\sigma} = \frac{\sigma + \beta[S_w p_w + (1 - S_w)p_g]I}{1 - d} \quad (5-74)$$

where S_w is water saturation, $p_w(p_g)$ is water (gas) pressure, β is a coefficient for the generalized effective stress. The second constitutive model is an elastic perfect plastic model based on the classic Hoek and Brown failure criterion. This model is also adapted to unsaturated

rocks by using the effective stress concept without damage ($d = 0$). The parameters of the two models have been determined from triaxial compression tests on the East argillite and according to the mechanical properties provided by the geological referential of ANDRA. The two models have been calibrated so that they give the same failure strength in uniaxial compression test.

A 2D model of a circular vertical shaft is considered. By assuming that the shaft is very long and two horizontal main stresses are different, the plane strain condition seems to be suitable when a representative section of shaft is of concern. Each calculation is composed of three phases:

- Excavation phase performed in one day, the initial stress and pore pressure are decreased from their initial values to atmospheric pressure;
- Ventilation during 8 days with a relative humidity of 90% in the shaft;
- Setting-up of concrete lining at 8 days and then ventilation during 10 years always with the relative humidity of 90% in the shaft.

Note that the relationship between relative humidity and capillary pressure is given by the Kelvin law. The relative permeability for water and gas are defined as function of water saturations.

The probable increase of rock intrinsic permeability In EDZ due to cracks and plastic dilatancy can lead to is modelled with a simplified empirical relationship. For the IdepLML model, the rock permeability is a function of the equivalent tensile plastic strain:

$$k = k_0 (1 + \lambda \cdot (\varepsilon^{+p})^3), \quad \varepsilon^{+p} = \sqrt{\sum \langle \varepsilon_i^{+p} \rangle^2}, \quad \lambda = 0,8 \cdot 10^{10} \quad (5-75)$$

where ε^{+p} denotes the i^{th} positive (tensile) principal plastic strain. However, for the perfect plastic model (H&B), two zones with different permeability are introduced; the intact zone with the initial permeability and the failure zone where the permeability is multiplied by 100.

Some simulation runs were reported to investigate the sensitivity of the hydromechanical changes in the near vicinity of the modelled shaft to desaturation (ventilation) and to plastic deformation and failure due to excavation. It is shown that the desaturation process is mainly controlled by hydraulic properties (intrinsic permeability, liquid relative permeability) and hydraulic parameters (water retention curve). The damaged and failure zones are related to the initial in situ stresses and pore pressure, the constitutive behaviour of rock. The variation of rock permeability in the damaged zone is an important feature regarding the evolution of desaturation process and failure zone extent.

5.4 Transport Models for Bentonite Buffers

Three possible basic mechanisms have been proposed for gas invasion of water saturated compacted bentonite /HOC 04/:

1. Behaviour of the bentonite as a conventional porous medium, with the gas flow governed by conventional concepts of capillary pressure and relative permeability.
2. 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.
3. 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.

The experiments have shown, in varying degrees, the following features of gas transport in clay formations:

- A threshold pressure for gas entry. This has been related by some to the bentonite swelling pressure.
- Apparently, the displacement of only small volumes of water.
- 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.
- Changes in pore-water pressure in response to the applied gas pressure.
- Evidence of macroscopic fracturing events with radial flow from a central source.

Pusch et al. 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) /PUS 85/. In isotropically constrained experiments, 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 /HOR 94/. 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 co-workers explained the gas entry pressure as the capillary entry pressure for pre-existing pathways through the clay /PUS 87/. 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 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 under a confining axial stress of 10 MPa similarly showed 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 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 the 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 the swelling pressure plus back pressure was estimated to be about 10 MPa but the peak gas injection pressure was nearly twice this at about 19,4 MPa. Two other features of this test were presented as follows /NEA 96/:

1. 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
2. evidence of very small precursor flows that took place when the pressure exceeded 13,7 MPa. It may be 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 exhibited a more complex behaviour /HOR 94/:

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

- 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 $\mu\text{L hr}^{-1}$ 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.
- 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)
- 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 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 /NEA 96/.

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 geometry mentioned above, during both water flow and gas injection experiments. These results were discussed in the GAMBIT Phase 2 report /HOC 04/. An anomaly found with this response was that the porewater pressure did not appear to relax back to the applied back pressure.

The given above discussion shows that the transport mechanisms in compacted bentonite are comparable with the transport mechanisms in clay formations. The presence of the entry pressure, fissuring-fracturing by high fluid pressures, effect of the mechanical-chemical processes on flow and diffusion are common concepts. Some numerical concepts to model the gas and two-phase transport in bentonite mediums are given in the following section.

5.4.1 Two-phase Flow through a Deformable Porous Medium

In the framework of GAMBIT-GW project, a model was developed by considering 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. The theory was originally developed by *Biot*

/BIO 41/. The necessary extensions for Biot theory to be applicable to gas invasion of water-saturated bentonite are presented in /HOC 04/.

5.4.1.1 Mathematical Formulations

It is assumed that the solid grains are incompressible.

The model consists of:

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

$$\frac{\partial}{\partial x_j} \sigma_{ij} + \rho X_i = 0 \quad (5-76)$$

where x is the spatial co-ordinate [m], σ_{ij} is the stress tensor [Pa]; ρ is the density of the material [kg m^{-3}]; X is the material force per unit mass [m s^{-2}].

- b) Macroscopic stress-strain relations that are the generalisation of Equation Hooke Law for a porous medium with both a liquid phase and a gas phase. For this formulation, the solid grains are assumed incompressible:

$$\Delta \varepsilon_{ij} = \frac{1+\nu}{E} \Delta \sigma_{ij} - \frac{3\nu}{E} \frac{\Delta \sigma_{ij}}{3} \delta_{ij} + \frac{1}{3K} \Delta p_w \delta_{ij} + \frac{1}{3H_m} (\Delta p_g - \Delta p_w) \quad (5-77)$$

and

$$\phi S_w = \frac{1}{H_m} \left(\frac{\Delta \sigma_H}{3} + \Delta p_w \right) + \left(\frac{1}{R_m} - \frac{S_g}{H_m} \right) (\Delta p_g - \Delta p_w), \quad (5-78)$$

where

$\Delta \varepsilon_{ij} = \frac{\Delta V_p}{V}$; E is the Young's Modulus [Pa], H_m is the modulus of elasticity for the porous material with respect to a change in matrix suction, $(p_g - p_w)$ [Pa] and p_g is the pressure of the gas phase [Pa], S saturation as fraction and is the volumetric modulus of the gas phase with respect to a change in matrix suction, $(p_g - p_w)$ [Pa].

- c) Continuity equations for the pore fluids (i.e. liquid phase and gas phase), in which the fluid velocities are determined by Darcy's Law. Continuity equation for gas phase is generalised as combined equation for dissolved and free gas flow as follows:

$$\begin{aligned}
& -\frac{\partial}{\partial x_i} \left[\frac{M_g}{H_g} \left(p_g q_i - S_w \phi \frac{d_m}{\tau} \frac{\partial p_g}{\partial x_i} \right) - \rho_g \frac{k_{g,ij}}{\mu_g} \left(\frac{\partial p_g}{\partial x_i} + \rho_g g \delta_j \right) \right] \\
& = \frac{1}{V} \frac{D}{Dt} \left[p_g \left(S_w \frac{M_g}{H_g} + S_g \frac{M_g}{RT} \right) V_p \right]
\end{aligned} \tag{5-79}$$

Where ρ is the density of the gas [kg m⁻³]; $k_{g,ij}$, is the permeability tensor for the gas phase [m²]; μ_g is the viscosity of the gas [Pa s]; p_g is the pressure of the gas [Pa]; M_g is the molar mass of the gas [kg mol⁻¹]; R is the ideal gas constant [J K⁻¹ mol⁻¹]; T is the temperature [K].

5.4.1.2 Physical Properties of Bentonite Clay

To complete the framework of the model some physical properties of the compacted bentonite had also to be determined. The functional form of elastic parameters and the permeability tensor were given as the following:

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 poisson ratio, ν , Elastic modulus E , the modulus of elasticity for the porous material with respect to a change in matrix suction, $(p_g - p_w)$; H_m and the volumetric modulus of the gas phase with respect to a change in matrix suction, $(p_g - p_w)$; R_m . Since the volume occupied by the gas phase is small (i.e. deformations of the bentonite are small), both Poisson's ratio, ν , and Young's modulus, E , is taken to be constant from measured values.

Considering the other elastic moduli (H_m and R_m), if Equations (5-78) and (5-79) are to apply also in the case when there is just a pure liquid phase (i.e. the equations reduce to one phase in the limit $S_w \rightarrow 1$), then there has to be a gas entry condition, Γ , which depends only on the scalar invariants of the stresses, such that

$$\begin{aligned}
p_g < \Gamma & \Rightarrow \text{no free gas} \\
p_g > \Gamma & \Rightarrow \text{free gas}
\end{aligned}$$

With the property that:

$$p_g < \Gamma \Rightarrow \frac{1}{H_m} = \frac{1}{R_m} = 0 \tag{5-80}$$

The form of Equations (5-77) and (5-79), as well as experience with the GAMBIT-GW model suggests that it may be appropriate always to set:

$$\frac{1}{H_m} = 0 \tag{5-81}$$

In the case where gas pressure is above of the gas entry pressure, the following criterion for R_m , is suggested.

$$\frac{1}{R_m} = \frac{1}{R_1} \sum_{i=1}^3 \theta [p_g - (-\sigma_i - p_w + \tau_s)] \quad (5-82)$$

If the interface between gas and liquid is unstable, including a term representing the interfacial tension, the Eq. (5-82) turns to:

$$\frac{1}{R_m} = \frac{1}{R_1} \sum_{i=1}^3 \theta [p_g - (-\sigma_i - p_w + \tau_s) - \sum \kappa] \quad (5-83)$$

Where Σ is a numerical parameter, used to control any instability at the interface between gas and liquid [Pa m]; κ is the curvature of a contour of the gas pressure [m^{-1}].

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 (5-83):

$$\frac{1}{R_m} = \frac{1}{R_1} \sum_{i=1}^3 \theta [p_g - (-\sigma_i - p_w + \tau_s) - \sum \kappa] + \frac{1}{R_2} \theta (S_g - S_{gi}) \quad (5-84)$$

Finally, previous experiences of modelling the migration of gas in bentonite suggest that the gas saturation (actually, the permeability of the gas phase) should evolve with an exponential dependence on matrix suction, $(p_g - p_w)$. Therefore, the form for the elastic modulus R_m was taken to be:

$$\frac{1}{R_m} = \frac{1}{R_1} \sum_{i=1}^3 \theta [p_g - (-\sigma_i - p_w + \tau_s) - \sum \kappa] + \frac{1}{R_2} \theta (S_g - S_{gi}) S_g \quad (5-85)$$

To summarise, it is proposed that:

a) The usual elastic moduli, that are ν and E , should be taken as constants;

b) The modulus H_m should satisfy the equation $\frac{1}{H_m} = 0$;

c) The modulus R_m should be modelled by Equation (5-85).

Permeability tensor for the gas phase

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

$$\Delta k_{g,ij} = k_{g,0} \delta_{ij} + k_{g,1} \Delta \sigma_{ij} + k_{g,2} \Delta \sigma_{ij} \Delta \sigma_{ji} \quad (5-86)$$

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 f 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, 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 is assumed that:

$$\begin{aligned}
 k_{g,0} &= \Delta[(\theta(S_g - S_{gc}))k_0 S_g^2] \\
 k_{g,ij} &= \theta(S_g - S_{gc})k_0 S_g^2 \delta_{ij} \Rightarrow \begin{aligned} k_{g,1} &= 0 \\ k_{g,2} &= 0 \end{aligned}
 \end{aligned} \tag{5-87}$$

Here, S_{gc} is a critical gas saturation [-]; k_0 is a parameter that is characteristic permeability of the bentonite [m^2].

5.4.2 Coupling with Hydromechanics; Swelling Model /XIE 04/

An upscaling concept for swelling/shrinking phenomena in expansive porous media, which are triggered by the mineral composition of the material is presented by /XIE 04/. The microscopic approach is based on the mineral structure and the diffusive double layer (DDL) theory. A constitutive equation to transform microscopic volume into macroscopic porosity changes is derived, which is the link between the two scales. Main processes during swelling/shrinking are hydraulic (water transport, re-saturation, de-saturation), chemical (particle-water-cation interaction) and mechanical ones (volume and porosity changes, swelling pressure), which are highly coupled. These processes are described at the macroscopic level.

5.4.2.1 Microscopic Level; Mineral Structure Model

Bentonite is a mixture of clayed minerals, in which montmorillonite is the main mineral for swelling. The unique mineral structure of montmorillonite is composed of two structural units, the silica tetrahedron and the alumina octahedron. These units are interconnected and extend to form thin sheets (only about 10^{-9} m in thickness). Several such sheets are stacked one above the other, to form a crystal particle. Microscopic view of the individual particle of montmorillonite can only be obtained by Scanning Electron Microscopy (SEM) or Transmission Electron Microscopy (TEM) methods. The particles are normally composed of thin sheet montmorillonite minerals. Owing to the weak connection between the sheets, water is easily to entrance between them with the help of the electron attraction which results from the net charge of the bentonite particle. The particles may be consequently separated into smaller pieces and macroscopically leads to swelling. Based on these results, a simplified microstructural model of bentonite is set up. The model before fluid uptake is illustrated in Figure 5-13 (a). With fluid intrusion a film of water/solution builds up around the surface of particles owing to the special structure of the net negative charge on the surface of the expansible minerals in bentonite (e.g. montmorillonite). In the meanwhile fluid can also be absorbed into the interlayer gaps of bentonite particles and results in expansion of the particles. Consequently the bentonite will swell macroscopically. If the volumetric expansion is confined, a swelling pressure appears. This mechanism is schematically illustrated Figure 5-13 (b).

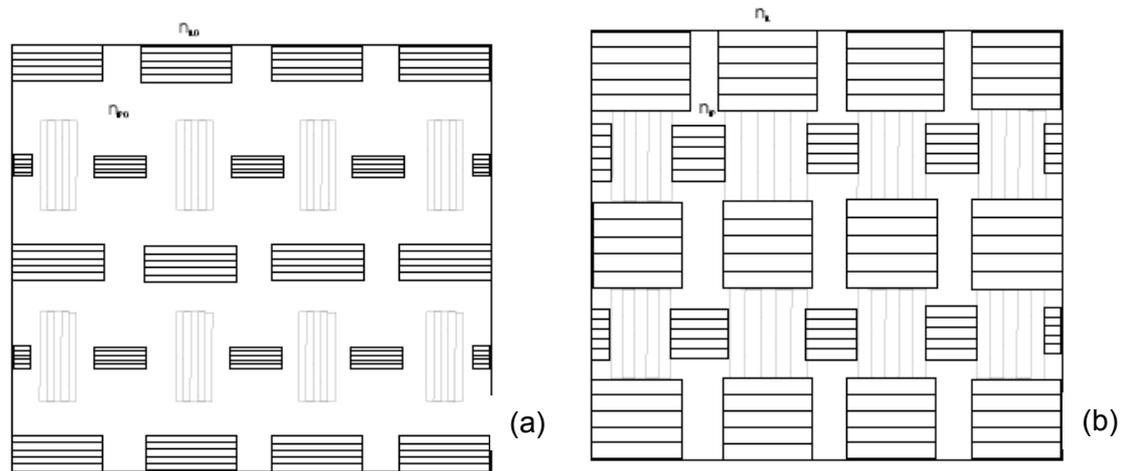


Figure 5-13: Simplified microstructural model of bentonite before and after saturation /XIE 04/

5.4.2.2 Microscopic Level; Diffusion Double Layer (DDL) Theory

Montmorillonite is the main component of bentonite. These mineral particles appear negative charge at the surface owing to the substitution of Al for Si in the tetrahedral sheet during the mineral formation. By contact with water, the mineral surface will attract positive ions to balance the negative charge. This can result in the formation of the diffusion double layer around the mineral surface. The thickness of the DDL decreases with the increase of concentration and charge of the ions in the fluid, which can be theoretically described by Gouy-Chapman theory.

For a flat surface with low net charge the electric potential is described as:

$$\psi = \psi_0 \cdot e^{-x/\delta} \quad (5-88)$$

where ψ is the electric potential at the surface, F is the Faraday constant ($=96485.309$ [C.mol⁻¹]). The Debye parameter δ reveals the "thickness" of the diffuse double layer (in meters) which is inversely proportional to the ionic strength I :

$$\delta = \left(\frac{\epsilon \epsilon_0 RT}{2F^2 I \times 10^3} \right)^{0.5} \quad (5-89)$$

5.4.2.3 Interlayer Porosity (Microscopic)

By the saturation process the solution will be absorbed and transported through the pores. In the meanwhile it can also enter the interlayer space of the particles. Thus the volume of each particle increases with the fluid intrusion. Consequently the sample as a whole tends to expand. If the sample is not confined, the particles can extend freely. Around the particles and within the interlayer space Diffuse double layers tend to build up completely in case of free swelling. The number of layers m within one particle of expansive minerals in bentonite is a

mineral structural parameter. Effective layer number is defined here as those layer numbers that contribute to the swelling effect. As the montmorillonite particles are very fine in size, the average value is used to calculate the interlayer porosity. So that it can be determined from the specific surface experiments as the ratio of maximal specific surface area S_{max} (including the surface between layers, which can separate by swelling) and external specific surface area $S_{external}$ (only the surface of particles). Thus the maximal interlayer porosity for one particle with m effective layers can be calculated:

$$\phi_{IL} = \frac{2m \cdot A \cdot \delta}{V_0}, \quad (5-90)$$

where a simplification for the surface area A of the particle can be made assuming that the particles are circles with diameter d .

