FORGE

Fate Of Repository Gases

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State of the art report on gas transport through interfaces

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State of the art report on gas transport through interfaces

Knowledge of gas transport properties through sealing or buffer materials is independently from the respective radioactive waste repository concept of vital importance for long term performance assessments because some gas generation may take place as a consequence of different processes (for instance corrosion of iron and degradation of organic materials).

Field tests about gas migration within the engineered barrier systems (EBS) demonstrated that, in addition to the matrix properties of the sealing material and the host rock, conductive discrete interfaces inside the sealing elements itself and to the host rock may act not only as mechanical weakness planes but also as preferential gas path ways. For instance despite the self sealing capacity of bentonite inherent existing interfaces may be reopened during gas injection.

The report gives an overview about the occurrence and consequences of interfaces in the EBS affecting gas migration processes of the repositories dealing to the following topics:

- Description of the disposal concept, comprising the repository layout, operational conditions and post-closure scenarios;
- Description of the fundamental processes of gas flow in the EBS and the host rock;
- Summary of direct qualitative and quantitative observations of water and gas flow through EBS-interfaces from lab and field tests;
- Outline about conceptual models for the simulation and prediction of gas migration and its consequences through interfaces.

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1. Introduction

The long-term safety of the disposal of nuclear waste is an important issue in all countries with a significant nuclear programme. Repositories for the disposal of high-level and long-lived radioactive waste generally rely on a multi-barrier system to isolate the waste from the biosphere. The multi-barrier system typically comprises the natural geological barrier provided by the repository host rock and its surroundings and an engineered barrier system (EBS), i.e. the backfilling and sealing of shafts and galleries to block any preferential path for radioactive contaminants.

The “engineered barrier system” represents the man-made, engineered materials placed within a repository, including the waste form, waste canisters, buffer materials, backfill and seals. The “near field” includes the EBS and those parts of the host rock in contact with or near the EBS, whose properties have been affected by the presence of the repository. The “far-field” represents the geosphere (and biosphere) beyond the near-field (OECD, 2003).

This multi-barrier principle creates an overall robustness of the system that enhances confidence that the waste will be successfully contained. However, gas generation from either the waste form or the engineered barriers is an unavoidable but generally undesired effect in most European repository concepts for radioactive waste. Gas generation and migration can potentially alter the hydraulic and mechanical properties of the repository (possibly the thermal and chemical properties as well) and thus affecting the performance of the repository. A comprehensive summary about gas generation and migration in the various repository concepts, respectively handling of the gas issue in performance assessment (PA) is given in Norris (2009). It states that due to the complexity of the repository system as a whole (waste, buffer, engineering disturbed zone - EDZ, host rock), in particular the gas issue is still poorly understood. Assessment of the possible gas transport modes at repository scale requires consideration of different gas transport properties in different materials and construction components.

Whereas the properties of the geological barrier depend on the natural conditions of the rock formation, the performance of the engineered barriers is a result of their adequate design and execution. To guarantee the overall safety the used technique for the emplacement of the waste canisters and the associated engineered barriers in the underground space are key issues. In this context, during the last two decades reliable information about the potential host rocks and the sealing materials (e.g. bentonite mixtures, concrete, rock backfill) has been obtained but only limited knowledge exists about the importance of contacts or interfaces between these different materials or construction parts, i.e. seal plugs. Reviews of research into gas migration (Metcalf et al., 2009) highlighted that very little has been done to investigate the implications of possible preferential gas transport along and through the EDZs of engineered structures (compare Figure 1-1).

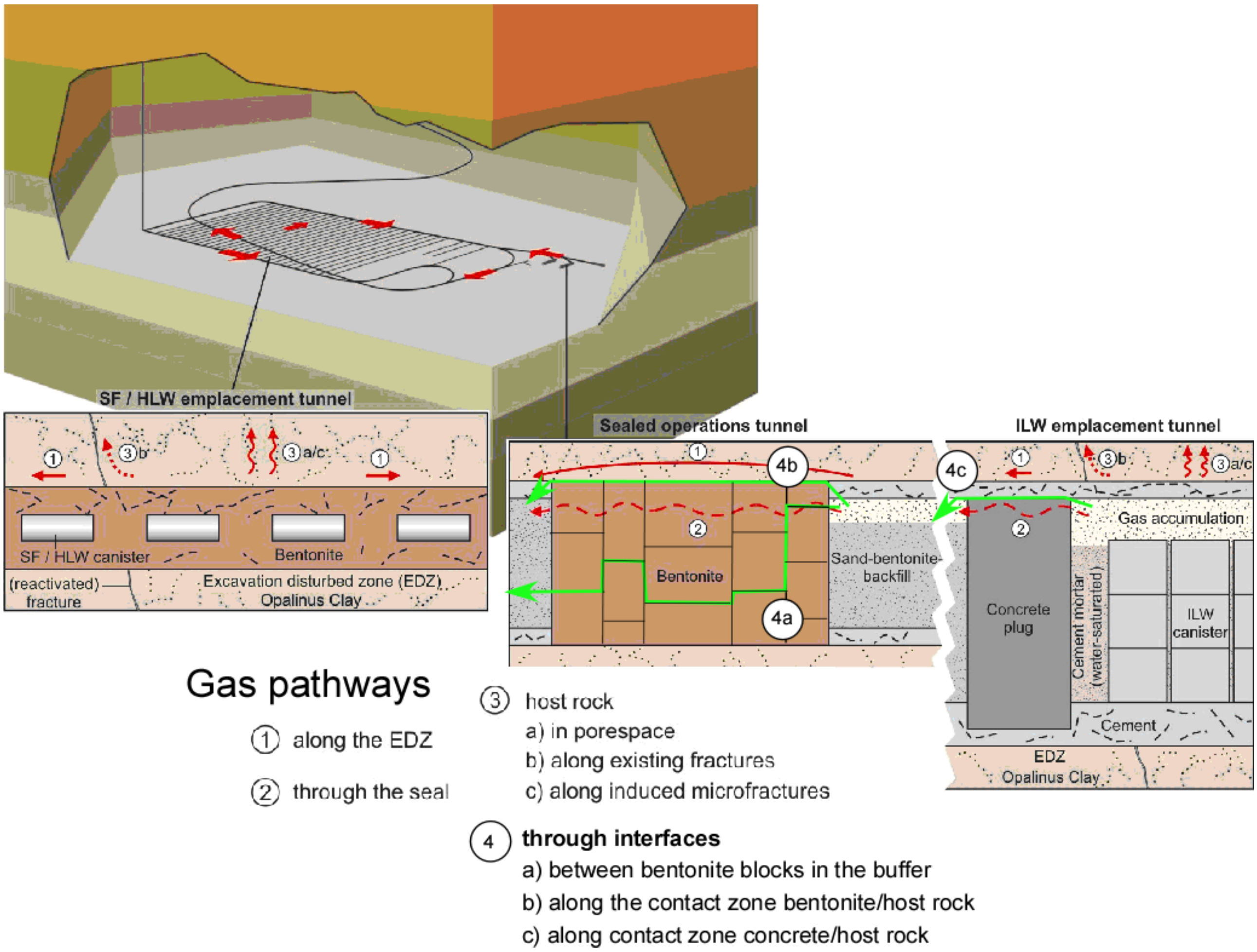


Figure 1-1. Potential migration paths for degradation and corrosion gases accumulated in the SF/HLW tunnels and ILW tunnels. An important factor for gas build-up in the ILW tunnels is the pathway through and around the sealing system. Note that the respective interface types (green labelled) may act as short circuits. The access tunnel, and the construction and operations tunnel represent a potential storage volume for gas (modified after Marshall et al., 2008).

These flow paths may act as hydraulic short circuits quite similar to rock joints (Kodikara et al., 1994; Seidel and Haberfield, 2002; Buzzi, 2004), thus channelling the fluid flow.

However, field tests on different EBS-systems demonstrated that during pressurisation of the main sealing element leakage occurred through several prominent flow-paths, which are inherent existent during the seal construction reducing the overall tightness of the EBS (see Figure 1-1). In addition to some minor flow through the partially saturated buffer material a significant flow occurred through

- the contact between the host rock and the engineered barrier, e.g. through the EDZ and the mechanical contact zone
- interfaces or hydraulic weakness zones within the buffer element.

The relative importance of the damage zone in relation to the backfill and the interface between the backfill and rock can be simply demonstrated for water flow (Chandler et al. 2003):

- Assuming a rock cylinder with a radius of 20 m, a circular tunnel with a radius of 2 m, and the extent of the damage zone to be 0.33 m, then the EDZ would need to be 300 times more permeable than the host rock or 3 times greater than the backfill to become the preferred hydraulic pathway. A smaller, but more permeable EDZ would need to be 1,000 times more permeable than the host rock or 10 times more permeable than the backfill to become the preferred flow path;

- Referring the backfill-tunnel interface Chandler et al. (2002) concluded that an interface between the tunnel and carefully placed pre-compacted blocks of sand-bentonite materials and voids filled with a pneumatically-placed mixture of sand and bentonite, had a transmissivity of 10^{-11} m^2/s or less, but an open air gap of only 0.6 mm would convert to a transmissivity of 10^{-4} m^2/s assuming a parallel plate model.

Thus the tight interface is very important for guaranteeing the backfilled deposition tunnel a barrier function. Therefore, the “damage zone” is not only the properties of the damage outside the periphery but also the geometry of the periphery itself. A rugged surface due to poor drilling, poor blasting or excessive scaling will influence the ability to backfill the tunnel and if so, the consequences might be more severe than the EDZ in itself. The rugged profile will also contribute to higher local stresses around the opening.

The purpose of this state-of-the-art-report is to summarize the knowledge about the occurrence and consequences of interfaces in the EBS affecting gas migration processes of the repositories corresponding to the following topics:

- Description of the disposal concept, comprising the repository layout, operational conditions and post-closure scenarios,
- Description of the fundamental processes of gas flow in the EBS and the host rock,
- Summary of direct qualitative and quantitative observations of water and gas flow through EBS-interfaces from lab and field tests
- Outline about conceptual models for the simulation and prediction of gas migration and its consequences through interfaces.