5.4.3 Macroscopic Level; CHM Swelling

Microscopic volume changes should be translated into macroscopic changes of porosity. As a consequence, hydraulic properties of the porous media, such as capillarity and permeability, have to be affected as well. The concept of the Chemo-Hydraulic-Mechanic (CHM) swelling model for the first step of coupling is based on the microstructural models in Figure 5-13 and the Gouy-Chapman theory. For the CHM model it is assumed that the total porosity ϕ can be divided into porosity between particles ϕ_{IP} and that within the particles or interlayer porosity ϕ_L :

$$\phi = \phi_{IP} + \phi_{IL} \quad (5-91)$$

If the interlayer porosity is expressed as function of the measured specific surface, combining Eq. (5-88), the following formulation is obtained for the maximal interlayer porosity:

$$\phi_{IL} = m S_0 \rho_0 \left(\frac{\varepsilon \varepsilon_0 R T}{2 F^2 I x 10^3} \right)^{0,5} \quad (5-92)$$

For the highly compacted samples of bentonite/sand mixtures, volume change in case of free swelling can be calculated from the interlayer porosity change (ϕ_L). For an absolutely dry sample, ϕ_L is assumed to be the reference value, set as zero. The maximal interlayer porosity can be reached only under free swelling case. Further the expansive minerals are assumed to be the only contributor for the swelling. Therefore it is reasonable to assume that for bentonite or bentonite/sand mixture ϕ_L is a function of water saturation S_l and volume fraction of expansive minerals β :

$$\phi_{IL} = f(S_l) \cdot \beta \cdot \phi_{IL \max} \quad (5-93)$$

For completing the model, a two-phase flow system is considered; the mass balance and fluid momentum balance equations are developed in a conventional way. For calculating the capillary pressure and relative permeability curves van Genuchten Model is proposed. After the discretization of the formula with finite differences approach and implementation in the

software ROCKFLOW, the obtained model was validated using two experimental drying/wetting cases /XIE 04/.

5.4.4 Modelling of Transport and Reaction in an Engineered Barrier

An attempt to model the chemical transformations of the engineered barrier and chemical-elements diffusion impact resulting from the temperature increase (disintegration reactions of wastes), the presence of fluids coming from the geological barrier, and from the liberation of iron (degradation of the containers) is presented by /MON 05a/. For that, a thermo-kinetic hydro-chemical code (KIRMAT: Kinetic Reactions and Mass Transport) was used. This code considers a 1D multi-solute mass transport system and is based on the steady-state or stationary-state properties of the thermo-kinetic Eulerian reactive transport mass balance equations. In KIRMAT, solute transport is added to kinetic dissolution and/or precipitation reactions. A chemically controlled time step (noted Dt_c) allows preserving accuracy of the calculations. Its value is chosen inversely proportional to the largest of the first derivative variations among all the solute concentrations, and is controlled by setting the h parameter (inversely proportional to Dt_c). The following aspects were considered to simplify the modelling system.

Geochemical transformations in a fluid saturated medium

Based on recent study showing that a bentonite barrier is fully water-saturated within approximately 3–4 years after deposition it was supposed that the interface contact “engineered barrier- geological medium” operates as a permeable membrane only to the water during the hydration phase of the engineered barrier (Figure 5-14). In this case, the chemical species contained in the geological fluid will only be adsorbed (or retarded) in the first few centimetres of the engineered barrier. These comments allow the assumption that initially the engineered barrier is saturated with a fluid of low concentration. In the present study, the engineered barrier is initially saturated with pure water or with a fluid of low concentration.

Solute diffusion

In the water-saturated engineered barrier of bentonite, the interstitial fluid is almost static because of the very low permeability in the medium. In these conditions, the convection transport can be negligible. Then, the significant transport phenomenon through the engineered barrier is uniquely the diffusion of chemical elements, mainly iron diffusion toward the geological medium and K, Ca, Na, Si, etc. diffusion toward the metallic container.

Reducing conditions

Following the closing of the repository system, the hydrolysis reactions of the mineral constituents “of the engineered barrier” take place in reducing conditions ($p_{O_2}=0$; $E_h = -200$ mV) because the oxygen is consumed rapidly.

Container corrosion

In the KIRMAT code, it is difficult to take the container corrosion directly into account. At the present time, two possibilities are considered:

- A significant concentration of total iron (0.001 mol/kg H₂O) in the boundaries of container. That is, this possibility does not consider the container corrosion rate. Here, the total concentration was taken arbitrarily constant during 1000 years of simulation.
- The second possibility allows to consider the container corrosion as a dissolution reaction in reducing conditions:



This perturbation into the system was simulated by a standard kinetic equation of mineral dissolution where the rate constant of iron dissolution was estimated considering a linear rate of corrosion of 5 μm/year during 100 years. The rate constant of iron dissolution [mol/m².year] was then estimated using the following formula:

$$k_{dFE} = \frac{v_{corrosion} \cdot \rho}{M} \quad (5-95)$$

with $v_{corrosion}$ as the rate linear corrosion, ρ as the specific (grain) density, and M as the molar mass of iron.

Two scenarios were taken into account: in the first scenario, the engineered barrier is initially in disequilibrium with the interacting solution (pure water). In this case, the system is “very reactive”. In contrast, in the second scenario, the stationary state of the system was reached by a previous simulation in closed system, i.e., without mass transport. Here, the interacting fluid is slightly charged in Na⁺, H₄SiO₄, and K⁺. The system modelled herein was considered to consist of a 1-m-thick zone of water-saturated engineered barrier of bentonite clay. This non-equilibrated or stationary-state system was placed in contact with a geological fluid on one side, which was then allowed to diffuse into the barrier, while the other was kept in contact with iron-charged water (0.001 mol/kg H₂O) or with a source of metallic iron.

The results show that Na/Ca–montmorillonite-to-Ca–montmorillonite conversion, the montmorillonite-to-chlorite conversion and dissolution/precipitation of accessory minerals were the most relevant chemical processes. The first chemical transformation represents about 22% in the worst case, i.e., near of the engineered barrier interfaces, while the second chemical transformation only represents about 3% (near the container), i.e., a high concentration of iron favours the chlorite–FeAl precipitation. Concerning the dissolution/precipitation of accessory minerals, in general, it was observed that the quartz, microcline, and albite were re-precipitated in the system; the calcite and biotite were partially dissolved, and the pyrite kept inactive. On the other hand, only a short augmentation of total porosity was observed near of engineered barrier interfaces.

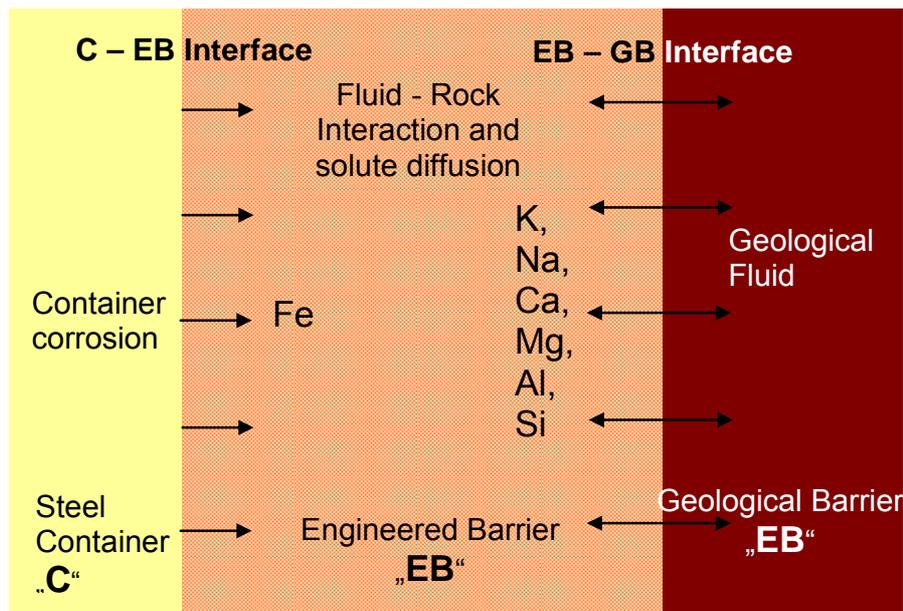


Figure 5-14: Schematic representation of fluid–rock reaction and solute diffusion in an engineered barrier, concept /MON 05a/.

5.5 Executive Summary

A summary of studied conceptual models is given in Table 5-3. In basic, the transport of gases is modelled by diffusion and dispersion supported advection. Gas moves either dissolved in liquid phase or together with liquid phase. In natural clay systems the flow of one-phase gas is not expected. There are few open questions regarding on the phase behaviour of gas-liquid phase properties excepting support the equation of states with empirical parameters such as solubility of gases in water with various ionic activities. The main problem arises from two sides. The first one is the physico-chemical interactions in gas-water-clay interfaces. The second one is the geometrical coupling of the flow pathways coupled with mechanics. Both are key features for the formulation of the gas retention in transport models. As can be concluded from the Table 5-3, more modelling efforts have been made for plastic clays than for indurated clays. Capillary bundle model or similar models coupled with geomechanics intent to conceptualize the preferential pathways introducing the capillary effects i.e. threshold pressure in two-phase flow. The validations of these models are reported to give sufficiently good results in matching the experimental data. The modelling of gas transport in indurated clays necessitates a better understanding of the fracture physics and its application in conventional and probably non-conventional flow formulations. If indurated clay contains already open fractures, then the problematic reduces to the flow in fractured geological media in which the petroleum industry offers a very big experience with network or continuum models with various concepts for taken the configuration of the fractures into considerations. Modelling of the gas transport, as two-phase or with diffusion supported one-phase flow in tight indurated clays necessitates the strong coupling with fracture mechanics to model induced fracturing.

As the case in other host rocks, the EDZ's should be taken in modelling efforts into consideration. The most important feature is the coupling of the hydraulic properties with mechanical changes. In clay formations the chemical coupling in EDZ's is also important. The fracture mechanics considered in modelling the gas transport in near and far field of the indurated clay formations can also be used for this purposes. A validated hydraulic-mechanical coupling does not exist for clay formations.

To be applied in full scale performance analysis of the repositories all modelling concepts should be incorporated into numerical codes, if the capacity of these codes is not sufficient to model the transport in clay formations. In the following section the numerical codes that are used or that can be used for clay formations are briefly given and discussed. In order to facilitate the evaluation of these codes and related phenomena in clay formations a summary of all aspects, mechanisms and parameters related to gas transport is made and determined with codes, acronyms and presented in Table 5-4.

Table 5-3: Summary of the conceptual models developed for gas transport in clay formations

Approach, Modelling Attempt	Short Description	Validation, Application, Attempts	Ref.
Empirical formulations	Definition of the gas breakthrough pressure and gas flow rate as function of gas saturation, vertical stress and temperature	Applied for plastic clay formations, Boom and Pontida clays	/ROD 99/
Consolidation after Terzaghi	Compressible behaviour of both the solid matrix and the pores. Changes in the volume is induced by changes in the internal fluid pressure p or an externally imposed stress	Coupled with mathematical formulations of the flow in fractures within the code FRAC3DS and tested for one-dimensional modelling of transport through Opalinus Clay.	/KOS 04/
Transient flow in deforming poro-elastic medium	Definition of the transient flow in a saturated linear elastic porous medium based on Biot's Theory of consolidation and Terzaghi effective stress	General formulation applicable for saturated flow (water with gas dissolved) in clay rocks	/HOR 96/ /PAL 89/
Thermo-Hydro-Plastic Coupling	An equation for coupling the pore pressure, solid displacement (Terzaghi concept, elastic and plastic) and heat flow	Application for plastic clays Boom and Pontida, satisfactory results comparing the experiments.	/LAL 02/
Thermo Hydro-Mechanical Coupling	Classical phenomenological approach by Biot using the effective stress concept of Terzaghi. The set of equations is conceptionally split into a solid and a fluid problem.	Two case studies are presented as saturated and unsaturated single phase flows. In unsaturated case it is assumed that the desaturation takes place due to gravitational effects. The capillary pressure and relative permeability curves are taken from the experimental studies.	/KOH 04/
Episodic Flow with Fracture as Pathway	A simplified conceptual model with a fracture as pathway with stress dependency width (as function of effective stress).	Conceptual model to be applicable for gas, two-phase flow in plastic as well as indurated clays neglecting TC coupling	/HOR 96/

Approach, Modelling Attempt	Short Description	Validation, Application, Attempts	Ref.
Capillary Bundles,	Porous media is composed from series of non-intersecting capillaries. Two-phase flow modelling defining gas entry pressure, saturation distribution in the model, no dependency on the stress dependency.	The numerical model, TOPAZ based on the above given formulation for two-phase flow through clay formations is used to simulate the experiments performed with Boom Clay core samples. Good agreements.	/ORT 96/
Capillary Bundles with Geomechanical Effects	“Capillary bundles” model coupled with a simple geomechanical concept, the width of the capillary, therefore the saturation in the capillary are dependent on the effective stress	Attempts to match the experimental results in Boom Clay, gas flux, breakthrough time with various tortuosity factors. Agreement is good.	/ORT 97a/ /ORT 97b/
Multiple Front Propagation	Fluids (wetting and non-wetting) advance through the clay of the tip of the propagating gas flow channel. The gas-filled pathways are assumed to dilate elastically for small displacements. The number of paths is set by an input channel density.	Tested for modelling experiments performed on Boom Clay and Mx80 bentonite buffer. Good prediction, the estimation of the empirical parameters of the equation may be a problem.	/HOR 96/
Crack Opening	Representation of single fractures embedded in a continuous finite element, the aperture of the fracture is estimated as a function of deformation,	Some examples to show the capabilities of the formulation in /ALO 02/ /DEL 02/ /OLI 05/. Modelling attempts of the tests conducted to study gas flow through compacted clays /ALO 02/.	/ALO 02/ /DEL 02/
Dual-Continua	The model is combined with two systems: a macropore or fracture pore system at the macroscopic level by fracture continuum (FC) and a less permeable matrix pore system by matrix continuum (MC). The transfer value between these two continua is important.	Application in Decovalex Project	/DUY 06/
Brush Model	Advection-dispersion in fractures and diffusion to the matrix with lower permeability	Implemented in ROCKFLOW, applied for the test tracer toxic waste disposal site of Mönchhagen, Not applied yet for clay formations	/LEG 96/

Table 5-4: Aspects, parameters and concepts related to gas transport in clay formations

Group	Process – Parameters	Acronym	Comment
Basic	Mass-Hydraulic Flux-Conservation	B_HC	
	Energy Flux-Conservation	B_EC	
	Mechanical Equilibrium	B_ME	
	Chemical Equilibrium	B_CE	
	Inverse Modelling	B_IM	
Geology	Faults	GF_F	
Geometry	Litho-Facies	GF_L	

	Areal Heterogeneities, Regions	GF_AH	
	Up-Scaling	GF-US	
	Tortuosity	G_TR	
	Porous Media	G_PM	
	Bundle Model	G_BM	
	Bundle Model with Geomechanics	G_BMG	
	Multiple Front Model	G_MFM	
	Crack Dilation Model	G_CDM	
	Fractures	G_F	
	Dual Porosity	G_F_DP	
	MINC	G_F_MINC	
	Discrete Fractures	G_F_DF	
	Statistical Configuration	G_F_SC	
	Dissolution/Precipitation	G_DP	
	Porosity-Permeability Relation-Method	G_PP_X	X, Method
	Relative Permeability Models		
	Corey	G_RP_Corey	
	Van Genuchten	G_RP_Gen	
	Grant	G_RP_Grant	
	Verra et al.	G_RP_Verra	
	Fatt &Klikoff	G_RP_Klikoff	
	Capillary Pressure Methods		
	Pickens	G_CP_Pick	
	Milly	G_CP_Milly	
	Leverett	G_CP_Lever	
	Van Genuchten	G_CP_Gen	
	Threshold Pressure	G_TP	
	Capillary Hysteresis	G_CH	
Phase Behaviour	Water properties	P_WP	
Thermodynamic	Brine Properties	P_BP	
	Vapour	P_VP	
	Air	P_AP	
	Gas, CO2, empirical correlations	P_CO2_EC	
	Gas, CO2, cubic equation of state	P_CO2_EOS	
	Gas, other gases, empirical correlations	P_X_EC	X: Gas type
	Gas, other gases, cubic equation of state	P_X_EOS	X: Gas type
	Gas, gas mixtures, cubic equation of state	P_GM_EOS	
	Solubility of Gas in Liquid_Gas_Method	P_SG_X_X	
	Thermodynamic Liquid_Gas Mixture, Correl.	P_LG_C_X	X: Method
	Thermodynamic Liquid_Gas Mixture, EOS	P_LG_EOS_X	X: Method
	Source (Gas Generation)	P_GG	
	Function of Time	P_GG_T	
	Function of Waste Type	P_GG_W	
	Function of Time/Waste	P_GG_TW	
	Precipitation/Dissolution	P_PD	
Hydraulic-Transport	One-phase Flow, Darcy	H_OP_D	
	Deviation from Darcy Law	H_DD	
	Two –phase Flow, Darcy	H_TP_D	

	Hagen-Poiseuille	H_HP	
	Cubic Law	H_CL	
	Dual Continua Model	H_DC	
	Intermittent/Episodic Flow	H_EF	
	Capillary Bundle Model	H_CB	
	Capillary Bundle Model with Geomechanics	H_CB_G	
	Fracture Flow-Matrix Diffusion	H_FMD	
	Mineral Structure Model	H_MSM	
	Dispersion	H_DIS	
	Diffusion, Fluids	H_DIF_F	
	Diffusion, Surface	H_DIF_S	
	Colloid Transport	H_CT	
	Adsorption		
	Precipitation/Dissolution-Porosity	H_PD_P_X	X: Method
Thermal	Liquid Properties	T_LP	
	Rock Properties	T_RP	
	Gas Properties	T_GP	
	Thermal Effect on Minerals	T_ME	
	Thermal Induced Consolidation	T_CO	
	Source Term	T_ST	
Mechanical	Elastic-visco-elastic modelling	M_EVE	
	Swelling	M_S	
	Geo_Stability	M_GS	
	Barcelona Basic Model, Elastoplastic Law	M_BBM	
	EDZ, Size. Structure	M_EDZ_S	
	EDZ, Time Effect	M_EDZ_TE	
	EDZ, Hydraulic Properties	M_EDZ_HP	
	EDZ, Self Sealing	M_EDZ_SS	
	EDZ, Desiccation Cracking	M_EDZ_DC	
	Crack propagation-Pathway Dilatation	M_CP	
	Clay-Water Interaction	M_CW	
Chemical, Physico- chemical	Redox	C_RX	
	Surface complexation	C_SC	
	Rock oxidation	C_OX	
	Chemical osmosis	C_CO	
	Dissolution/Precipitation	C_DP	
	Ion-Exchange	C_IE	
	Thermodynamic databank	C_TD_X	X, Data- bank
	Colloid Formation	C_CF	
	CHM Model for Swelling	C_CHM	
Coupled Processes	Thermal-Hydraulic	TH	
	Thermal-Hydraulic-Mechanical	THM	
	Thermal-Hydraulic-Chemical	THC	
	Thermal-Hydraulic-Mechanical-Chemical	THMC	

6 NUMERICAL MODELLING CODES

In this section the numerical codes that are used for modelling the transport in clay formations as host rock for geological repository are listed. These codes apply the basic concepts for modelling flow and related transport phenomena in porous and/or fractured media by discretization of the space and time with finite differences/elements methods. Some of them are commercial products; other codes are accessible for further developments by the user. The qualification and validation efforts continue for all of these codes; this is expected taken the difficulties related the physics of the transport in clay formations into account.