This overview will supply a basis for designing laboratory and field tests which will be performed in the framework of WP 3 “Engineered Barriers and Seals” to study the importance of interfaces between different materials or construction parts for the gas migration processes. The task of the tests is to deliver not only quantitative data for modelling, but also aid in the interpretation of other laboratory and field scale tests performed in the framework of FORGE.

2. EBS - Boundary conditions

2.1. Disposal concepts

In many countries (Canada, France, Sweden, Spain, Japan and others), the design of nuclear waste repositories is based on natural and engineered barriers to achieve long term confinement. Some Underground Research Laboratories (URL) have been developed to study the feasibility of such concepts.

The repository design in the context of the overall disposal concept determines to a great extent the *gas production*, but has also a severe impact on the *gas accumulation* in the emplacement tunnels and on the gas transport through the engineered barrier system. In contrary to the geological setting, the repository design can be adapted to the safety requirements such that the effects of gas accumulation and release on system performance are acceptable (design optimisation). The influence of the repository design on the treatment of the gas issue in PA can be broken down to the following aspects:

- waste inventory and materials used in repository construction
- repository layout
- operational and post operational system evolution

2.1.1. Waste inventory and construction materials

The primary processes determining the *gas species and the quantities of gas* produced in the emplacement tunnels of a nuclear waste repository are (Schulze, 2002, Rübel et al., 2004, Nagra, 2004):

- anaerobic corrosion of metals (H_2)
- radiolysis of porewater (H_2)
- degradation of organic matter (CH_4 and CO_2).

In the FORGE project the issue “gas generation” is part of the WP 2. For an overview of the relevant processes and their handling in PA depending on the various types of wastes and repository concepts see Norris (2009).

The production of gas is determined by the amount of degradable matter in the backfilled emplacement tunnels, comprising the waste inventory and the construction materials. The estimation of the total amount of degradable matter by species together with the knowledge of the stoichiometries for the relevant reactions provides an estimate of the upper limit of the total amount of gas which can be produced. The temporal evolution of gas production can be inferred from the metal corrosion rates and degradation rates of organic matter as given in Norris (2009). It is obvious, that the actual gas production depends also on the environmental conditions in the tunnel near field, such as porewater chemistry and the water saturation of the EBS.

2.1.2. Repository and EBS layout – reference systems

Pressure build-up in the backfilled emplacement tunnels is affected by the gas storage capacity (tunnel size, porosity of the backfill materials) and the gas transport capacity of the near field system (backfill, seals and EDZ). The design of the EBS and their geotechnical properties may differ considerably between the different national disposal concepts.

However, the prime features of a final repository for high-level nuclear waste are a canister, a buffer consisting of swelling clay around the canister and an excavation at mining depth in the bedrock that may host the package. These features are the same for present repository concepts in argillaceous formations and crystalline rocks, world-wide.

Depending on the functions to be fulfilled by the backfill or buffer materials various requirements exist, i.e. mechanical, hydraulic, geochemical and thermal, as exemplarily summarized Table 2-1 (based on the phenomenology considered in ANDRA's repository concept). However, as demonstrated in ESDRED the functional requirements as have to be fulfilled by the material properties and technical concept vary between the individual national repository concepts.

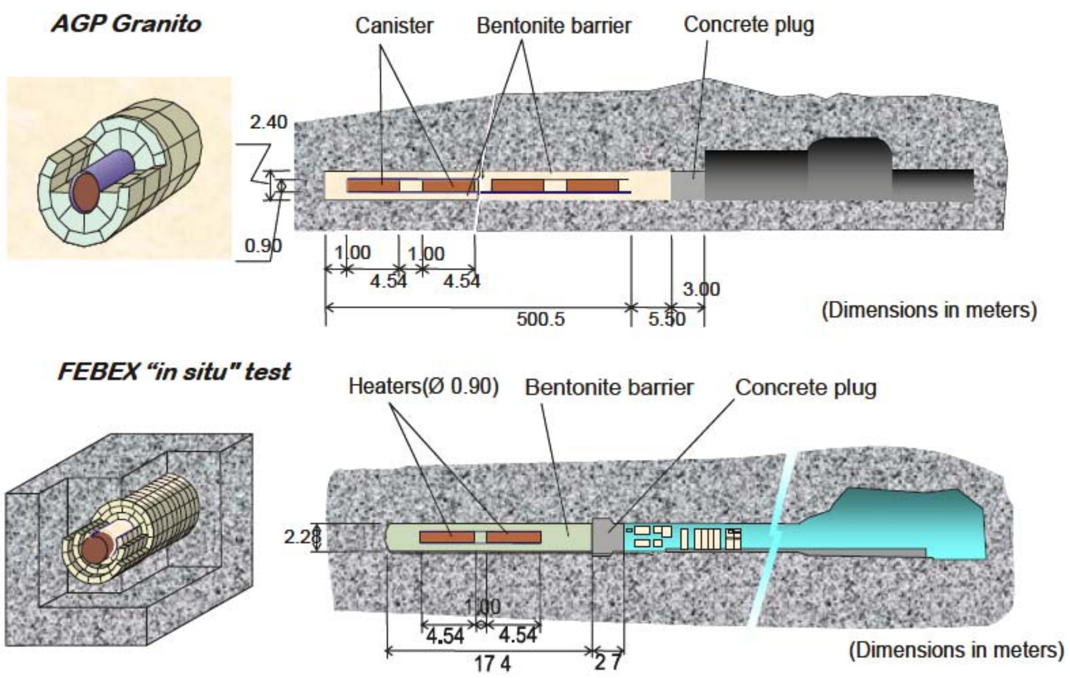


Figure 2-1. General scheme of the Spanish reference concept and the FEBEX "in situ" test (for details see Fuentes-Cantillana et al, 1998).

Within the various repository concepts there are two possible types of engineered barrier materials (backfill or buffer materials) that are considered, mainly used for different functions as illustrated exemplarily in Figure 2-1):

- Clays (generally clays are of the bentonite type) – sealing elements
- Cementitious materials (grout) based on Portland cement – abutment/temporary sealing elements.

For both engineered barrier material options the generation of gas within the repository presents a problem, due for the need for any generated gas to be able to escape through the barrier without degrading the subsequent performance of the barrier (Rodwell et al., 1999).

Table 2-1. Functional requirements of buffer material in ANDRA HLW disposal concept (taken from ESDRED, 2009).

FUNCTIONAL REQUIREMENTS OF BUFFER MATERIAL IN ANDRA HLW DISPOSAL CONCEPT			
Description of Objective	**Time Frame of Objective**	**Associated Material Parameters and Criteria**	
FUNCTIONS			
To isolate the canister from the rock and to support and protect it against rock displacements.	**Before** canister loss of integrity, i.e. $<$ a few thousand years	Plasticity	As high as possible (most swelling clays on the market are satisfactory)
To isolate the canister from groundwater flow and transport processes taking place in the surrounding rock; achieved by providing a low-permeability medium for water flow around the waste packages.		Hydraulic conductivity K	$K < 10^{-12}$ m/s
		Swelling pressure P	$P > 1$ MPa after sliding of the concrete plug $P < 7$ MPa at any time
To create a geochemical environment that will protect against corrosion		Compatibility with steel (pH)	pH not too low
		Hydraulic conductivity	$K < 10^{-12}$ m/s
To create a geochemical environment that will promote the stability of the matrix glass and U/Pu oxides	**After** canister loss of integrity, i .e. $>$ a few thousand years	Compatibility with glass	
		Hydraulic conductivity	$K < 10^{-12}$ m/s
		Swelling capacity	$P > 1$ MPa after sliding of the concrete plug $P < 7$ MPa at any time
To delay radionuclides release by retarding the transport of radionuclides		Hydraulic conductivity	$K < 10^{-12}$ m/s
		Swelling pressure P	$P > 1$ MPa after sliding of the concrete plug $P < 7$ MPa at any time
		Sorption	
CONSTRAINTS			
Buffer should allow gas to escape (as long as steel parts are present)	Many thousands of years	Gas permeability	As high as possible
Buffer should be a good thermal conductor (as compared to rock mass) i.e. should not act as an insulator	Most critical during thermal climax, i.e. a few tens of years. Likely to occur before saturation	Thermal conductivity λ (which depends on dry density, nature of additives, water content)	$\lambda > 1.2$ W/m/K (before saturation and swelling-loss of conductivity due to gaps to be added)
	Also important during the remainder of the thermal phase, i.e. from a few centuries to a few thousands of years		$\lambda > 1.5$ W/m/K (after saturation and swelling- no more gaps)

Special design features such as an EDZ cut-off along seal sections could have a significant impact on the gas-induced pressure build-up in the backfilled tunnels. Excavation and redistribution of the stress around the tunnel lead to the development of an excavation damage zone (EDZ). However, as demonstrated in Table 4-2 various technical solutions to control and limit the EDZ hydraulic effects exists. If the bulkheads of an EBS are keyed into the rock wall of the tunnel they may act as cut-offs for the EDZ of the tunnel and technical induced interfaces between the plug and the buffer. In addition, clay grouting conducted around the clay bulkhead is an additional measure to interrupt the connectivity of EDZ at the bulkhead.

However, due to the complexity of EBS this overview about gas transport and interface properties is related only to the following terms of references:

- The EBS is constructed in either crystalline rock, typified for example by sparsely fractured Äspö granite of the Scandinavian Shield, or by clay rock (including both plastic and indurated clay), typified, for example, by the Callovo-Oxfordian clay from Meuse-Haute Marne or Opalinus Clay from the Mont Terri Site).
- Waste placement options consider both, (1) vertical silo type option (e.g. the in-floor borehole (KBS-3V-type) option) and (2) the horizontal type options (e.g. the horizontal borehole (KBS-3H-type) option or a NAGRA-type option involving placement in long horizontal cylindrical tunnels).
- Repository depths considered for the analysis are 500 to 1000 m for crystalline rock, 300 to 900 m for clay formations.