The evaluation of the software TOUGH2 and TOUGHREACT was straightforward because of the long-time experience of the authors on these codes. The codes available for testing purposes e.g. PORFLOW and Code-BRIGHT were downloaded and with some simple applications characterized. Some other codes such as THAMES, ROCKMAS could only be evaluated based on the provided information in related literature. In all cases the applications performed with listed numerical codes were tried to be taken into consideration in the evaluating efforts. However this part of the study can not and should not be taken as a benchmark similar to Project EVEGAS /MAN 97/. This is rather a listing and a preliminary evaluation of the related codes. As a conclusion this part of the study is due to a continuous care and revalidation. For listing, a ranking based on the knowledge and experience on the corresponding codes is preferred.

6.1 TOUGH2

TOUGH2 is a numerical simulator for non-isothermal-fluid flows of multi-component, multi-phase fluids in one, two, and three-dimensional porous and fractured media. It was developed at Berkeley National Laboratory in the USA and is continuously maintained. TOUGH2 is used world-wide by more than 150 institutes. Several different fluid property modules and enhanced process modelling capabilities exist. TOUGH2 is written in standard Fortran 77 and can be run on any platform. The source code has a modular architecture and can be easily modified for any user specific problem. TOUGH2 uses unstructured grids which enables the flow simulation in complex structures. Several numerical parameters (e.g. time step function or weighting) and different auxiliary functions for capillary pressure and relative permeability are available for an optimum adaptation to the physical problem.

TOUGH2 is used since many years (since 1992) for the numerical solution of the physical problems from wide variety of spectrum; geothermal, groundwater, waste isolation, underground storage and oil-gas engineering. Therefore many version of TOUGH2 exists in the literature adapted for the specific cases with necessary implementations.

6.1.1 Technical Description /PRU 99/

Fluid advection is described with a multiphase extension of Darcy's law; in addition diffusive mass transport in all phases is considered. Heat flow occurs by conduction and convection. Several modules for different fluid systems in non-isothermal multiphase flow exist. These

are e.g. a module for the flow of tracers (e.g. radionuclides) including the effects of advection, diffusion, dispersion, adsorption, volatilisation and radioactive decay, a module for the system water-salt and a non condensable gas including the effect of precipitation and dissolution of salt, and another module for the flow of water-air and a volatile organic compound.

A summary of the modelling properties of TOUGH2 is given in Table 6-1.

6.1.2 Applications in Clay Formations

Significant number of application of TOUGH2 for modelling the transport of the fluids in geological repositories can be found in related literature. However studies on clay formations are limited. Several investigations are published on modelling the flow through fractures or fractured media. In /HOC 95/ for example, the equivalent continuum (ECM) and dual permeability (DK) models for flow in fractures are assessed and compared. The numerical modelling of flow in artificial fractures in a clay matrix is first investigated in /KRO 98/ in a modelling study of the remediation of semi-volatile contaminants. The effect of the mechanical effect respectively rock compaction, swelling and the damage at the excavated damaged zone are first implemented in /JAV 98/, /JOB 98/, /FRE 98/.

A numerical study was conducted, representing the backfilled disposal tunnels repository in the Opalinus Clay formation (SF and ILW, respectively) and the surrounding host rock formation by a two-dimensional cross-section /POP 03/. The simulations were carried out with the TOUGH2 EOS5 module. A sensitivity study aimed at investigating the impact of repository-induced processes (heat, gas generation) and parameter uncertainties on the evolution of porewater pressure was carried out. The following features of TOUGH2 were used for modelling:

- gas dissolution in the pore water (Henry's law)
- gas migration into backfill materials and rock under the assumption of multiphase flow in an homogeneous porous medium
- pore water displacement and
- thermal conduction and expansion.

In /ENG 03/ hydraulic parameters of unsaturated SPV Vol clay/crushed rock mixtures were calculated in the presence of water with different ionic concentrations by using the inverse modelling module of TOUGH2, ITOUGH. The influence of the swelling pressure as well as the use of pure water on the capillary pressure is investigated. The inversion with the van Genuchten model results in parameter estimates that are consistent with the values obtained from the experimental data.

During the last TOUGH symposium (2006) three study that are explicitly investigating the hydro-mechanical problems in clay formations were presented. In /POD 06/ the episodic or intermittent flow that is one of the dominant flow mechanisms in clay formations is numerically investigated. The gas threshold pressure test (GTPT) in a deep borehole at Andra's Underground Research Laboratory near Bure, France was analyzed using the two-phase simulator TOUGH2 /SEN 06/. Even though the standard version of TOUGH2 does not consider coupled mechanical processes associated with the observed fracturing, an analytical

fracture mechanics analysis was used to estimate the fracture volume, aperture, and extent. The simulation of the initial fracture response used a restart option to incorporate the inferred fracture characteristics in the numerical model. The closure and re-opening of the fracture during the subsequent recovery and second gas injection phase was implemented by calibrating a pressure-dependent permeability relationship for the fracture elements.

A preliminary numerical model of the full-scale test of gas transport in bentonite at the Aspö Hard Rock Laboratory in Sweden was conducted with a modified version of TOUGH2 /ASP 05/,/CAL 06/. Development of the gas-transport model required modifications to TOUGH2 to simulate expected gas transport mechanisms. While the mechanism for gas transport within bentonite is not well known, three potential mechanisms have been proposed:

- conventional two-phase flow through a porous medium
- stress- or pressure- induced microscopic fracturing of the bentonite to provide pathways for gas flow
- stress- or pressure- induced macroscopic fracturing of the bentonite to provide pathways for gas flow

Each of these mechanisms may work individually or simultaneously. TOUGH2 was modified to include a pressure-dependent permeability function to simulate micro- or macro- fracturing and a permeability-dependent capillary pressure function to simulate fracture dilation. Additional modifications to TOUGH2 were implemented to simulate He gas.

As can be concluded from the above summarized scientific activities published in TOUGH Symposiums as well as many other works published elsewhere, TOUGH2 is a convenient tool for the numerical modelling of fluid/gas transport in clay formations. However a fully coupled version for modelling the hydraulical, thermal and mechanical phenomena is not available yet. The main difficulty of applying TOUGH2 for clay formations arises from the lack of a chemical module that can model the chemical processes taking place during the transport.

Table 6-1: Properties of TOUGH2 in terms of modelling gas transport in clay formations

Governing equations		
		Basic mass and energy balance, B_HC, B_EC, B_IM
Hydraulic transport modelling		
	Advection/dispersion	H_TP_D, Advective mass flux is a sum over phases. H_DIS, Hydrodynamic dispersion with longitudinal and transversal dispersion coefficients
	Diffusion	H_DIF_F, Molecular diffusion taken into account, Fick's law, multi-phase diffusion
	Phases/Components	P_WP, P_AP, P_VP, P_AP, P_CO2_EC, P_X_EC 3 Phases according to the EOS module considered, the thermodynamical and thermophysical properties of the components and phases considered are calculated in each individual EOS module Components considered in related modules ; water, brine, air, radionuclide 1-2, non-condensable gas with salt precipitation, CO2/CH4/H2
	Sorption	H_A, Reversible instantaneous linear sorption, taken into account in mass accumulation term
Geology-Geometry modelling		
	Porous media	GF_F, GF_L, GF_AH, G_TR Conventional, with tortuosity and capillary characteristics Relative permeability functions, G_RP_Corey, G_RP_Gen, G_RP_Grant, G_RP_Verra, G_RP_Klikoff Capillary pressure functions, G_CP_Pick, G_CP_Milly, G_CP_Lever, G_CP_Gen
	Fractured media	G_F, G_F_MINC, G_F_DP Classical double-porosity concept after Warren and Root. Rock matrix and fractures may exchange fluid or heat by means of interporosity flow
	Changes in petrophysical parameters	G_DP, G_DP_KK, G_DP_CL,
Heat transport modelling		
	Convective/conductive	B_EC; Heat flux with conductive and convective components
	Effect on phase properties	Considered
Mechanical coupling		Individual Implementations
	Rock convergence	Limited and individual efforts /LOR 99/ after /PSE 85/ , /JAV 06/
	EDZ	Not fully coupled, time dependent EDZ porosity /FRE 98/
	Swelling	/JOB 98/, /LOR 99/ permeability related to swelling through void ratio and swelling pressure, validated with measured values in a Na-Bentonite
	Fracturing, pathway dilatation	Implementation after /CAL 06/, /SEN 06/,
Chemical coupling		
	Physical	P_PD, Physical precipitation considered for NaCl
Application for clay formations		
	Fracturing, pathway dilatation	Implementation after /CAL 06/, /SEN 06/

Discretization	
Space	Integral finite difference method. The discretized flux is expressed in terms of averages for the neighbouring cells. The grid geometry flexible.
Max grid size	100000
Time	First order finite differences, flux terms fully implicit
User friendliness	
User Manual	A good developed user manual, upgraded versions
Pre-post facilities	Mesh-maker, individual processing software such as Tecplot, Surfer, commercial version available with pre-post code Petrasim

6.2 TOUGH-FLAC

Two existing computer codes—TOUGH2 and FLAC-3D— are joined to develop a numerical simulator (named TOUGH-FLAC) for analysis of coupled THM processes in complex geological media under multiphase flow conditions /RUT 02a/. Both codes are well established and widely used in their respective fields. The TOUGH2 code is designed for geohydrological analysis of multiphase, multi-component fluid flow and heat transport, whereas the FLAC-3D code is designed for rock and soil mechanics with thermomechanical and hydro-mechanical interactions. The two codes are executed on two separate meshes and joined with two coupling modules. A set of coupling modules can be exchanged with another set, depending on the type of rock and the studied problem.

6.2.1 Technical Description

TOUGH-FLAC is a simulator based on the coupling of two well established computer codes: TOUGH2 used for coupled thermal-hydrological analysis and FLAC3D used for mechanical analysis. Simulated processes include heat transfer by conduction and convection, liquid and vapour water movements, rock stress and deformation, and stress-induced changes in fracture permeability. In this paper, model predictions of coupled THM responses are compared to in situ measurements of temperature, water saturation, rock-mass displacement, and changes in fracture permeability. A schematic description of the resulting simulator is shown in Figure 6-1.

6.2.2 Applications in Clay Formations

A direct use of TOUGH-FLAC in clay formations is not known. A published application of the simulator for the assessment of the geologic repository systems is the project Yucca Mountain /RUT 02b/, /RUT 03a/. Yucca Mountain is a ridge-line in Nye County, Nevada, composed of volcanic material (mostly tuff) ejected from a now-extinct caldera-forming supervolcano. The "mountain" is most notable as the site of the proposed Yucca Mountain Repository, a U.S. Department of Energy terminal storage facility for spent nuclear reactor and other radioactive waste. Like many nuclear facilities, the proposed Yucca Mountain facility is controversial. The ability of the numerical simulator to model relevant coupled THM processes at the DST (Drift Scale Test) was evaluated by comparison of numerical results to in situ measurements of temperature, water saturation, displacement, and fracture permeability. Of par-

ticular relevance for coupled THM processes are thermally induced rock-mass stress and deformations, with associated changes in fracture aperture and fractured rock permeability. Thermally induced rock-mass deformation and accompanying changes in fracture permeability were reasonably well predicted using a continuum elastic model, although some individual measurements of displacement and permeability indicate inelastic mechanical responses. It is concluded that fracture closure/opening caused by a change in thermally induced normal stress across fractures is an important mechanism for changes in intrinsic fracture permeability at the DST, whereas fracture shear dilation appears to be less significant. Observed and predicted maximum permeability changes at the DST are within one order of magnitude. These data are important for bounding model predictions of potential changes in rock-mass permeability at a future repository in Yucca Mountain.

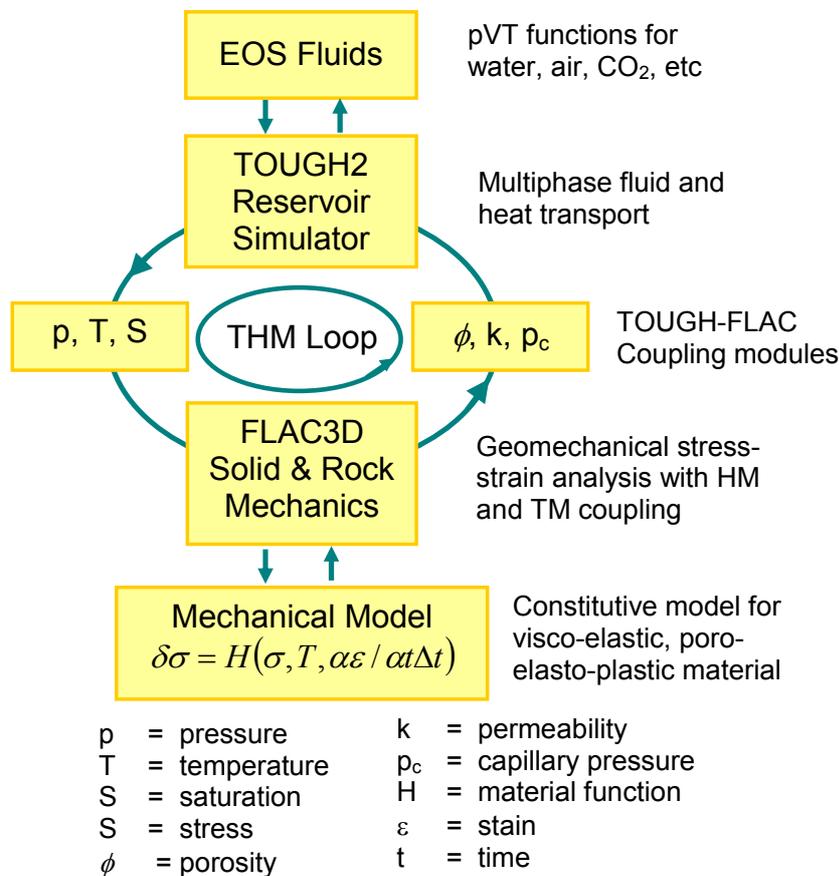


Figure 6-1: Schematic of linking TOUGH2 and FLAC3D for a coupled THM simulation /RUT 02a/

The application of Yucca Mountain gave promising results in terms of probable application of TOUGH-FLAC for clay repositories. The use of TOUGH-FLAC at the benchmark conducted in the framework of DECOVALEX project for the performance assessment of a crystalline rock repository with bentonite buffer in excavation as well as succeeding phases is reported in /XIE 06a/. In this project five simulators are compared in terms of mechanical processes

coupled with fluid transport. Thermal-hydrological results such as fluid pressure, saturation, and vertical flux are also modelled. The five models were in reasonable agreement, despite the fact that different approaches were used to describe swelling pressure in the bentonite and that only one code solves for complex multiphase flow behaviour of liquids and gases. However TOUGH-FLAC gives especially good results in modelling the heat-induced flow perturbations are affected by a complex interaction between the abundant fractures and the rock matrix. The executive summary of TOUGH-FLAC is given in Table 6-2.