2.1.3. Evolution of the repository system

According to the terminology of NFPRO the development of the EDZ respectively of technical interfaces inside the EBS is divided into three major stages:

- initial phase during repository construction (EDZ initiation and development)
- short-term evolution during the operational phase / installation of the EBS (hydromechanical and chemical EDZ evolution)
- long term EDZ evolution post repository closure (self-sealing, gas transfer and alkaline plume effects[1]).

It is obvious, that the entire history of the repository system and in particular the evolution of the near field affects the gas pressure build-up in the backfilled emplacement tunnels. For example, an extended initial EDZ or significant interfaces inside the EBS could delay the gas pressure build-up for long times, because the produced gas is piped along the existing pathways.

[1] Over time, concretes based on Ordinary Portland Cement (OPC), leached by the ground waters, will give rise to the release of significant quantities of ions, mainly OH-, K+, Na+ and Ca2+. The resulting leachate could have a pH as high as 13.5. This leaching water might perturb other repository materials such as the engineered barriers (bentonite buffer and backfill material) and the near-field host rock. In literature this phenomenon is known as the hyper alkaline plume.

Due to stress release after tunnel excavation and EBS-installation, the gallery wall converges and a negative radial displacement is measured until the clay comes in contact with the installed plug. This process is amplified by swelling of the buffer. Once the contact is established, displacement rate will decrease but self-sealing processes in the tunnel near field and inside the EBS start to establish the isolation conditions according to the designed overall barrier function of the repository system.

Furthermore, long operational times could give rise to a marked de-saturation of the tunnel near field, creating a residual gas phase in the rock mass around the emplacement tunnel. As a consequence, long operational times are expected to delay the build-up of gas pressures and reduce the pressure magnitude in the backfilled emplacement tunnels.

Such examples illustrate the need for a targeted assessment of the system evolution for any given disposal programme. Scenarios of gas release may be defined, combining alternative histories in repository system evolution with possible gas transport processes and gas paths. As pointed out by Marshall et al. (2008) the definition of defendable gas release scenarios, i.e. under consideration of the possible gas transport pathways, is therefore the starting point for any quantitative assessment of the gas issue and its impact on long term repository safety.

2.2. Bentonite buffer materials and plug installation techniques

2.2.1. Bentonite-based buffer materials

In the literature a variety of different possible bentonite mixtures or clay minerals has been projected as backfill material in the nuclear waste context. Pure bentonite has been rarely proposed for the engineered barrier due to technical reasons, e.g. low mechanical strength of the blocks or aggregates, limitation of swelling pressure. Therefore, usually some aggregates (e.g. sand or crushed rock) are added to the bentonite in order to enhance its mechanical properties.

Table 2-2. Comparison of technical and petro-physical properties of various bentonite-sealing elements designed for usage in various national EBS-concepts or field tests (after Sitz, 2003 – references see there).

Parameter	Swiss concept	Sweden	FEBEX	Canada	Wiß	Wetro FS50
Pressing Power	100 MPa	50 – 100 MPa	40 – 50 MPa	?	>170	40 – 50 MPa
Size	Up to 1 m	?	Ca. 20kg blocks	(10 * 36 * 17) cm^3	Cubes with 13,2 cm edge length	(25 * 12.5 6.25) cm^3
Material	Bentonite MX-80	Bentonite IBECO C	Spanish Bentonite	70 Bentonite Kunigel V1 + 30% sand	Bentonite Deponit CCA	50% Bentonite Calcigel + 50% sand
Bentonite dry density	1.9 -2.0 (g/cm^3)	1.69 (g/cm^3)	1.70 - 1.77 (g/cm^3)	1.69 (g/cm^3)	Ca. 2.0 (g/cm^3)	1.63 – 1.72 (g/cm^3)
Water content	8 – 14%	ca. 18%	13.6 – 14.4%	ca. 14.5%	ca. 12.6%	7 – 10%
Technical level	?	Small series for testing	ca. 140t for plug construction	In situ test: (9000 bricks ≈ 105t)	Testing in small mock-up scale	In situ test: (ca. 120t)

The manufacturing of bricks or blocks comprises two main steps: mixing the bentonite with sand and water to a homogeneous mixture and with correct degree of saturation, and compaction under high pressure – 50-100 MPa. A comparison of different technical and petro-physical properties of various bentonite-sealing elements corresponding to different national concepts are summarized in Table 2-2.

Bentonite-sand mixtures with half mass content of bentonite have been widely studied (e.g. Dixon et al., 1985, 2002; Tang et al., 2002; Tang and Graham, 2002; Graham et al., 2001) but, other mixtures are also used for the same purpose. The sand can be used at different mass fractions, ranging from 10 to 90%, (Santucci de Magistris et al., 1998; Chapuis, 2002; Al Shayea, 2001; Chijimatsu et al., 2000) and crushed rock can be used as an additive (Borgesson et al., 2003; Mata et al., 2001). In case of other kinds of waste for which the confinement is also crucial, some bentonite cement mixtures are sometimes employed (Koch, 2002; Garvin and Hayles, 1999). These authors have shown the influence of the mixture composition on its mechanical properties and hydraulic conductivity.

2.2.2. Bentonite plugs – granular backfill vs. pre-fabricated blocks

Technical interfaces inside bentonite-plugs or the contact zones to the host rock are an important aspect of EBS-design that needs special attention. Their occurrences depend mainly on the backfilling method of the disposal drifts after placement of the waste canisters with buffer material. The design and improvement of bentonite based EBS was part of the ESDRED topics. As illustrated in Figure 2-2 various emplacement techniques of bentonite buffers exist, whereby both, horizontal and vertical configurations are possible.

The following sub items refer to uncertainties of the various concepts (after ESDRED, 2009):

- Pellet filling method, i.e. usage of granular Bentonite (smectitic clay) which is mechanically compacted to obtain a relatively high bulk dry density of the buffer as well as a quite homogeneous buffer
  - Selection of Pellet Material, i.e. mixtures of bentonite, sand and cement + additive
  - Design of Feed & Filling Method of Pellet Material, e.g. shot-gun techniques
- Block method, i.e. pre-fabricated bentonite blocks (masonry of different brick – monolith)
  - Bentonite Block Manufacturing Technique - Single Axis Static Compaction
  - Degradation of Bentonite Block at atmospheric condition because the bentonite starts to suck water and swells due to humidity in the drift.
  - Bentonite Block Remote Handling Technique, e.g. usage of a vacuum suction cup

In order to fulfil the requirements, several specifications have to be met:

- The buffer material has to backfill the whole excavation space (larger gaps inside the backfill or to the host rock can not be tolerated. Especially for masonry construction follows:
  - No persistent interfaces between blocks – hydraulic and mechanical weakness planes ⇒ optimised block arrangement
  - Flat host rock contour ⇒ depending on the excavation type, e.g. blasting or cutting

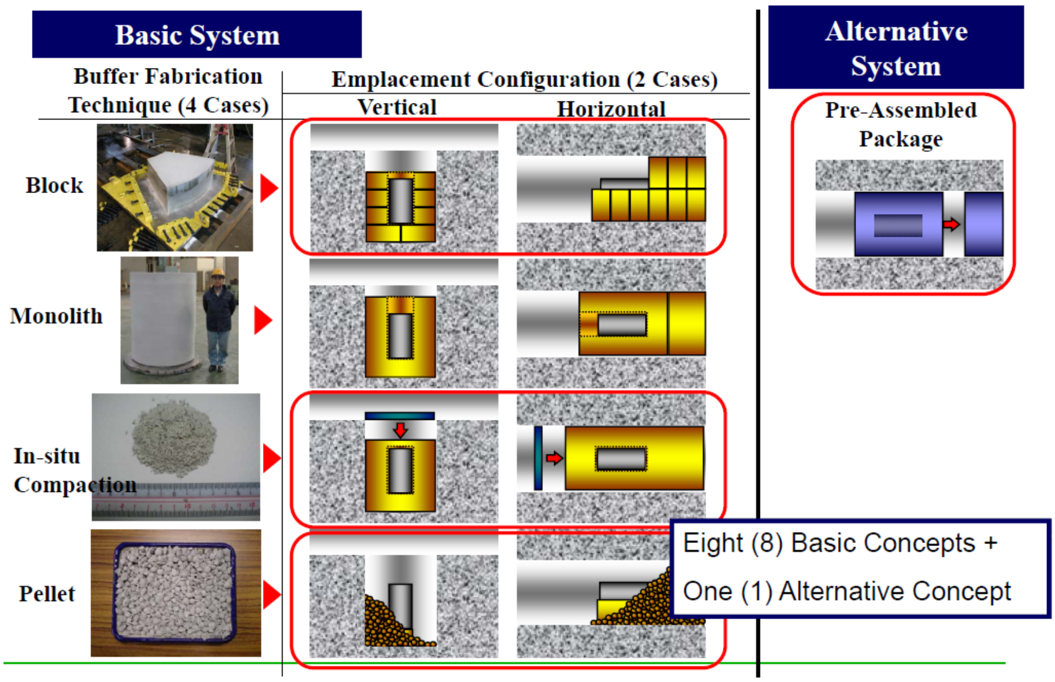


Figure 2-2. Emplacement concepts of bentonite based EBS depending on the buffer fabrication (block ⇔ granular media, i.e. pellet) and emplacement configuration (i.e. vertical / horizontal) – taken from Toguri (2008).

  - The installation of larger blocks needs to take the time constrain into consideration to avoid block alteration
- The range of acceptable bulk densities of the buffer material has to be pre-defined to avoid significant inhomogeneities, i.e. optimisation of the buffer material has to be related to:
  - Prevention of segregation during the backfilling with subsequent inhomogeneous density distribution;

  - Optimum particle size distribution, particle shape and roughness of the buffer material to reach the required high and homogeneous bulk density;
  - The backfill process has to be performed and controlled automatically by remote operations, i.e. to ensure constant quality of the backfill.

In summary, it has to be stated, that, although backfilling is a standard procedure in mining, the unique demands in relation to radioactive waste disposal require non-standard procedures and techniques. Based on the results of ESDRED from lab and field tests further development has to be directed towards optimisation of concepts and refinement of details as well as on design of efficient, safe and reliable equipment and machines.