Table 6-2: Properties of TOUGH-FLAC in terms of modelling gas transport in clay formations

Governing equations		
		Basic mass and energy balance, B_HC, B_EC, B_IM, B_ME
Hydraulic transport modelling		
	Advection/dispersion	H_TP_D, Advective mass flux is a sum over phases. H_DIS, Hydrodynamic dispersion with longitudinal and transversal dispersion coefficients
	Diffusion	H_DIF_F, Molecular diffusion taken into account, Fick's law, multi-phase diffusion
	Phases/Components	P_WP, P_AP, P_VP, P_AP, P_CO2_EC, P_X_EC 3 Phases according to the EOS module considered, the thermodynamical and thermophysical properties of the components and phases considered are calculated in each individual EOS module, TOUGH2 Modules.
	Sorption	H_A, Reversible instantaneous linear sorption, taken into account in mass accumulation term
Geology-Geometry modelling		
	Porous media	GF_F, GF_L, GF_AH, G_TR Conventional, with tortuosity and capillary characteristics Relative permeability functions, G_RP_Corey, G_RP_Gen, G_RP_Grant, G_RP_Verra, G_RP_Klikoff Capillary pressure functions, G_CP_Pick, G_CP_Milly, G_CP_Lever, G_CP_Gen
	Fractured media	G_F, G_F_MINC, G_F_DP, Classical double-porosity concept after Warren and Root. Rock matrix and fractures may exchange fluid or heat by means of interporosity flow
	Changes in petrophysical parameters	G_DP, G_DP_KK, G_DP_CL Considered in EWASG, ECO2N due to change in pore volume, the porosity-permeability relationship is taken into account with selective various methods
Heat transport modelling		
	Convective/conductive	Heat flux with conductive and convective components
	Effect on phase properties	Considered

Mechanical coupling		Coupling of FLAC3D, constitutive model for visco-elastic-poro-elastic material
	Rock convergence	M_RC
	EDZ	M_EDZ_S, M_EDZ_TE, M_EDZ_TE
	Visco-elastic-poro-elastic behaviour	M_EVE
	Swelling	M_S_X
	Fracturing, pathway dilatation	M_CP
Chemical coupling		
	Physical	P_PD, Physical precipitation considered for NaCl
Application for clay formations		Direct application not known
	Drift Scale Test	/RUT 03a/, Yucca Mountain, fracture flow
	THM modelling	/XIE 06b/, DECOVALEX Project
Discretization		
	Space	Integral finite difference method. The discretized flux is expressed in terms of averages for the neighbouring cells. The grid geometry flexible.
	Max grid size	100000
	Time	First order finite differences, flux terms fully implicit
User friendliness		
	User Manual	A good developed user manual for TOUGH2 and FLAC3D
	Pre-post processing facilities	Mesh-maker, individual processing software such as Tecplot, Surfer

6.3 TOUGHREACT

TOUGHREACT is applicable to one-, two-, or three-dimensional geologic domains with physical and chemical heterogeneity. Basically TOUGHREACT is a version of TOUGH2 with chemical coupling. TOUGHREACT can be applied to a wide range of subsurface conditions. Temperature ranges from 0 °C to 300 °C, because the present most available geochemical database is up to 300 °C such as EQ3/6. Pressure can be from 1 bar (atmospheric pressure) to several hundred bars (at several thousand meter depth). Water saturation can range from completely dry to fully water saturated. The model can deal with ionic strength from diluted to highly saline water (up to 6 mol/kg H₂O for NaCl dominant solution). TOUGHREACT is applicable to a variety of reactive fluid and geochemical transport.

6.3.1 Technical Description /XUT 06/

TOUGHREACT covers full capability of standard TOUGH2 and in addition a chemical module permitting the reactive transport of the phases. The gas, liquid phases are active for multiphase fluid flow, mass transport and chemical reactions. The solid phase coupled is also coupled and taken into consideration based on precipitation and dissolution. Transport of aqueous and gaseous species by advection and molecular diffusion is considered in both liquid and gas phases. Any number of chemical species in liquid, gas and solid phases can be accommodated. Aqueous complexation, acid-base, redox, gas dissolution/exsolution, and cation exchange, are considered under the local equilibrium assumption. Mineral dissolution and precipitation can proceed either subject to local equilibrium or kinetic conditions. Linear adsorption and decay can be included. A detailed description is given in Table 6-3.

6.3.2 Applications in Clay Formations

A known application of TOUGHREACT for clay formations is given by /BUR 06/. The two-phase non-isothermal base-case standard simulation presented in this study reveals significant coupled thermal, hydrological and chemical processes (THC): a limited carbonation along the entire width of the concrete barrier and a possible drastic change of the porosity at the concrete/clay interface before 2000 years. A first sensitivity analysis shows that the re-saturation and the heating will be large enough and of long enough duration to cause a limited carbonation in all concrete. On the other hand, the change in porosity is maximal at the concrete/clay interface but the extent of this change depends on many parameters. Therefore, these results should be considered as preliminary. The effect of mineral precipitation under kinetic constraints, rather than local equilibrium, will deserve further investigation. The use of TOUGHREACT for coupling the hydraulic with mainly thermally induced chemical aspects for various types of geologic formations can be found in the literature. They are up to present on geothermal /KIR 04/ or on the geological storage of CO₂ /XUT 06/.

Table 6-3: Properties of TOUGHREACT in terms of modelling gas transport in clay formations

Governing equations		
		Basic mass and energy balance, B_HC, B_EC, B_CE, B_IM
Hydraulic transport modelling		
	Advection/dispersion	H_TP_D, Advective mass flux is a sum over phases. H_DIS, Hydrodynamic dispersion with longitudinal and transversal dispersion coefficients
	Diffusion	H_DIF_F, Molecular diffusion taken into account, Fick's law, multi-phase diffusion
	Phases/Components	P_WP, P_AP, P_VP, P_AP, P_CO2_EC, P_X_EC 3 Phases according to the EOS module considered, the thermodynamical and thermophysical properties of the components and phases considered are calculated in each individual EOS module TOUGH2 Modules, ECO2N; water, NaCl, CO2/CH4/H2, salt precipitation
	Sorption	H_A, Reversible instantaneous linear sorption, taken into account in mass accumulation term
Geology-Geometry modelling		
	Porous media	GF_F, GF_L, GF_AH, G_TR Conventional, with tortuosity and capillary characteristics Relative permeability functions, G_RP_Corey, G_RP_Gen, G_RP_Grant, G_RP_Verra, G_RP_Klikoff Capillary pressure functions, G_CP_Pick, G_CP_Milly, G_CP_Lever, G_CP_Gen
	Fractured media	G_F, G_F_MINC, G_F_DP, Classical double-porosity concept after Warren and Root. Rock matrix and fractures may exchange fluid or heat by means of interporosity flow
	Changes in petrophysical parameters	G_DP, G_DP_KK, G_DP_CL Considered in ECO2N due to change in pore volume, the porosity-permeability relationship is taken into account with selective various methods
Heat transport modelling		
	Convective/conductive	Heat flux with conductive and convective components
	Effect on phase properties	Considered
Mechanical coupling		Not known
Chemical coupling		Fully
	Physical	P_PD, Physical precipitation considered for NaCl
	Chemical	C_RX, C_SC, C_OX, C_DP, C_IE,
	Databank	C_TD_EQ3/6, flexible
Application for clay formations		
	Reactive flow	/ALK 06/ /BUR 06/
Discretization		
	Space	Integral finite difference method. The discretized flux is expressed in terms of averages for the neighbouring cells. The grid geometry flexible.
	Max grid size	8000 - ?
	Time	First order finite differences, flux terms fully implicit
User friendliness		
	User Manual	User manual, not sufficient, should be developed
	Pre-post facilities	Mesh-maker, individual processing software such as Tecplot, Surfer, commercial version available with pre-post code Petrasim /ALC 06/

6.4 CODE BRIGHT

CODE_BRIGHT is a simulator for coupled Deformation, Brine, Gas and Heat transport problems /OLI 94/. It solves the equations of mass and energy balance and stress equilibrium and, originally, it was developed for application to repositories in salt formations where convergence of the rock and its effect on the permeability and porosity of crushed salt backfill, which is thereby compacted, is a fundamental issue in the evaluation of the performance of the repositories. The governing equations also include a set of constitutive laws and equilibrium conditions. The main peculiarities of saline media are in the dissolution/precipitation phenomena, presence of brine inclusions in the solid salt and creep deformation of the solid matrix. A comprehensive description of the code is given by /ZHA 04/ /GUI 06/.

6.4.1 Technical Description

CODE_BRIGHT is a finite element code for the analysis of THM problems in geological media. A porous medium composed by solid grains, water and gas is considered. Thermal, hydraulic and mechanical aspects will be taken into account, including coupling between them in all possible directions. As illustrated Figure 6-2, the problem is formulated in a multiphase and multi-species approach.

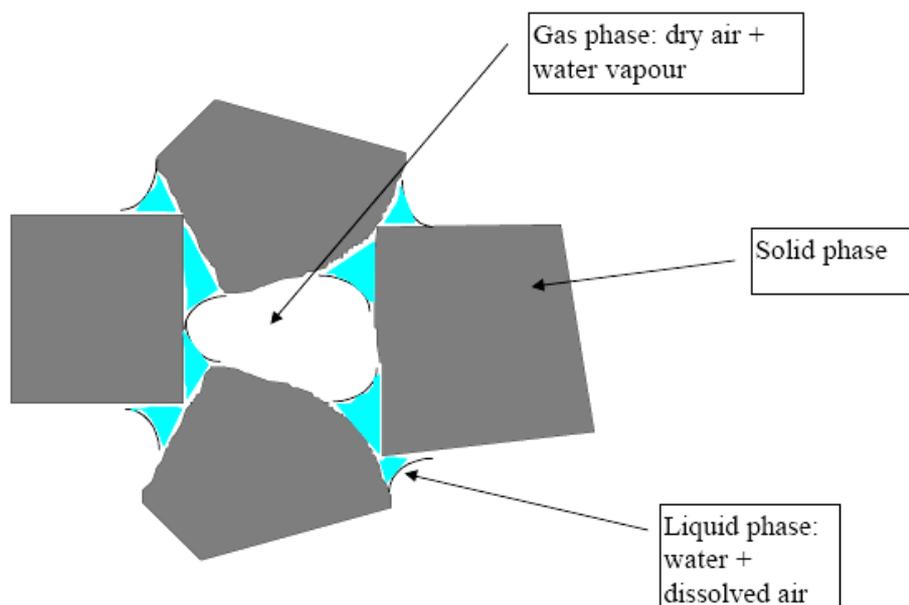


Figure 6-2: Phase and species consideration in Code-BRIGHT

The three phases modelled are:

- solid phase (s):
- liquid phase (l): water + air dissolved
- gas phase (g): mixture of dry air and water vapour

The three species are:

- solid (-):
- water (w): as liquid or evaporated in the gas phase
- air (a): dry air, as gas or dissolved in the liquid phase

The following assumptions considered in the formulation of the problem:

Dry air is considered a single species and it is the main component of the gaseous phase. Henry's law is used to express equilibrium of dissolved air.

Gas phase is consisted of dry air + water vapour and solid phase is consisted of liquid phase: water + dissolved air. Some simplifications of the model are as follows:

- Thermal equilibrium between phases is assumed. This means that the three phases are at the same temperature
- Vapour concentration is in equilibrium with the liquid phase, the psychrometric law expresses its concentration.
- State variables (also called unknowns) are: solid displacements, \mathbf{u} (three spatial directions); liquid pressure, P_l ; gas pressure, P_g ; and temperature, T .
- Balance of momentum for the medium as a whole is reduced to the equation of stress equilibrium together with a mechanical constitutive model to relate stresses with strains. Strains are defined in terms of displacements.
- Small strains and small strain rates are assumed for solid deformation. Advective terms due to solid displacement are neglected after the formulation is transformed in terms of material derivatives (in fact, material derivatives are approximated as Eulerian time derivatives). In this way, volumetric strain is properly considered.
- Balance of momentum for dissolved species and for fluid phases are reduced to constitutive equations (Fick's law and Darcy's law).
- Physical parameters in constitutive laws are function of pressure and temperature. For example: concentration of vapour under planar surface (in psychrometric law), surface tension (in retention curve), dynamic viscosity (in Darcy's law), are strongly dependent on temperature.
- An elastoplastic law named Barcelona Basic Model (BBM) is implemented in CODE_BRIGHT, which is able to represent many mechanical features of unsaturated soils in a consistent and unified manner.

A summary of the technical properties of the CODE_BRIGHT is given in Table 6-4.

6.4.2 Applications in Clay Formations

CODE_BRIGHT is applied for the performance assessments of waste disposal in clay formations. The present applications are mainly on the scientific basis. In /ZHA 04/ the theoretical

framework and the capacity of CODE_BRIGHT is briefly reviewed with duplicating the experimental and in-situ data. Various clay formations such as Boom, Opalinus and Callovo-Oxfordian Clays were studied. The thermal, hydraulic and mechanical parameters were selected from the previous studies mainly and listed in the corresponding references. Among the experimental studies which were modelled with CODE_BRIGHT, the swelling behaviour of Serata Bentonite, desaturation of Opalinus Clay and ventilation of a borehole in clay can be cited.

Numerical simulations were performed in order to establish the necessary heat output and to get a first estimate of the desaturation/resaturation time-scale and of the temperature levels for modelling heat and moisture transport in the Andra/SKB temperature buffer test. Prior to test start, a program for predictive modelling was defined. Modelling teams organized by Andra, SKB and Enresa made blind predictions of the thermal, hydraulic and mechanical evolution of the test /HÖK 05/.

The influence of trapped air in the backfill on the water saturation process was studied with CODE_BRIGHT version 2.2. At the model's outer boundary, water and gas pressure boundary conditions were set and the water supply to the backfill was varied by varying the rock permeability. The rock was kept saturated. Thus, the air present in the initially unsaturated backfill had to escape by diffusion through the rock. For reference, models assuming unlimited escape of air, i.e. with a constant atmospheric gas pressure inside the backfill, were also analyzed.

The formulation and constitutive models used in CODE_BRIGHT have also been applied to the simulation of the large scale tests of the FEBEX project namely the "mock up" tests and the "in-situ" test /SAN 05a/, /SAN 05b/.

Table 6-4: Properties of CODE_BRIGHT in terms of modelling gas transport in clay formations

Governing equations		
	Balance of Energy	B_EC
	Balance of water mass	B_HC
	Balance of air mass	B_HC
Hydraulic transport modelling		
	Advection/dispersion	G_PM , Darcy Law for liquid and gas flow, permeability tensor
	Diffusion	Molecular diffusion of vapour in air, Fick's law
	Phases/Components	P_WP, P_VP, P_VP, P_AP
	Sorption	-
Geology-Geometry modelling		
	Porous media	H_TP_D, Conventional, with tortuosity and capillary characteristics Relative permeability functions G_RP_Gen Capillary pressure functions G_CP_Lever, G_CP_Gen
	Fractured media	-
	Changes in petrophysical parameters	Porosity to permeability
Heat transport modelling		
	Convective/conductive	Convective terms in energy balance, conductive heat flow via Fourier law
	Effect on phase properties	T_LP, T_RP, T_GP, T_ST
Mechanical coupling		
	General	Stress tensor, M_EVE, M_BBM, Effective stress concept, Elastoplastic law Barcelona Basic Model (BBM)
	Rock convergence	M_GS, Considered
	EDZ	M_EDZ_S, M_EDZ_HP, M_EDZ_DC
	Swelling	permeability related to swelling through void ratio and swelling pressure, validated with measured values in a Na-Bentonite
	Fracturing, pathway dilatation	-
Chemical coupling		Fully
	Physical	P_PD,
	Chemical	C_RX, C_SC, C_OX, C_CO, C_DP, C_IE
	Databank	Individual versions
Application for clay formations		
	THM Coupling	/ZHA 04/ Numerical modelling of THM Coupling for Callovo-Oxfordian and Opalinus Clay
	THM Tests	/HÖK 05/.Andra/Skb Temperature buffer test
	HM Response of Bentonit to Heating and swelling	/ZHA 04/ Response of bentonite buffer to heating, saturated, unsaturated cases
	Mock-up tests	/SAN 05a/ the simulation of the large scale tests of the FEBEX project
Discretization		
	Space	Finite difference method
	Max grid size	Flexible
	Time	Linear, fully implicit with Newton Raphson Method
User friendliness		
	User Manual	User manual, individual references
	Pre-post facilities	

6.5 HYTEC

HYTEC is a reactive transport model coupled with geochemical code CHES which is speciation model specifically developed to simulate the equilibrium state of complex aquatic systems, including oxides or minerals, organics, colloids and gases. CHES stands for Chemical Equilibrium of Species and Surfaces and is actually used in many scientific areas, notably in environmental engineering, safety and performance assessment of waste repositories and ground- and surface water pollution studies. About seven different thermodynamic databases have been made available for use with CHES and they are readily extended with new species. HYTEC coupled with CHES is used for groundwater pollution studies, safety assessment of nuclear waste disposals, general geochemical studies, mining problems and interpretation of laboratory column experiments. It is developed by Ecole Des Mines De Paris, Centre De Géosciences and widely applied in corresponding research activities mainly for modelling reactive flow /LEE 05/.

6.5.1 Technical Description /LEE 05/

HYTEC is a numerical tool for 1D-2D transport through porous or fractured media and deals especially with geochemically and hydrodynamically heterogeneous media. HYTEC handles precipitation, dissolution, kinetics, complexation, cation exchange and redox equations.

It accounts for porosity changes as mineral phases precipitate or dissolve, full feedback on hydrogeology with integrating efficient algorithms. The current version includes the ability to call an externally running transport model via MPI (Message Passing Interface), a communication protocol generally reserved for coding of codes running on parallel computers. The only requirement is that the transport model contains a similar communication interface, i.e. function calls which respect the MPI. So far, HYTEC has been interfaced with METIS (developed at the CIG) and RT1D (a one-dimensional transport model). Coupling with other dynamic codes is currently in progress. Accordingly, the user may specify at run-time which model should be used to perform the hydrodynamic part of the calculations. The structure is schematically illustrated below:

The present versions of HYTEC (up to version 2.5) were based on a one-dimensional transport model. The main purpose of HYTEC-1D was to simulate column experiments. Standard hydrodynamic conditions and geometry and dimensions of laboratory systems allowed us to simplify the hydrogeological model, notably with respect to boundary conditions: HYTEC-1D imposes a constant flux, a zero-gradient condition at the outlet and a constant concentration condition at the inlet of the column. From a geochemical viewpoint, however, HYTEC-1D is quite complete and handles mineralogical heterogeneity in the column, sources and sinks and variable input concentrations. The latest version of HYTEC-1D is 2.5. A two- or three dimensional approaches as well as a transport model which solves the flow equations (i.e., imposed hydraulic head boundary conditions) were required for field scale modelling. A new generation of HYTEC has been developed to full these modelling designs, HYTEC version 3.0 and later. The MPI technology applied for coupling of codes appears a very efficient and useful approach for the reactive transport model. Note that the one-dimensional transport model derived from HYTEC-1D, RT1D, has been abandoned since version 3.0. Accordingly,

the user may specify which model should be used to perform the hydrodynamic part of the calculations.

A summary of the technical properties of the HYTEC is given in Table 6-5.

6.5.2 Applications in Clay Formations

Preliminary simulations with the geochemical code HYTEC have been used to reproduce the corrosion of iron in clay media. Some prospective simulations both on clay interstitial water and iron corrosion provide interesting results which must be compared with experiments. Both thermodynamic and kinetics parameters were used to fit and further predict evolution of the system. The kinetic parameters have been fitted to reproduce the experimental iron corrosion rate. The thermodynamic parameters are chosen in order to reproduce the observed precipitated phases /COM 05/.

Table 6-5: Properties of code HYTEC in terms of modelling gas transport in clay formations

Governing equations		
	Balance of Energy	B_EC
	Balance of water mass	B_HC
	Balance of air mass	B_HC
Hydraulic transport modelling		
	Advection/dispersion	H_OP_D
	Diffusion	
	Phases/Components	P_WP, P_BP
	Sorption	H_AD,
Geology-Geometry modelling		
	Porous media	Conventional, with tortuosity and capillary characteristics Relative permeability functions, G_RP_Corey, G_RP_Gen, G_RP_Grant, G_RP_Verra, G_RP_Klikoff Capillary pressure functions, G_CP_Pick, G_CP_Milly, G_CP_Lever, G_CP_Gen
	Fractured media	H_CL, H_DC
	Changes in petrophysical parameters	Porosity to permeability, G_PP_Kozeny-Karman
Heat transport modelling		
	Convective/conductive	Convective terms in energy balance, conductive heat flow via Fourier law
	Effect on phase properties	T_RP, T_LP, T_ME
Mechanical coupling		Not considered
Chemical coupling		Fully with CHESS
	Physical	P_PD
	Chemical	C_RX, C_SC, C_OX, C_CO, C_DP, C_IE
	Databank	Flexible
Application for clay formations		
	Chemical	/COM 05/ to reproduce the corrosion of iron in clay media
Discretization		
	Space	Finite difference, the grid geometry flexible.
	Max grid size	Not tested
	Time	First order finite differences, flux terms fully implicit
User friendliness		
	User Manual	User manual, in French
	Pre-post facilities	Self pre-post processing programs

6.6 ASTER

Code_ASTER is open-source software for finite element analysis. Originally, the program was developed as an in-house application by the French company “Electricite de France“, it was released under the terms of the GNU General Public License, in October 2001, /EDF 07/. Code ASTER is a numerical code used for general applications for analysis of structures and thermomechanics for surveys and research. It offers a full range of multiphysical analysis and modelling methods that go well beyond the standard functions of thermomechanical calculations. Code ASTER can evaluate from seismic analysis to porous environments via acoustics, fatigue, stochastic dynamics, etc. Its modelling, algorithms and solvers are constantly undergoing work to improve them and add to them (1,200,000 lines of code, 200 operators). Resolutely open, it is chained, coupled and encapsulated in numerous ways.

6.6.1 Technical Description

The application of ASTER is primarily oriented on the modelling of the deformable solids. It is reported that a variety of constitutive laws are available in Code ASTER: isotropic and anisotropic elasticity, elasto-viscous plasticity (isotropic hardening, kinematics and viscoplasticity, Chaboche and Lemaître models), laws describing progressive strain (Taheri model, polycrystalline), brittle or ductile damage laws (Rousselier model) and all laws originating from targeted issues (plasticity of and damage to the concrete, steels, assemblies, cohesive elements, etc.). Thermomechanical chaining by strongly coupling the thermal, hydraulic and mechanical (thermo-hydro-mechanical) equations for investigation of temperature dependent materials with thermal or hydration-drying-shrinkage changes is also provided. ASTER modelling all of the repository disturbances has therefore many coupled possibilities for computing the transport phenomena in various media. The mechanical behaviour is modelled to estimate the internal and external state of the materials submitted to a statical or dynamical load. Code Aster is especially powerful on modelling the fracture physics. The conventional release rate, the key parameter in fracture mechanics, makes it possible to reach a conclusion regarding whether a crack will propagate or not. The ASTER operators calculate it for diverse situations: 2D, 3D, temperature dependent materials, surface or volume forces, lip pressure, etc. This is the case in both elasticity and elastoplasticity, provided the load remains monotonous and radial. The coupled phenomena are external thermal, acoustical and hydraulic under stationary and transient disturbances. For hydraulic considerations, the code is coupled with Code-Saturne and the saturated or unsaturated media can be modelled. The other usual criteria in elasticity, which are stress intensity factors, are accessible in 2D and in certain 3D configurations

A very detailed description of the code is given in a manual written in French /AST 03/. The last known version is 8.2 delivered at December 2005. A good pre and post processing possibility is provided by coupling the programme with various pre-post processing programmes and especially with the code Salamon. These facilitate the works on creating of grids and on the visualisation of the results greatly.

A summary of the technical properties of the code ASTER is given in Table 6-6.

Table 6-6: Properties of code ASTER in terms of modelling gas transport in clay formations

Governing equations		
	Balance of Energy	B_EC
	Balance of water mass	B_HC
Hydraulic transport modelling		
	Advection/dispersion	H_OP_D
	Diffusion	H_DIF_S
	Phases/Components	P_WP, P_BP
	Sorption	H_AD
Geology-Geometry modelling		
	Porous media	For hydrodynamics coupled with Code-Saturne, conventional, with capillary characteristics Relative permeability functions, G_RP_Corey, G_RP_Gen, G_RP_Grant Capillary pressure functions, G_CP_Lever, G_CP_Gen
	Fractured media	Good possibilities for modelling fracture physics
Heat transport modelling		
	Convective/conductive	Convective terms in energy balance, conductive heat flow via Fourier law
	Effect on phase properties	T_RP, T_LP, T_ME
Mechanical coupling		
	General	95 various constitutive laws are provided, for additional, the flexibility is provided.
	EDZ	Various modelling possibilities by adapting the available constitutive laws
	Swelling	M_S_X, permeability related to swelling through void ratio and swelling pressure, validated with measured values in a Na-Bentonite
	Fracturing, pathway dilatation	M_CP, M_EDZ_TE, M_EDZ_HP, M_EDZ_DC
	Crack propagation	M_CP, very powerful for modelling fracture physics
Chemical coupling		-
Application for clay formations		
	TH Coupling	Thermo-hydraulic behaviour of a system composed of an engineered clay barrier and a host rock, /BAR 04/.
Discretization		
	Space	Finite element method
	Max grid size	Flexible grid creating.
	Time	Linear and non-linear methods
User friendliness		
	User Manual	User Manual in French
	Pre-post facilities	Good pre-post processing tools coupled with Salome for mesh creating and post processing

6.6.2 Applications in Clay Formations

Hydraulic, geochemical and geoelectrical laboratory tests have been also performed to characterize the Opalinus clay properties /MAY 06/. In the framework of these studies, the "in situ" VE tests have been interpreted and modelled with Code-Aster. In another study, the impact of a heat source on the thermo-hydraulic behaviour of a system composed of an engineered clay barrier and a host rock, namely an argillite is investigated firstly by benchmark test case with code CAST3M and code ASTER /BAR 04/. The results of both codes are in good agreement, except for the gas pressure. Nevertheless, gas pressure does not seem to influence the saturation process, although the saturation kinetics is governed by the Darcy water flow. The saturation process is accelerated when the heat source is taken into account. More precisely, this acceleration is due to dynamic viscosity increase with heating. In a second time, five other heating sources have been tested in code ASTER. Compared with the reference calculations, some give an identical response. However, the highest heating sources provoke a desaturation phenomenon because of the air pressure increase with temperature. The liquid saturation of the engineered barrier is then delayed.

6.7 CAST3M

Originally, CAST3M is a computer code for the analysis of structures by the finite element method. With the origin, this code was developed by the Department of Mechanics and Technology of the French Police station with Atomic Energy. The development of CAST3M enters within the framework of an activity of search in the field of mechanics; the goal being to define a high level instrument, being able to be used as support valid for the design, dimensioning and the analysis of structures and components, in the nuclear field as in the traditional industrial sector. Accordingly, CAST3M presents a complete system, integrating not only the functions of calculation themselves, but also of the functions of construction of the model (pre-processor) and of processing of the results (post-processor). CAST3M makes it possible to deal with problems of linear elasticity in the fields statics and dynamics (extraction of eigenvalues), of the thermal problems, the nonlinear problems (elasto-visco-plasticity), of the dynamic problems step by step, etc /CAS 00/.

6.7.1 Technical Description /CAS 00/

CAST3M is a general Finite Element/Finite Volume code for structural and fluid mechanics and heat transfer. CAST3M is a multi-purpose numerical code which allows different spatial schemes for diffusion-dispersion-convection transport equation: A mixed hybrid finite element scheme with RT0 Raviart-Thomas elements for the diffusive part and a specific scheme for the advective one; A Finite Volume scheme of Multi Point Float Approximation (MPFA) type for the diffusive part and a decentred scheme for the convective one. Different comparisons have been done between these schemes on analytical cases and characteristic problems of waste storage simulation.

A summary of the technical properties of the code CAST3M is given in Table 6-7.

6.7.2 Applications in Clay Formations

One of the experiments performed in order to characterize the confinement properties of the Opalinus Clay in the Mont Terri underground laboratory, called HE-C, has consisted in measuring in situ the time evolution of the rock temperature submitted to a thermal source. Inverse simulation by using the Code CAST3M has been used to estimate the thermal longitudinal and transversal conductivities of the host rock /CAR 05/. First a 3D direct numerical simulation of this experiment has been performed with the code CAST3M, with a mesh done of 37 708 zones. It showed that the thermal behaviour of the clay was not homogeneous around the borehole where was installed the heater. Furthermore, it was necessary to introduce a new parameter to model the heater dissipation from the heater power regulation unit to the location of the heater at the bottom of the borehole. Inverse simulation consists in minimizing an objective function that is the sum of the squared differences between the measured and calculated temperatures. This method induced a lot of CAST3M simulations /MON 06/. CAST3M was also one of the software integrated in programme ALLIANCE which aim to accumulating within the same simulation environment the already acquired knowledge and to gradually integrate new knowledge /MON 05b/.

Table 6-7: Properties of code CAST3M in terms of modelling gas transport in clay formations

Governing equations		
		Basic mass and energy balance, B_HC, B_EC
Hydraulic transport modelling		
	Advection/dispersion	H_TP_D, Advective mass flux is a sum over phases. H_DIS, Hydrodynamic dispersion with longitudinal and transversal dispersion coefficients
	Diffusion	H_DIF_F, Molecular diffusion taken into account, Fick's law, multi-phase diffusion
	Phases/Components	P_WP, P_AP,
	Sorption	H_A, Reversible instantaneous linear sorption, taken into account in mass accumulation term
Geology-Geometry modelling		
	Porous media	GF_F, GF_L, GF_AH Conventional, with tortuosity and capillary characteristics Relative permeability functions, Capillary pressure functions
	Fractured media	good possibility of modelling fractured media
	Changes in petrophysical parameters	?
Heat transport modelling		
	Convective/conductive	Heat flux with conductive and convective components
	Effect on phase properties	Considered
Mechanical coupling		Constitutive model for elasto-viscoplastic constitutive law with isotropic hardening
	Rock convergence	M_RC
	EDZ	A good coupled elastic and plastic damage model
Chemical coupling		Fully coupled version by /MÜG 03/ with CHESS and PHREEQC
	Chemical	C_RX, C_SC, C_OX, C_DP, C_IE,
Application for clay formations		
	Thermal properties	Inverse modelling for thermal properties of Opalinus Clay /CAR 05/
	Mechanical coupling	Alliance Project /MON 05b/
Discretization		
	Space	Finite elements method
	Max grid size	?
	Time	First order finite differences, flux terms fully implicit
User friendliness		
	User Manual	A good developed user manual, upgraded versions
	Pre-post facilities	Not known

6.8 FRAC3DVS

The numerical code FRAC3DVS is and can be used to calculate the transport of radionuclides through the geosphere. The code is described in detail in /THE 96/. It solves the three-dimensional groundwater flow and solute transport equations in discretely fractured and porous media. Its commercial version is released by the "WATERLOO HYDROGEOLOGIC".

6.8.1 Technical Description /KOS 04/

Processes and phenomena explicitly included in FRAC3DVS are:

- Transient flow of fluids in partially- or fully-saturated porous media, in fractures and in fractured-porous media
- Advective, dispersive and diffusive transport of solutes
- Diffusion of solutes from a fracture into a limited porous rock matrix
- Linear sorption of solutes on fracture surfaces and in the rock matrix
- Radioactive decay of solutes
- Chain decay of solutes

Other flow and transport processes are included implicitly, for example through the selection of appropriate parameter values and boundary conditions. With FRAC3DVS it is possible to calculate variable-saturated groundwater flow, but this is not used and all calculations described in this report are based on flow in a fully saturated medium.

FRAC3DVS needs as input boundary conditions the radionuclide release rates from the near-field models, and provides radionuclide release rates, which are used for the biosphere-transport modelling.

Due to its modular design, FRAC3DVS allows the use of different modelling strategies. Main model concepts are possible for continuum models, discrete fractured porous-medium models and discrete fracture models. The appropriate model concept for a problem depends on the model scale, the significance of inhomogeneities (geological and/or artificial), and of course on the knowledge about the system under consideration.

Continuum models are applied if it is possible to divide the inhomogeneous domain into homogeneous sub domains. This is based on the concept of the representative elementary volume (REV). The size of the homogeneous sub domains should be chosen in such a way that there are no fluctuations of the physical parameters and that it is possible to allow the inclusion of significant heterogeneities.

Discrete fracture network models can be applied if large-scale heterogeneities dominate the flow and/or transport in the domain. In this case it is not possible to approximate single connected fractures with a porous medium and the REV is larger than the model domain.

Discrete fractured porous medium models are applied if the exchange processes between fractures and matrix are important. In such hybrid models discrete fractures are placed into a porous matrix, and the matrix is implemented, e.g. for the Opalinus clay, in terms of a continuum model. It is important to mention that for an approximation by a (normally more com-

plex) discrete fractured porous medium model the knowledge about the real system has to be much better than for a (normally simpler) continuum model. The complexity of a model also increases the effort needed for the whole modelling process, e.g. more complex model setup, longer numerical calculations and more complicated data analysis. A schematic description of the features of FRAC3DVS related to near and far field of the geological repositories is given in Figure 6-3.

A summary of the technical properties of the code FRAC3DVS is given in Table 6-8.

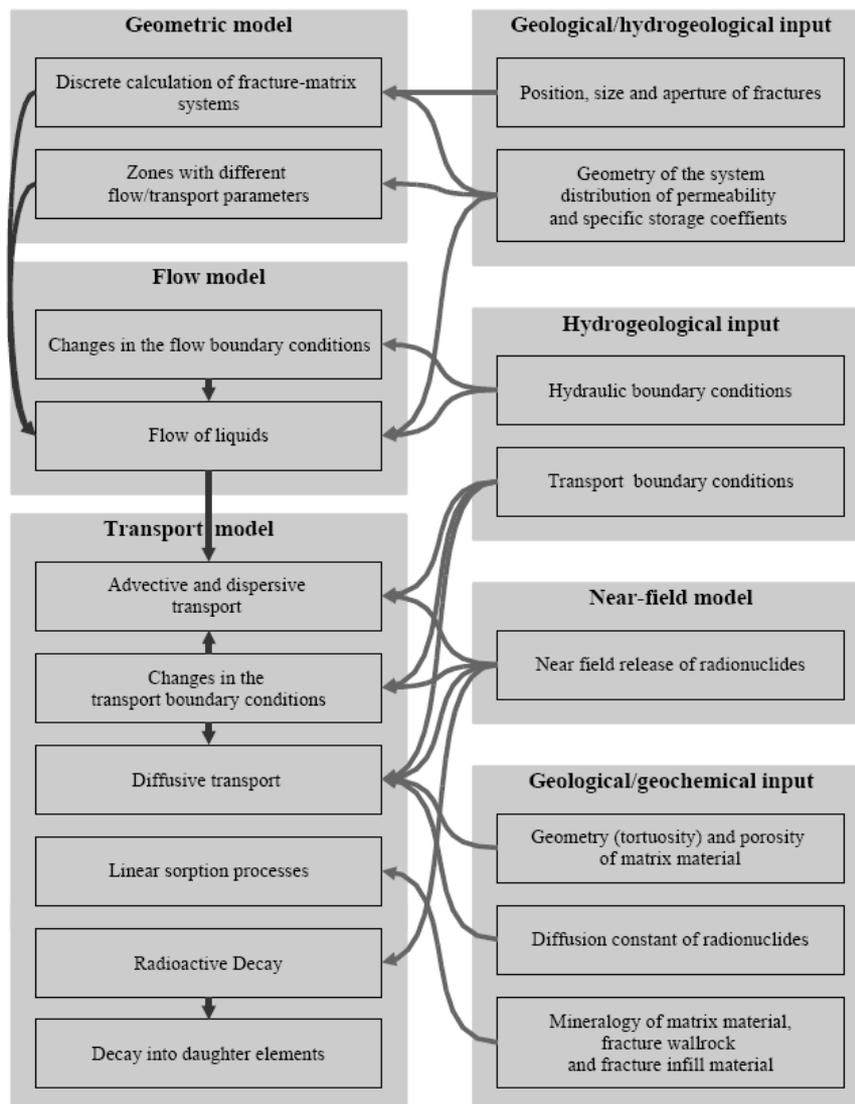


Figure 6-3: Modelling features of FRAC3DVS of the geologic repository systems and related input /KOS 04/

6.8.2 Applications in Clay Formations

The influence of time dependent flow processes on the radionuclide transport in the geosphere for Opalinus Clay is investigated numerically by using FRAC3DVS /KOS 04/. In the Opalinus Clay diffusion dominates the transport of radionuclides, but processes exist that can locally increase the importance of the advective transport for some time. Two important cases were investigated:

- glaciation-induced flow due to an additional overburden in the form of an ice shield of up to 400 m thickness and
- fluid flow driven by tunnel convergence.