2.3. Cementitious based abutment/temporary sealing elements

As formulated in the ESDRED-project (ESDRED, 2009) the construction of underground repositories for the disposal of high activity wastes (high level vitrified waste and spent fuel) will require the use cementitious materials for:

- **construction of plugs as auxiliary structures**, e.g. abutments (for rock support or to facilitate build-up of swelling pressure) and temporary or permanent sealing plugs needed for the operation of the repository. The plugs are used to provide temporary mechanical (and sometimes hydraulic) confinement to buffer and seal materials arranged around the waste containers; other plugs provide the same functions for the seals placed at different locations in the underground disposal facilities.

  Plugs are required for confining backfills in underground repository drifts. The principal design criterion is that the plug sustains the mechanical loads in the different conditions to which it is subjected during the evolving conditions: during the operating phase one of the sides of the plug is essentially at atmospheric pressure, whereas the other is progressively loaded with the pressure imposed by the backfill materials (due to the mechanical pressure of a swelling clay and to the hydraulic pressure imposed by the rock formation as resaturation of the confined volume progresses). The plug itself is not a safety barrier of the repository; nevertheless it is considered as a functional requirement that it as far as possible provides the same degree of groundwater containment as the surrounding rock.
- **ground structural support**. Specifically the use of concrete for rock support will be a key issue for repository concepts in clayey rock to guarantee the stability of the excavations (shafts, main tunnels and deposition drifts), but they may also be necessary in repositories built in crystalline rock as well.

Seals may consist of two mechanical abutments (e.g., plugs constructed from low-pH cement and rock blocks) on either side of a sealing section to provide mechanical stability for the bentonite seal in between. Depending on the design of the drifts, the abutments may be keyed in recesses in rock to provide mechanical stability and to project through the EDZ (for details of this topic see Table 4-2). Seal sections may require the removal of liners and partial (slots) or full re-excavation of the EDZ in weak rocks to avoid preferential flow along or through the EDZ and/or engineered structures which will degrade with time.

The construction material for the plugs differs in the national concepts, according to the requirements (Table 2-3). Most concepts favour the use of concrete but in some cases (e.g. Switzerland) alternative materials are under discussion for the final seals to ensure that the degradation of the cement with time does not influence the function of the seal. Frictional gravel supports or constructions including specially designed rock blocks are being considered.

The reliable emplacement method of the concrete for rock support is shotcreting. However, several experiments showed that the shotcrete method also could be used to achieve a closer contact between plug and host rock, as well as significantly optimise plug construction costs. Cast-in-place concrete, i.e. pouring of the concrete as it is usual for conventional fundaments seems not be useful, e.g. due to higher temperature development and horizontal inhomogeneities.

The most common shotcrete method is the wet one. By this method a wet concrete mix is fed into the shotcrete gun and sprayed onto the rock surface using compressed air. A set accelerator is fed into the air stream and mixed with the concrete during shotcreting to provide a “false-setting”, which helps to hold the concrete in place on the rock surface while hydration is occurring.

An advantage of the shotcrete-method is also that the peak-temperature is limited to around 40°C, which minimizes the risk of cooling-induced shrinkage. However, volume constancy or small swelling during setting of the cement is required to ensure that no gap between the plug and the host rock may open.

Table 2-3. Functional requirements for concrete plugs (taken from ESDRED, 2009)

Item	ENRESA	SKB	ANDRA	POSIVA
Hydraulic conductivity	$k \le 10^{-10}$ m·s^{-1}	$k \le 10^{-10}$ m·s^{-1}	Depends on length L: $k / L \le 10^{-12}$ s^{-1}	$k \le 10^{-10}$ m·s^{-1}
Final mechanical properties: **- Young modulus** **- Poisson's ratio** **- Tensile strength** **- Friction angle** **- Cohesion** **- Compressive strength**	›20000MPa 0,2 – 0,3 > 1 MPa ≥ 37° ≥ 2 MPa ≥ 10 MPa	›20000MPa 0,2 – 0,3 > 1 MPa ≥ 37° ≥ 2 MPa ≥ 10 MPa	High strength is not required as such, but the requirements on durability lead to prescribe mix compositions corresponding to high performance concrete (≈ 60 MPa at 90 days)	›20000MPa 0,2 – 0,3 > 1 MPa ≥ 37° ≥ 2 MPa ≥ 10 MPa
Durability	≥ 100 years	≥ 100 years	as high as possible (and sulphate resistant)	≥ 100 years
Workability	≥ 2 hours	≥ 2 hours	≥ 2 hours	≥ 2 hours
Pump ability	250m	250 m	> 100 m	250 m
Peak hydration temperature	≤ 40°C	≤ 40°C	≤ 30°C	≤ 40°C
Thermal conductivity	1,2 W/m°C	1,2 W/m°C	Access drift plugs: not specified Disposal cell plugs: 1,75 W/m°C	1,2 W/m°C
Construction rate	1 m/day		Not specified	
Use of organic components (fibres or admixtures)	To be studied	Not at all but if this is not possible, quantities and types of organic material must be described	Not at all but if this is not possible, quantities and types of organic material must be described	Not at all but if this is not possible, quantities and types of organic material must be described
Estimated pressure at the plug/buffer interface	7 MPa	15 MPa	Access drift plugs: 3 MPa Disposal cell plugs: 4.5 MPa	15 MPa
Length of plug		As short as possible but it must be able to withstand the estimated pressure with a safety factor	Access drift plugs: not defined Disposal cell plugs: 4 to 6 m	As short as possible but it must be able to withstand the estimated pressure with a safety factor
Rock surface		No slot shall be necessary		No slot shall be necessary
Diameter		1860 mm-1840 mm	Access drift plugs: 7 m Disposal cell plugs: 0.7 to 3.5 m	1860 mm-1840 mm
Ground water conditions		Saline (3.5%)		Saline (3.5%)
Time between start of construction and full function of plug		To be studied	Not specified	To be studied
Rest products		It must be possible to describe and quantify the rest products after degradation of the plug	It must be possible to describe and quantify	It must be possible to describe and quantify the rest products after degradation of the plug
Drainage		It must be possible to drain water through the plug during construction (including curing time). It must be possible to seal the drainage hole after the construction of the plug.	Not specified. However, piping might be needed for artificial water supply to buffer (to be eventually grouted)	It must be possible to drain water through the plug during construction (including curing time). It must be possible to seal the drainage hole after the construction of the plug.