In addition to the two assessment cases conducted with FRAC3DVS the applicability of the one-dimensional approximation for modelling transport through the Opalinus Clay is also investigated. For the reference case of the safety assessment the model chain STMAN-PICNIC-TAME is used. In order to evaluate radionuclide release and transport, the geometry of the repository near field/geosphere system is simplified and the Opalinus Clay is treated as a one-dimensional layer. In this study the code FRAC3DVS is used to assess the effects of the simplifications by calculating a two-dimensional model which includes both the Opalinus Clay and the SF/HLW bentonite annulus. The one-dimensional approximation gives results similar to the geometrically more realistic FRAC3DVS model. Discrepancies introduced by the one-dimensional approximation are shown to be small and the results are always conservative compared with the FRAC3DVS calculations. This modelling exercise thus gives strong support for the applicability of the one-dimensional approximation.

Table 6-8: Properties of code FRAC3DVS in terms of modelling gas transport in clay formations

Governing equations		
		Basic mass and energy balance, B_HC, B_EC
Hydraulic transport modelling		
	Advection/dispersion	H_TP_D, Advective mass flux is a sum over phases. H_DIS, Hydrodynamic dispersion with longitudinal and transversal dispersion coefficients
	Diffusion	H_DIF_F, Molecular diffusion taken into account, Fick's law, multi-phase diffusion
	Phases/Components	P_WP, P_AP, P_VP, P_AP
	Sorption	H_A, Reversible instantaneous linear sorption after Freundlich isotherm
Geology-Geometry modelling		
	Porous media	GF_F, GF_L, GF_AH Conventional, with tortuosity and capillary characteristics Relative permeability functions, G_RP_Corey, G_RP_Gen, Capillary pressure function
	Fractured media	G_F, G_F_MINC, G_F_DP, Classical double-porosity concept after Warren and Root, Discrete fractures in porous media
	Changes in petrophysical parameters	G_DP, G_DP_KK, G_DP_CL
Heat transport modelling		Not considered
Mechanical coupling		Not coupled
Chemical coupling		Not considered
	Physical	Multi-species transport of either straight or branching decay chains
Application for clay formations		
	Radionuclide transport in the geosphere for	Opalinus Clay, /KOS 04/
Discretization		
	Space	A control-volume finite element, Galerkin finite element or finite difference method. A highly efficient conjugate-gradient-like solver based on CGSTAB acceleration is used.
	Time	An efficient, adaptive time-stepping procedure adjusts time-step size based on the system response and user-defined criteria
User friendliness		
	User Manual	A comprehensive user's manual
	Pre-post facilities	A separate post-processor (F3DPLOT) for PC-based systems uses an interactive, menu-driven graphical interface to generate 2D slices through the 3D domain which show hydraulic head, saturation or concentration output from FRAC3DVS. F3DPLOT also has the ability to generate TECPLOT compatible output files in 2-D or 3-D, and also supports the generation of output in postscript, HP-GL or raster graphics format

6.9 PORFLOW

PORFLOW is a commercial product of ANALYTIC & COMPUTATIONAL RESEARCH, INC. PORFLOW is a comprehensive computer program for simulation of transient or steady state flow, heat, salinity and mass transport in multi-phase, variably saturated, porous or fractured media with dynamic phase change. The geometry may be 2D or 3D, Cartesian or cylindrical, the porous/fractured media may be anisotropic and heterogeneous, arbitrary sources of sinks (injection or pumping wells) may be present and, chemical reactions or radioactive decay may take place. It accommodates alternate fluid and media property relations and boundary conditions

PORFLOW is a highly modular program which has been applied to a wide range of practical problems in petrochemical, hydrological, geological, nuclear and chemical industry applications. Typical petrochemical industry application include ground water pollution and resource management, disposal and management of hazardous wastes, environmental impact of hot or cold pipes buried in geologic media, thawing/freezing of permafrost in terrestrial or marine environment, flow in porous beds, formation of geologic basins, and a range of reservoir engineering problems.

6.9.1 Technical Description /POR 02/

A good technical description of PORFLOW is given in User Manual, Version 5. PORFLOW numerically solves a variable set of equations for general transport, multi-phase pressure, temperature and one or more chemical species. Constitutive equations, phase-change relations, equations of state, and initial and boundary conditions supplement the governing equations. The equations are coupled through convection, buoyancy, temperature, phase change, fluid density and viscosity effects. These equations may be solved individually or simultaneously in a coupled or uncoupled manner, depending on the needs of a specific problem and the options selected by the user. The current version of PORFLOW permits simulation of flow systems with up to three phases. Examples of such systems are water-oil-vapour-air, water-steam-air, water-steam, water-ice or water-air systems.

The problem geometry can be defined in terms of either Cartesian (x, y, z) or cylindrical (x, r, θ) coordinates. Either transient or steady state problems can be solved. Except for the geometry and spatial grid, all problem parameters can change with time. The source terms, the boundary conditions, the values of field variables, and the fluid and porous matrix properties can all change either continuously or abruptly with time. The values of most parameters are allowed to vary within the spatial grid. The model domain can be divided into zones, each differing from the others in one or more distinct way, such as in material properties. The material properties can also be either isotropic or anisotropic.

PORFLOW addresses dynamic liquid-vapour (e.g., water-steam) and liquid-solid (e.g., water-ice) phase changes. The phase change algorithm is reversible and generalized, and provides for non-equilibrium thermodynamics. The user may arbitrarily change the phase-change parameters and fluid-property relations. PORFLOW assumes a pore structure that can be classified in terms of three types of pore space. The largest of these porosities is total porosity,

which is the volume fraction of the total pore space to the total volume of the host matrix. However, all of these pores do not actively participate in the movement of fluid. Some pores are completely isolated from the interconnected flow pathways; others form dead-end pathways. Consequently, effective porosity is defined as the fraction of the pore space volume through which fluid flow occurs compared to the total matrix volume. A third porosity of interest is diffusional porosity; this porosity is defined as the ratio of the volume of the pores that participate in diffusion to the total matrix volume. It includes the pores through which fluid movement occurs plus the dead-end pores that are assumed not to contribute to fluid flow, but which are assumed to facilitate the diffusion of heat and mass. By definition, its numerical value is between the total and effective porosity values. The processes incorporated to PORFLOW are schematically given in Figure 6-4.

In addition to the capability to consider heterogeneity and anisotropy of the porous media, PORFLOW incorporates an option that permits the user to consider planar geologic features such as fractures, faults, clastic dikes and linear features such as boreholes.

A summary of the technical properties of the code PORFLOW is given in Table 6-9.

Table 6-9: Properties of code PORFLOW in terms of modelling gas transport in clay formations

Governing equations		
		Basic mass and energy balance, B_HC, B_EC
Hydraulic transport modelling		
	Advection/dispersion	H_TP_D, Advective mass flux is a sum over phases. H_DIS Hydrodynamic dispersion with longitudinal and transversal dispersion coefficients
	Diffusion	H_DIF_F, Molecular diffusion taken into account, Fick's law, multi-phase diffusion
	Phases/Components	P_WP, P_AP, P_VP, P_AP
	Sorption	H_A
Geology-Geometry modelling		
	Porous media	GF_F, GF_L, GF_AH Conventional, with tortuosity and capillary characteristics Relative permeability functions, G_RP_Corey, G_RP_Gen, Capillary pressure functions, G_CP_Pick, G_CP_Gen (selective, linear, after Pickens, TRUST, Leverett, van Genuchten)
	Fractured media	G_F, G_F_DF
	Changes in petrophysical parameters	Not considered
Heat transport modelling		
	Convective/conductive	Heat flux with conductive and convective components
	Effect on phase properties	Considered
Mechanical coupling		In standard release not considered
Chemical coupling		In standard release not considered
Application for clay formations		
	Safety analysis	/AND 01/, /MOT 05b/
Discretization		
	Space	Finite difference method, flexibility in creating grid geometry
	Max grid size	Flexible
User friendliness		
	User Manual	Version 5, very good presented
	Pre-post facilities	Good developed self pre and post processing

6.9.2 Applications in Clay Formations

With its described capacity, PORFLOW is able to model various repository problems encountered in clay formations. The studies of ANDRA reports on the use of PORFLOW for quantitative evaluation of various scenarios are as part of the quantitative safety analysis /AND 01/. In the framework of the software platform ALLIANCES, PORFLOW is used as one of the numerical tools with the objective of:

- The simulation of the characteristic phenomena of all disposal and storage situations;
- The choice and coupling of different numerical codes;
- The simulation of multi-physical and multi-scale phenomena;
- The uncertainties analysis related to data and models;

- The studies management and trace ability.

Some results of this attempt is presented in /MAZ 01/, /MON 05a/.

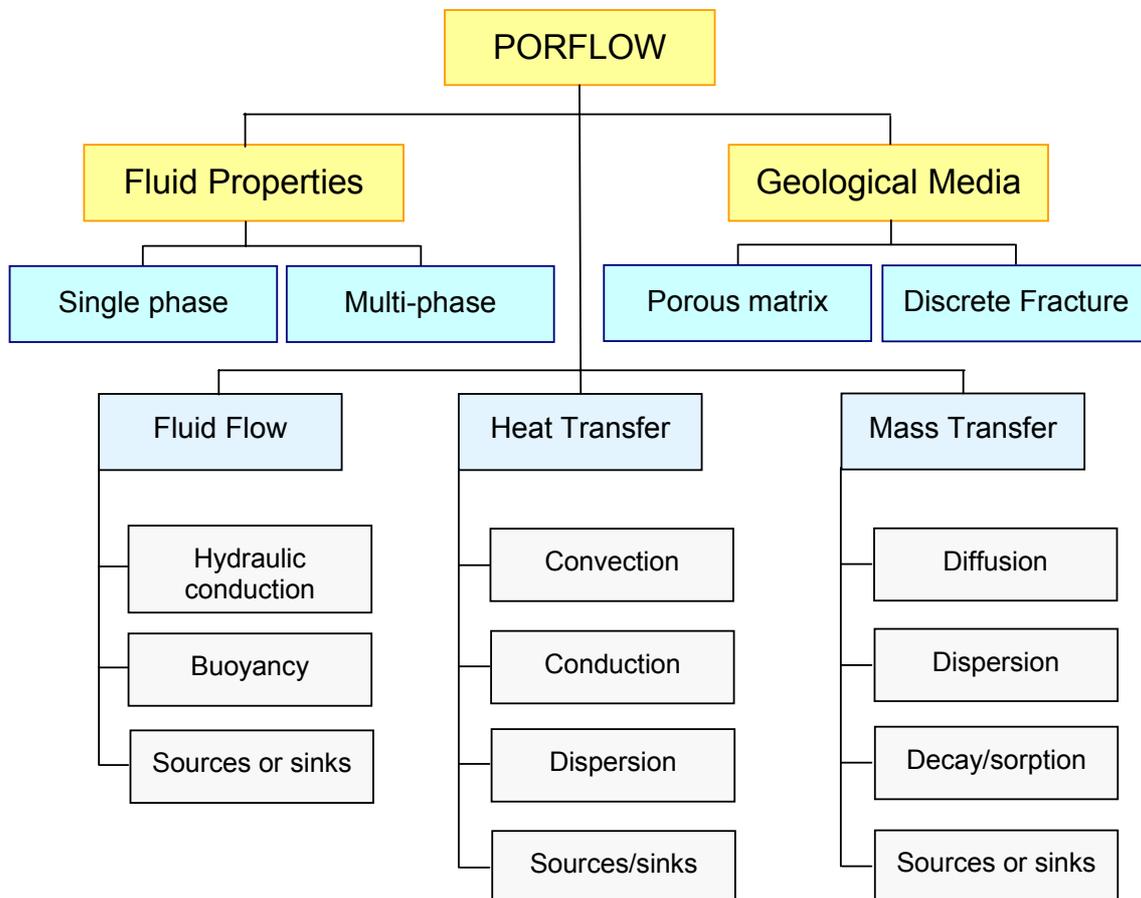


Figure 6-4: Processes considered in PORFLOW /POR 02/

6.10 ROCKFLOW

ROCKFLOW is a 3-D numerical code designed for converting the multiphase model formulations into a fully coupled thermo-hydraulic (TH/M) model for non-isothermal flow processes. Rockflow is an object oriented modelling program. The multiphase flow modelling capabilities implemented in the program are mainly based on the work done by /THO 01/ who developed the corresponding Rockflow kernels. However, to account for non-isothermal processes including phase changes of fluid components some implementation were made /JON 02/.

6.10.1 Technical Description

A good description of ROCKFLOW is given in /JON 02/. The material balance equations are written for water and air components. In the expression for the advective fluxes, the relative velocity of the liquid phase or gaseous phase relative to the solid phase in the water species

is used. Because of this, terms containing the solid phase displacement velocity in the water species have to be added to the balance. However, since this method does not include displacement, the solid velocity terms cancel out of the equation. A standard equation is used for the energy balance. For porous media containing more than one fluid, the concept of relative permeability is introduced. The relative permeability is used to calculate the effective permeability, which is described in the extended Darcy law. The relationship depends on the saturations. Different relationships are possible: constant values, user-defined functions, linear functions, potential functions, or functions found in literature, such as the van Genuchten Model. The governing equations are written for water and air components.

The reactive flow ability of the programme has been developed by introducing the geochemical code PHREEQC to ROCKFLOW. The capacity of the code has been extended to cover discrete or single continuum; unsaturated liquid flow; thermal vapour diffusion; advection/diffusion of total concentrations (sequential) /XIE 06c/. It is reported that the new model enables the program Geo-Sys/Rockflow to simulate reactive transport under extreme conditions (e.g. high pressure, high temperature, high concentration or even dry out cases). The validation of the improved code was made with a 1D transport and calcite dissolution case.

A summary of the technical properties of the code ROCKFLOW is given in Table 6-10.

6.10.2 Applications in Clay Formations

One of the non-isothermal drainage experiments conducted with mixtures containing sodium-(SPV Volclay) or calcium-bentonite (Calcigel) and crushed rock to investigate the thermal and hydraulic properties of the buffer and backfill under conditions expected to exist in a permanent repository for radioactive waste in Äspö test site was treated as a benchmark between TOUGH2 and RockFlow/RockMech. The simulation of the experiment served also a validation for RockFlow/RockMech /ENG 04/

In order to analyse and understand the bentonite behaviour under various repository conditions, a variety of aspects concerning THMC coupled problems is considered by using with PHREEQC improved ROCKFLOW /SHA 05/. To investigate the possible changes in pore water chemistry resulting from thermal gradients and hydration processes. A 1D model was used to calculate the distribution of temperature, water content, and concentration of different chemical specimens in a highly compacted FEBEX-bentonite simultaneously subjected to heating and hydration. The results show a good agreement of simulated and measured pore water chemical compositions.

Table 6-10: Properties of code ROCKFLOW in terms of modelling gas transport in clay formations

Governing equations		
		Basic mass and energy balance, B_HC, B_EC, B_ME
Hydraulic transport modelling		
	Advection/dispersion	H_TP_D, Advective mass flux is a sum over phases. H_DIS, Hydrodynamic dispersion with longitudinal and transversal dispersion coefficients
	Diffusion	H_DIF_F, Molecular diffusion taken into account, Fick's law, multi-phase diffusion
	Phases/Components	P_WP, P_AP
	Sorption	H_A, Reversible instantaneous linear sorption, taken into account in mass accumulation term
Geology-Geometry modelling		
	Porous media	GF_F, GF_L, GF_AH Conventional, with tortuosity and capillary characteristics Relative permeability functions, Capillary pressure functions
	Fractured media	good possibility of modelling fractured media
	Changes in petrophysical parameters	G_PP
Heat transport modelling		
	Convective/conductive	Heat flux with conductive and convective components
	Effect on phase properties	Considered
Mechanical coupling		
	Swelling	CHM Model after /XIE 05/ /XIE 06b/
	Deformation model	Using generalized Hooke's law in /KOH 04/
Chemical coupling		
	Physical	Multi-species transport of either straight or branching decay chains
	Chemical	PHREEQC improvement /SHA 05/
Application for clay formations		
	THM Coupling	/ZHA 04/ Numerical modelling of THM Coupling for Callovo-Oxfordian and Opalinus Clay
	THM Tests	/HÖK 05/.Andra/Skb Temperature buffer test
	HM Response of Bentonit to Heating and swelling	/ZHA 04/ Response of bentonite buffer to heating, saturated, unsaturated cases
	Mock-up tests	/SAN 05a/ the simulation of the large scale tests of the FEBEX project
Discretization		
	Space	Finite element method
	Time	Finite differences schemes
User friendliness		
	User Manual	A comprehensive user's manual

6.11 GAMBIT-GWS/ENTWIFE

In the framework of GAMBIT Club programme a programme of a computational model that (i) would 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 was developed /HOC 04/.

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. New implementations performed on GAMBIT-GW model in this phase are cited as:

- a) Introduction of a dual porosity model to provide a more realistic representation of the clay fabric; and
- b) Implementation of 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.

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.

6.11.1 Technical Description /HOC 04/

The theory is considered first with coupling of 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 /BIO 41/ 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 also taken into account. 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 Law.

A summary of the technical properties of the code GAMBIT-GWS/ENTWIFE is given in Table 6-11.

6.11.2 Applications in Clay Formations

The simulation of some gas migration experiments have been performed on cylinders of pre-compacted Mx80 bentonite using a Constant Volume and Radial Flow (CVRF) apparatus. A two-dimensional mesh with a cylindrical geometry was used to represent the bentonite sample in experiment Mx80-8 /HOC 04/. 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. 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.

Table 6-11: Properties of code GAMBIT-GWS/ENTWIFE in terms of modelling gas transport in clay formations

Governing equations		
		Basic mass and energy balance, B_HC, B_EC
Hydraulic transport modelling		
	Advection/dispersion	H_TP_D, Advective mass flux is a sum over phases. H_DIS Hydrodynamic dispersion with longitudinal and transversal dispersion coefficients
	Diffusion	H_DIF_F , Molecular diffusion taken into account, Fick's law, multi-phase diffusion
	Phases/Components	P_WP, P_AP, P_VP, P_AP
	Sorption	H_A
Geology-Geometry modelling		
	Porous media	GF_F, GF_L, GF_AH Conventional, with tortuosity and capillary characteristics Relative permeability functions, G_RP_Corey, G_RP_Gen, Capillary pressure functions, G_CP_Pick, G_CP_Gen (selective, linear, after Pickens, TRUST, Leverett, van Genuchten)
	Fractured media	G_F, G_F_DF
	Changes in petrophysical parameters	Not considered
Heat transport modelling		
	Convective/conductive	Heat flux with conductive and convective components
	Effect on phase properties	Considered
Mechanical coupling		In standard release not considered
Chemical coupling		In standard release not considered
Application for clay formations		
	Safety analysis	/AND 01/
Discretization		
	Space	Finite difference method, flexibility in creating grid geometry
	Max grid size	Flexible
User friendliness		
	User Manual	Version 5, very good presented
	Pre-post facilities	Good developed self pre and post processing

6.12 ROCMAS

ROCMAS is a finite-element code for analysis of coupled THM processes in partially saturated geological media /NOO 96/. In ROCMAS, the Biot formulation is extended to partially saturated media for heat- and moisture-flow in soil. This results in a comprehensive coupled THM formulation for partially saturated geological media that includes the coupled processes show in Figure 6-5.

In ROCMAS, solid, liquid, and gas phases are considered. However, it is assumed that the gas pressure p_g is constant and equal to atmospheric pressure throughout the porous medium. As a consequence, vapour transport occurs only through molecular diffusion driven by a gradient in vapour concentration. The heat transfer may take place through conduction over all phases and by advection with water in both liquid and gas phases.

6.12.1 Technical Description

ROCMAS considers liquid water flow as well as vapour flow in air-filled pores due to molecular diffusion, and both are coupled with temperature and mechanical deformation/. The liquid flow is driven by the pressure gradient and depends on the relative permeability, K_r which is a function of saturation. The vapour flow is driven by the vapour density gradient and depends on an effective molecular diffusion coefficient D . Air flow and convection of vapour with bulk air flow are not considered. Thus, this approach may be limited to relative low temperature (weakly non-isothermal) or low-permeability systems where the steam convection can be neglected. The basic governing equations in ROCMAS for coupled thermo-hydro-elasticity in weakly non-isothermal, variably saturated media are:

- Mass conservation of water and vapour
- Energy conservation
- Momentum conservation

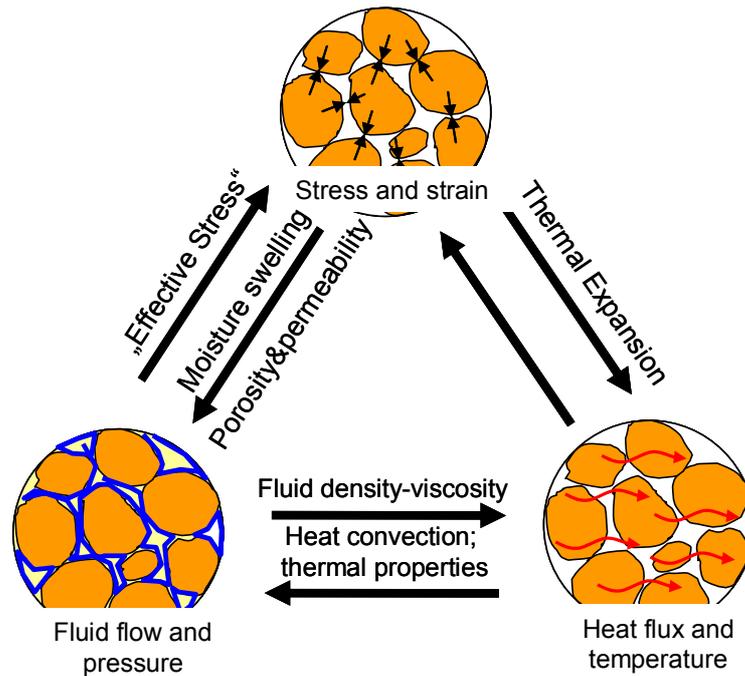


Figure 6-5: Coupled processes considered in ROCMAS /NOO 96/

In ROCMAS the fractured media can also be modelled by the permeability k , depending on the current fracture aperture and can be calculated using the “cubic law”. The permeability of a fracture can easily change several orders of magnitude because of mechanical fracture-aperture changes accompanied by stress changes.

A combined methodology of discrete and continuum approaches DFN DEM (discrete fracture network-distinct element method) is implemented to ROCMAS which provide the mechanical and hydraulic properties of fractured rock masses, and their stress-dependencies/MIN 05/. Sound representation of rock mechanical behaviour at different scales is accommodated in ROCMAS through the stress-deformation matrix or discrete fractures derived from rock mechanical constitutive relations of normal and shear deformation in rock fractures. Implemented fracture normal closure deformation implies that the normal deformation, mechanical, and hydraulic aperture is a nonlinear function of the current local normal stress across the fracture. Shear is accommodated by a dilating, strain-softening, elastoplastic model where shear failure is triggered by Mohr Columb criteria. A summary of the technical properties of the code ROCMAS is given in Table 6-12. More detailed description of ROCMAS is given in /RUT 99/.

6.12.2 Applications in Clay Formations

ROCMAS is used in many numerical validation, testing and comparison studies /MAK 95/, /CHI 00/,/MIN 05/.

In Decovalex Project, modelling of the full-scale heater experiment is given as the applicability of ROCMAS for practical field problems. The simulation is performed based on two model

calibrations: the calibration for the rock property field by Task 2B and calibration of the bentonite behaviour using laboratory experiments. Therefore, Task 2C is a prediction of the fully coupled THM behaviour of the heater-bentonite-rock system and the interaction between the different components. Because of the complexity and uncertainties in the material behaviour, fracture geometry and properties, scale and time effects, and reliability of sensors and data for long-time experiments, good agreement between predicted and measured results should not be expected for all sensors. Despite these limitations, good agreement was achieved for most of the predicted variables in the buffer, especially temperature and water content distribution and rock temperature /CHI 00/.

The results do, however, show that the liquid flow from the rock into the bentonite was over-estimated by the numerical modelling. One possible explanation is that a sealing effect occurs at the rock-bentonite interface, retarding the wetting of the bentonite from the saturated rock surface. The overall conclusion from Task 2C is that the agreement between model and experiments are satisfactory good, with remaining uncertainties in the mechanics of the buffer and the hydraulics of the rock-bentonite interface.

In /MIN 05/ a combined methodology of discrete and continuum approaches is tested using ROCMAS. The results of a series of simulations based on the DFN–DEM (discrete fracture network–distinct element method) approach provide the mechanical and hydraulic properties of fractured rock masses, and their stress-dependencies. These properties are calculated on a representative scale that depends on fracture network characteristics and constitutive models of intact rock and fractures. It is indicated that the large scale domain can be divided into four regions with different property sets corresponding to the depth. The results derived by the DFN–DEM approach are then passed on to a large-scale analysis of the far-field problem for the equivalent continuum analysis.

ROCMAS was also used for modelling the full-scale engineered barrier experiment (FEBEX), currently conducted at the Grimsel Test Site in Switzerland. A three-dimensional fully coupled THM analysis of the FEBEX in situ test was carried out for the first 1,000 days of heating. Model geometry and material properties are presented /RUT 03b/. The material properties were obtained from various field and laboratory tests that were performed before the emplacement of the buffer and heaters. The results indicate that numerical modelling can provide highly reliable predictions for temperature distribution, and reasonably reliable predictions for moisture flow and stress in a bentonite barrier. Moreover, field observations and modelling shows that resaturation of the buffer was controlled by the properties of the bentonite barrier whereas the permeability of the rock was sufficiently high to act as an unrestricted water source.

Table 6-12: Properties of code ROCMAS in terms of modelling gas transport in clay formations

Governing equations		
		Basic coupled mass and energy balance, B_HC, B_EC, B_EC
Hydraulic transport modelling		
	Advection/dispersion	H_TP_D, Advective mass flux is a sum over phases.
	Diffusion	H_DIF_F , Molecular diffusion taken into account, Fick's law, multi-phase diffusion
	Phases/Components	P_WP, P_AP, P_VP
	Sorption	-
Geology-Geometry modelling		
	Porous media	GF_F, GF_L, GF_AH Conventional, with tortuosity and capillary characteristics Relative permeability functions, Capillary pressure functions
	Fractured media	G_F, G_F_DP, DFN DEM model
	Changes in petrophysical parameters	Coupled with mechanical changes.
Heat transport modelling		
	Convective/conductive	Heat flux with conductive and convective components
	Effect on phase properties	Considered
Mechanical coupling		Shear is accommodated by a dilating, strain-softening, elastoplastic model where shear failure is triggered by Mohr Columb criteria
	Rock convergence	M_RC
	EDZ	M_EDZ_S, M_EDZ_SS
	Swelling	M_S
	Fracturing, pathway dilatation	
Chemical coupling		Not considered
Application for clay formations		
	Swelling model	Implemented by /CHI 00/
	Fracture/stress relationship	Implemented by /MIN 05/
Discretization		
	Space	No Information
	Max grid size	No Information
	Time	
User friendliness		
	User Manual	No Information
	Pre-post facilities	No Information

6.13 THAMES

The coupled THM analysis numerical code THAMES was originally developed by Ohnishi, Kyoto University /OHN 85/. JAEA (Japan Atomic Energy Agency) has validated the code Thames with the help of Hazama Corporation and Kyoto University. The code Thames was applied to the simulation of the coupled THM phenomena in and around the EBS in the second progress report on research and development for the geological disposal of HLW in Japan. In order to perform a THMC coupled analysis of the processes in near field of the geological disposal system, THAMES was also tested in the framework of DECOVALEX project /WAN 06/.

6.13.1 Technical Description

The continuity equation is written for water/vapour movement and heat induced water movement. The energy conservation equation takes into account the heat transfer by conduction and convection as well as the energy by evaporation. The mechanical equilibrium equation takes the swelling behaviour of the partially saturated bentonite into account.

The code is based on the coupling analysis code Couplys (Coupling analysis system) including THMC-phenomena by existing analysis codes THAMES, and PHREEQC. The results are cited as follows/OHN 85/:

1. In order to obtain a reliable resolution the THAMES code was modified for 8 nodes element and each phenomenon was solved separately instead of full coupling.
2. In order to upgrade the model, gas diffusion has been introduced independent on aqueous element.
3. The geochemistry module has been adopted to take into account the dependence of the surface site density to the water conditions in the bentonite and the changes in CSH solid phase with changes in the ratio of C/S for cementitious material. The methodology of time mesh for kinetic model and separate method for pore water chemistry in the bentonite has been studied.

A summary of the technical properties of the code THAMES is given in Table 6-13.

6.13.2 Applications in Clay Formations

A validation of the code THAMES was performed with the simulation of the Big Bentonite facility (BIG-BEN) intended to demonstrate the function of the engineered barrier system, the large-scale experiment is conducted /CHI 00/. The facility consists of an electric heater surrounded by glass beads, carbon steel overpack, buffer material and man-made rock. The buffer is a mixture of bentonite and sand. The heater is operated at 0,8 kW. Water is injected from the interface between the buffer and the man-made rocks at the pressure of 0,05 MPa. The duration of the experiment is 20 months. The change in temperature and swelling pressure are continuously monitored and gravimetric water content is measured by sampling.

The coupled thermal, hydraulic and mechanical processes are simulated with the finite element code THAMES, which can simulate the fully coupled phenomena in the saturated and unsaturated clay under non-isothermal condition. To examine the validity of the code, all the parameters used in the model are evaluated from the other laboratory tests. The simulated results are compared with the measured ones without calibration of the parameter values using the results from the BIG-BEN experiment. It can be concluded that the changes in temperature and gravimetric water content within the buffer can be simulated reasonably well and that the mechanical effect such as swelling pressure is difficult to realize.

In DECOVALEX Project the JNC model introduced in THAMES is compared with other codes for modelling an in-situ T-H-M experiment in Kamaishi Mine in Japan. A granulated bentonite was compacted directly into a test pit, by layers of 10 m thickness. The initial water content of the bentonite is given as 15%. A heater was installed in the test pit, surrounded by the bentonite. The temperature at the centre of the heater was maintained at 100°C during a heating phase of 258 days. The temperature, water content and radial stress profiles are calculated with various codes. The JNC model implemented in THAMES gave consistent results with the experimental data in modelling strain behaviour in the near vicinity of the heater.

Table 6-13: Properties of code THAMES in terms of modelling gas transport in clay formations

Governing equations		
		Basic mass and energy balance, B_HC, B_EC JNC model is implemented in /CHI 00/, continuity Eq. for water/vapour movement
Hydraulic transport modelling		
	Advection/dispersion	H_TP_D, Advective mass flux is a sum over phases.
	Diffusion	H_DIF_F, Molecular diffusion taken into account, Fick's law, multi-phase diffusion
	Phases/Components	P_WP, P_AP, P_VP, P_AP
	Sorption	H_A
Geology-Geometry modelling		
	Porous media	GF_F, GF_L, GF_AH Conventional, with tortuosity and capillary characteristics Relative permeability functions, G_RP_Corey, G_RP_Gen, Capillary pressure functions
	Fractured media	?
	Changes in petrophysical parameters	Not considered
Heat transport modelling		
	Convective/conductive	Heat flux with conductive and convective components
	Effect on phase properties	Considered
Mechanical coupling		Momentum Balance in terms of stress for rock and bentonite
	Rock convergence	Considered
	EDZ	-
	Swelling/shrinking	M_S_JNA
	Fracturing, pathway dilatation	-
Chemical coupling		Coupled with PHREEQC
	Chemical	C_RX, C_SC, C_OX, C_DP, C_IE,
	Physical	P_PD
	Calibration and validation in the framework of BIG-BEN Project	/CHI 00/
Application for clay formations		
	Thermal properties	Inverse modelling for thermal properties of Opalinus Clay /CAR 05/
	Mechanical coupling	Alliance Project /MON 05b/
Discretization		
	Space	Finite difference method.
	Time	First order finite differences
User friendliness		
	User Manual	No information
	Pre-post facilities	No information

6.14 GEFDYN

GEFDYN is a program for static and dynamic linear 3D modelling, with or without consideration of hydraulic/mechanical coupling. It is indicated that it is particularly suitable for geomechanical problems with numerous non-linear rheological laws, such as civil engineering works where soil plays an important role, especially dams, surface or deep foundations, retaining walls, and tunnels. The implementation of the constitutive stress-strain-temperature relationship for the solid matrix is described in /LAL 02/. A thermo-plastic model is presented which takes into account thermal hardening and irreversible thermal strain.

6.14.1 Technical Description

The version of GEFDYN used to analyse the THM coupling in clay formations is developed by /LAL 02/. This thermo-hydro-mechanical (THM) formulation is obtained on the basis of the homogenisation theory (averaging principle) and is associated with a thermo-plastic constitutive model developed by the authors to take into account thermal hardening and irreversible thermal strains.. For modelling a saturated soil as a porous medium with two phases: solid (assemblage of grains) and fluid (water) is considered. External solicitations are considered as mechanical, hydraulic and/or thermal (three fields). Starting from a microscopic level where each phase is considered separately as a continuum, and using the homogenisation theory, it is possible to derive a mathematical formulation for an equivalent continuum at a macroscopic level. The coupled equations obtained govern the evolution of pore pressure, solid displacement and heat flow under mechanical, hydraulic and/or thermal loading. The equations for momentum, energy and mass conservations are coupled throughout the dependent variables solid displacement vector, fluid pressure and temperature in the medium. The constitutive stress strain- temperature relationship for the solid matrix is assumed to be governed by a thermo-plastic model (the LTVP model).

The LTVP model is a generalisation to non-isothermal conditions of the cyclic orthotropic elasto-plastic multi-mechanism model with kinematical hardening. This thermo-plastic constitutive model is different from others as:

- It is one of the first cyclic thermo-plastic constitutive models able to represent principal thermo-mechanical characteristics of clays over a wide range of loading conditions.
- It handles overconsolidated as well as normally consolidated clays in the same framework; the isotropic thermo-plastic mechanism appears to be the major element in the model.
- Other Cam-Clay-family models may be transformed into thermoplastic models by coupling such a mechanism with their standard yield surface.

The LTVP model describes behaviour using non-linear elasticity and four kinematic plastification mechanisms: one isotropic and three deviatoric. These four mechanisms are activated during monotonous as well as cyclic loading. Each deviatoric mechanism has its own hardening parameters related to the distortion in the corresponding plane. All four mechanisms are coupled by the isotropic hardening parameters. The limit criterion is very close to that of

Mohr-Coulomb. Temperature acts on the essential rheological parameters. The thermo-plastic strain rate is defined through a plastic flow rule. Thus it is related to the yield surface, which depends on stress state, temperature and internal variables.

A summary of the technical properties of the code GEFDYN is given in Table 6-14.

6.14.2 Applications in Clay Formations

To illustrate the capacity of the LTVP model to predict the major aspects of clay behaviour, two numerical simulations are performed. The first validation attempt was made for Boom clay and the second one for Pontida Clay /LAL 02/. For Boom Clay the material parameters were identified using undrained triaxial and consolidation tests at ambient temperature. To determine the thermomechanical parameters, experimental results of thermal loading from an ambient temperature of 21,5°C to a high temperature of 95°C were used. The test consists of applying a thermal load to a normally consolidated (case 1), a slightly overconsolidated (case 2) and an overconsolidated sample (case 3). Cases 1 and 3 were used to determine the thermal parameters of the model with the assumption that in case 3 the behaviour was thermo-elastic. Therefore, only case 2 corresponds to a numerical prediction. The comparison between the numerical predictions and experimental results is satisfactory during thermal loading and unloading.

For Pontida Clay the validation tests were made at two different temperatures for two different overconsolidation ratios. Experimental results show that temperature caused a shear resistance decrease and a decrease of dilatancy. The model parameters were determined using isothermal triaxial tests. Numerical simulations of the mechanical behaviour at 95°C are quite satisfactory for shear strength as well as for the volumetric variation.

Table 6-14: Properties of code GEFDYN in terms of modelling gas transport in clay formations

Governing equations		
		Basic mass and energy balance, B_HC, B_EC
Hydraulic transport modelling		
	Advection/dispersion	H_TP_D H_DIS, Hydrodynamic dispersion with longitudinal and transversal dispersion coefficients
	Diffusion	H_DIF_F, Molecular diffusion taken into account, Fick's law, multi-phase diffusion
	Phases/Components	P_WP, P_AP, P_VP, P_AP, P_CO2_EC, P_X_EC
	Sorption	H_A, Reversible instantaneous linear sorption
Geology-Geometry modelling		
	Porous media	GF_F, GF_L, GF_AH Conventional, with tortuosity and capillary characteristics Relative permeability functions, G_RP_Corey, G_RP_Gen, Capillary pressure functions (selective, linear, after Pickens, TRUST, Leverett, van Genuchten)
	Fractured media	G_F, G_F_MINC, G_F_DP, Classical double-porosity concept after Warren and Root. Rock matrix and fractures may exchange fluid or heat by means of interporosity flow
	Changes in petrophysical parameters	G_DP, G_DP_KK, G_DP_CL
Heat transport modelling		
	Convective/conductive	Heat flux with conductive and convective components
	Effect on phase properties	Considered
Mechanical coupling		thermo-plastic constitutive, non-linear elasticity and four kinematic plastification mechanisms
	Rock convergence	M_RC
	EDZ	M_EDZ_S, M_EDZ_TE, M_EDZ_TE
	Swelling	M_S_X
	Fracturing, pathway dilatation	M_CP
Chemical coupling		Not considered
Application for clay formations		
	Validation	Boom and Pontida Clay, /LAL 02/
Discretization		
	Space	Integral finite difference method. The discretized flux is expressed in terms of averages for the neighbouring cells. The grid geometry flexible.
	Max grid size	-
	Time	First order finite differences, flux terms fully implicit
User friendliness		
	User Manual	A good developed user manual, upgraded versions
	Pre-post facilities	

6.15 Comparative Evaluation of the Software

The general characteristics of the codes used for modelling transport and coupled phenomena in clay formations and clay based buffer materials are given in Table 6-15. Table 6-15 contains not only the codes studied in the chapter but also some other codes for which an evaluation was possible only with limited data from the literature. Two features are especially important by evaluating the compared codes. These are firstly available fluid phases and secondly, available coupled processes. Some codes permit computations only for saturated media, in other terms they make the calculations for one-phase flow (FRAC3DVS, HYTEC). Some others take the presence of a second phase only as air or vapour (Code_BRIGTH, Porflow). More developed codes in this term such as TOUGH2, TOUGHREACT offer more gas components like CO₂, H₂, CH₄. If the presence and generation of other gases than air has to be taken into considerations, neglecting the effect of these components may be an oversimplification. The coupling of thermal, mechanical and chemical processes to the transport phenomena should be another important factor in code evaluation. Almost all codes provide the coupling of the thermal processes and parameters to the hydraulic computations. FRAC3DVS or TOUGH2-FLAC have strong coupling with mechanics whereas some codes like TOUGHREACT and HYTEC provides gut qualified chemical components without any mechanical coupling.

A code with fully validated modelling capability is difficult to identify. This is due to many reasons:

The first reason is the complexity of the transport phenomena in clay formations and buffer materials. There are quite a number of open points in the explanation of the flow physics as well as of the coupled effects. Modelling of EDZ's and of the chemical and physico-chemical interactions in clay formations is dubious yet. The full mechanical coupling necessitates under both, physical and numerical aspects new developments and implementations.

The second reason is the necessity for the qualification and validation of the existing physical modelling approaches. Various physical solutions and their numerical implementations are used in the software for tackling the main problem; however, a real, interrelated validation of these implementations fails. The validation attempts are mainly case specific.

The third reason is about the universal applicability of this software. Almost all codes are developed as the result of many scientific and practical research studies. However, their applicability in terms of full scale geological modelling is limited. Modelling of faults or the up-scaling possibilities show deficits for most of the software. The limits on grid elements or flexibility on grid structures are other potential problems related to full scale geological modelling in repository assessments. An important deficit of many codes within this context is insufficiencies in pre- and post-processing of the input and output data. Some of the codes provide own processing possibilities, however, they are mostly inadequate for a geological THMC modelling.

Table 6-15: Comparison of the numerical codes studied

Code Name	Origin	Main features	Hydraulic media	Coupling	Notes about coupling	Application in clay	Association	ISTec Experience
TOUGH2	DOE/LBNL	3D, 3P Components flexible	PM DP	TH M	M not fully, individual developments for compaction and swelling	/JAV 06/ /CAL 06/ /POP 03/	ISTec, GRS, NAGRA	Since 1999, application and development
TOUGH-FLAC	DOE/LBNL	3D, 3P Components flexible	PM DP	TH M	TOUGH2 coupled with mechanical simulator FLAC3D (elastic, plastic and viscous)	/XIE 05/	GRS	not available
TOUGHREACT	DOE/LBNL	3D, 3P Components flexible	PM DP	TH C	TOUGH2 coupled with chemical module and EQ3/6 Database	/BUR 06/ /ALK 06/	ISTec,	Since 2005, application and development
CODE BRIGHT	T. University of Catalonia	3D, H2O-Air	PM FM	TH M C	BBM Elastoplastic law, plastic law	/ZHA 04/ /SAN 05a/ /MAY 06/	GRS, ANDRA, EN-RESA	not available
ROCKFLOW	Un. of Hannover, Un. of Tübingen	3D, H2O-Air	PM FM	TH M C	Extended to chemical coupling with PHREEQD, DDL swelling model, Brush Model	/WAN 06/ /XIE 06a/ /MAS 06/ /ENG 04/	Un. Of Hannover, Un. of Tübingen BGR,	A demo version has been installed and tested
PORFLOW	ACRI	3D, H2O-Air	PM	TH	FM limited as discrete fracture Chemical coupling limited with decay, chain reactions, constant reaction rate	/ZAL 00/ /MAZ 01/ /MON 05b/	ANDRA, SCK-CEN	A demo version has been installed and tested
ASTER	Electricite de France	3D, H2O-Air	PM	THM	Originally for modelling mechanical problem designed	/MAY 06/	ANDRA	Not available

Code Name	Origin	Main features	Hydraulic media	Coupling	Notes about coupling	Application in clay	Association	ISTec Experience
CAST3M	CEA	3D, H2O-Air	PM FM	TH C	No sufficient data about the validation of M and C coupling	/MÜG 03/ /MON 05b/ /CAR 05/	ENRESA	A demo version has been installed and tested
FRAC3DVS	Waterloo Hydrogeology	3D, 3P	PM FM	H M	M, limited by consolidation, Radionuclide decay	/KOS 04/	NAGRA	not available
HYTEC	École N. S. des Mines de Paris	2D, 2P	PM	H C	Hydraulic model coupled with chemical model CHESS, multi species in liquid phase	/COM 05/	AEA	A demo version has been installed, not tested
THAMES	JAEA, Japan Atomic Energy Agency	3D H2O-Air	PM FM	TH M	Swelling, thermo-elastic model	/CHI 00/	JAEA	Information on internet
FRT-THM	CAS, Chinese Academy of Science	3D H2O-Air	PM FM	TH M	Elastic, elastoplastic, viscoplastic model	/RUT 06/	CAEA	Information on internet
GEFDYN	SFIT, BRGM	3D	PM	THM	Thermo-elastic, thermo-plastic LTVP Model	/LAL 02/		not available
ROCMAS		3D, 3 Phase H2O-Air	PM FM	TH M	Mechanical coupling limited	/RUT 03b/ /CHI 00/ /MIN 05/	SKI, ANDRA	not available
CASTEM2000	DMT-ECA	3D, 3 Phase H2O-Air	PM FM	THM C	Limited chemistry with diffusion	/ROB 00/ /MÜG 04/	KTH, AEA	Information on internet

7 STATE OF THE ART OF TRANSPORT MODELLING IN GEOLOGICAL REPOSITORY SYSTEMS

Host rocks for geological repositories are initially considered as non-permeable systems as they are selected due to their sealing properties. Having this initial condition, the transport processes which can take place under the effect of various disturbances and events are investigated in the framework of a safety analysis. As expected, in near and far field of the geological repositories for hazardous waste, transport mechanisms exhibit comparable characteristics for all possible host rocks. The fluid advection-dispersion accompanying by diffusion is the basic mechanism. Various thermophysical, chemical and mechanical internal and external features, events and processes (FEP's) influence these mechanisms. For physical and numerical modelling of the basic transport mechanisms different approaches have been made. These approaches are supported by various disciplines related to flow in geological formations such as hydrogeology and petroleum engineering. The accompanying retardation processes sorption, dissolution, precipitation are dealt by researchers from various sectors very frequently. The advection accompanying by diffusion and also the retardation mechanisms form the basic structure of all modelling attempts of gas respectively fluid transport in repository host rocks.

To model the gas transport in geological milieu, gas generation must be defined first. Considerable amount of study on gas generation and rates due to various mechanisms, mainly corrosion, microbial degradation and radiolysis exist in the literature. Various models supported by stoichiometric analysis and experimental data permit sufficiently accurate predictions. However, the know-how on the gas generation due to microbial degradation is reported to allow for a rather large band width of uncertainties. Therefore some more investigation is recommendable on microbial degradation of the wastes to be disposed in all host rocks.

The gas generated by various mechanisms remains in gas phase or dissolves in liquid due to the dominating thermodynamics and petrophysics in geological milieu. The knowledge on thermodynamic aspects, phase behaviour and diffusion are almost complete if all components of the transport are known and applied for modelling. This is possible only on a theoretical basis. A frequently applied simplification is the lumping of all gases and liquid components into one gas and one liquid phase. That is mostly sufficient for modelling the transport processes. In clay formations the physico-chemical interactions between fluids and clay minerals play an additional role in determining the thermodynamic initialisation. Moreover, it should be indicated that in gas phase especially the individual consideration of the gas components can be an important modelling factor affecting the success.

Homogeneous porous media in terms of one/two phase Darcy formulation is the most often applied basic concept. Various attempts to integrate high flow gradients (e.g. flow through fractures) into the whole of the modelling system were also made. Presence of water and its initial saturation define the boundaries of the flowing conditions in all host rocks. The conventional models are often applied to define the advection and diffusion in crystalline and salt rocks. However, this approach is limited for clay formations because following of reasons. First, capillary and physico-chemical forces are higher in clay formations and play a major role in controlling the flow conditions. On the other side, these forces are mostly neglected in

crystalline and salt rocks. Second, the poro-elastic crack dilation due to effective stress concept causes intermittent, episodic flow processes in clay formations. Although physical understanding of intermittent flow in plastic clays is good; its numerical application is not perfectly operative. Third, the anisotropy and heterogeneity are more pronounced for clay formations. The difficulties on presetting a pathway network are obvious for clay formations whereas the crystalline boundaries or natural fractures and faults permit in some cases a definition for flow pattern. From a point of view of flow dynamics, more efforts to conceptualize the transport phenomena in plastic clays exist in the literature. This is not only because plastic clay needs more explanation on flow characteristics but also because an analogy likely exists between hard clay and crystalline rocks with the fracturing processes. However, the definition of a flow network in both clays is necessary although not easy.

It can be concluded that the application of the basic porous media and/or fracture flow concepts are more questionable for clay formations than for crystalline and salt formations.

Another complexity of modelling gas transport in clay formations arises from the deficits in numerical coupling of the geomechanics in clay formations. The long-term creeping behaviour, the geomechanical aspects of cavern excavation, the dilatancy boundary and extent and effects of EDZ's are not fully understood and quantified for both plastic and indurated clay formations making the coupling efforts difficult. A universally applicable, reliable coupling of the hydraulical properties to the mechanical properties does not exist yet for all host rocks; however this is especially important for clay formations taken the compaction and self-sealing features into considerations. The re-sealing capacity of the clay formations adds a positive aspect on their capacity as repository rocks. However, the know-how about the re-sealing of the clay formations is not sufficient and more studies are required on this aspect. It is affirmed that the plastic clays and bentonite based buffers show more promising properties in terms of self sealing.

A summary of the comparison of the state of the art of transport modelling in possible host rocks as geological repository is given in Table 7-1 based on the relevance of the process studied. A detailed ranking is avoided because of the dependence of the processes and properties related to transport on the type of the waste, buffer material and disposal concept. As can be concluded the weak points of modelling approaches for clay formations for both plastic and indurated are concentrated mainly on the following topics:

- Non-Darcy flow
- Poro-elastic pathway dilation
- Definition of the flow network, anisotropy, heterogeneities
- Effects of the physico-chemical forces
- Chemical processes, coupling with transport mechanisms
- Definition of the EDZ and deviator-dilatancy-permeability coupling

Finally, the modelling of the full scale transport processes in geological repositories is an important deficit common to all host rocks. The geological modelling, up-scaling of the geological features and petrophysical parameters is necessary for a full scale modelling of the cascade-like transport phenomena from the waste container to the biosphere. There exist numerous numerical simulators in the literature all with different major features. The compilation of these major features into one powerful simulator with an additional capacity of geological modelling should be one of the aims of the modelling efforts in geological repositories. The pre- and post-processing ability of such a simulator should also be capable for conducting effective modelling and following monitoring studies.

Table 7-1: Relevance and state of the art of the processes and properties of gas transport in host rocks for geological repository

Process/Property	Crystalline rock		Salt rock		Plastic Clay		Indurated Clay	
	R	SA	R	SA	R	SA	R	SA
Gas generation ¹	H	G	H	G	H	G	H	G
Thermodynamics	H	G	H	G	H	G	H	G
Advection/Dispersion	H	G	H	G	H	L	H	L
Flow/Porous Media	H	G	H	G	H	L	L	L
Flow/Fracture	H	L	H	L	H	P	H	P
Pathway network	H	G	H	G	H	P	H	L
Heterogeneity-Anisotropy	L	G	L	L	H	P	H	L
Diffusion	L	G	L	G	H	L	H	L
Retardation	H	G	H	G	H	L	H	L
Physico-chemical forces (Osmosis)	L	-	L	-	H	L	H	L
Heat flux	H	G	H	G	H	L	H	L
Thermal effects on petrophysics	H	G	H	G	H	G	H	G
Mechanics	H	G	H	G	H	L	H	L
Swelling-consolidation	L	-	L	-	H	L	H	L
EDZ's mechanics	H	G	H	G	H	L	H	L
EDZ; Dilatancy-permeability	H	G	H	L	H	P	H	P
Self-sealing	L	L	H	L	H	L	H	L
Chemical (Oxidation, complexation, etc)	L	L	H	L	H	L	H	L
Precipitation-Dissolution	L	G	H	G	H	L	H	L
TM Coupling	H	L	H	L	H	L	H	L
TC Coupling	L	L	H	L	H	P	H	P
Field Scale	H	L	H	L	H	L	H	L

¹ Except microbial degradation

R: Relevance, SA: State of the Art, H: High, L: Low, G: Good, L: Limited, P: Poor

8 CONCLUSION

Considerable amount of experimental as well as numerical data has been published in the last years on modelling the fluid transport in clay formations on physical as well as on numerical basis. The basic objective of this study is the evaluation of the results of this data in terms of their applicability in numerical modelling. A compilation of the physical interpretation of the characteristics of the fluid transport in clay formations and their mathematical implementations on existing or new computer codes simulating the hydrodynamic and related process in geological media is aimed.

Basically the transport of gases is modelled by diffusion supported advection and dispersion. Gas moves either dissolved in liquid phase or together with liquid phase. In natural clay systems the flow of single-phase gas is not expected. There is no significant lack of knowledge regarding on phase behaviour of gas-liquid phase properties, except supporting the empirical parameters of equation of states such as solubility of gases in water with various ionic activities. The main problem arises from two sides. The first one is the physico-chemical interactions in gas-water-clay interfaces. The second one is the geometrical coupling of the flow pathways coupled with mechanics. Both are key features for the formulation of the gas retention in transport models. The obvious insufficiency of Darcy approach, the local and global anisotropy and heterogeneity, lack of experimental data on EDZ's, the interactions of present fluids with clay formations are some other features creating the complexity.

More experimental and theoretical studies need to explain following topics in clay formations:

- Capillary forces and their relation to other petrophysical properties
- Configuration of the natural and induced fracture networks
- Effect of surface forces on the transport potential and mechanisms
- Effect of the physico-chemical mechanisms (swelling, osmosis, etc) on the retention and diffusion of gas
- Scaling and up-scaling of the anisotropy and heterogeneity
- The EDZ properties and effect of self sealing on the long time-behaviour

The numerical formulations of these physical explanations and concepts should be properly coupled with basic transport models.

The actual stand of the numerical implementations of the conceptual models and the use of conventional and non-conventional numerical modelling tools were surveyed in an individual chapter. A total of 15 codes which are used for modelling the transport phenomena in clay formations are detected from the literature. This survey showed the obvious necessity of a more comprehensive code for a coupled numerical modelling of the transport processes in clay formations. The code should also allow the modelling of the full scale geology and related features with sufficient pre- and post-processing possibilities.

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