NAGRA does not specify requirements for concrete plugs. The Swiss concept for the construction of the seals foresees the use of frictional non-cementitious materials for embankments. Concrete plugs will only be used to protect the seals from accidental flooding during the operational phase. The distance between such concrete plugs and waste packages will be large enough (metres) to rule out any influence of a potential pH-plume in a diffusion dominated system (bentonite and Opalinus Clay). Regular (not low-pH) concrete is therefore planned to be used.

Depending on the application the concrete will be in contact with the bentonite buffer materials and the host rock which may induce chemical reactions between the different materials, i.e. hyper alkaline plume reaction. Although this is not in the focus of the report it has to be mentioned that also due to such reactions altered interface properties may affect fluid transport along interfaces, i.e. resulting in a permeability increase due to corrosion or sealing due to precipitation.

Since concrete is not considered to be chemically stable due to the dissolution of the cement and, in reinforced concrete, the corrosion of some types of reinforcement, and because the hydrogen gas production associated with this corrosion can cause piping of adjacent backfills, therefore the operational lifetime of such plugs is estimated to be on the order of one or a few hundred years. Besides, installed concrete may have a degrading effect on other EBS components it may have to be removed and replaced by backfills or masonries of compacted clay blocks in conjunction with permanent closure of the repository (Pusch & Svemar, 2004).

3. The gas issue in a radioactive waste repository

3.1. Geological site conditions of EBS – host rock and buffer conditions

In accordance with Norris (2009) the assessment of the gas issue related to the gas transport through EBS - and in particular through existing interfaces as a potential main gas pathway - needs to consider a comprehensive picture of the dominating gas transport processes and of the composite gas pathway from the locus of generation through the engineered and geological barriers into the biosphere.

The most relevant documents giving an overview concerning "Gas Generation and Migration from a deep geological repository" in argillaceous formations respectively buffer materials are:

- Horseman et al. (1996), a review of the fundamental processes governing water, gas and solute migration through argillaceous media;
- Rodwell et al. (1999), a review of the status of understanding (in 1999) of gas migration and two-phase flow through engineered and geological barriers in deep repositories for radioactive waste;
- NEA/OECD (2001), the proceedings of an international workshop covering safety-relevant issues related to gas generation and migration in radioactive waste disposal;
- Rodwell et al. (2003), recording the views of GASNET, a network of researchers concerned with gas issues in safety assessments;
- Marshallet al. (2007), a review about gas transport from the point of the gas related PA-issues in various host rock repository types (i.e. crystalline, clay and rock salt formation);
- Metcalf et al. (2008), a review about Nirex/NDA's work relating to gas evolution and migration in a deep geological repository.

The geological conditions around the EBS and particularly the hydromechanical characteristics of both, the host rock formation and the buffer material of the seals, determine to a great extend the *significance of gas accumulation for the assessment of repository performance*. Referring explicitly only to the migration of repository generated gases through EBS, it seems reasonable to assign the variety of influencing factors to the following key aspects:

- The hydraulic properties of the intact host rock and the buffer material, which control (1) the resaturation of the repository and (2) its gas transport capacity after complete resaturation. Long resaturation times could slow down the build-up of gas overpressures in several respects. During the early resaturation phase gas generation rates due to anaerobic corrosion could be reduced due to the low air humidity in the buffer system. After resaturation, residual gas in the buffer system may enhance the system compressibility and thus reduce the build-up rates of gas pressure in the emplacement tunnels.
- The geomechanical rock properties and in-situ stress conditions, which control after tunnel construction (1) the creation and development of the EDZ and (2) after closure of the tunnel sealing processes. The EDZ around the backfilled disposal system and, in particular poten-

tial interfaces between the seal and the host rock can hold two functions with regard to gas pressure build-up, namely enhanced gas transport in axial direction (“gas piping”) and storage of gas due to enhanced EDZ and interface porosities. Due to swelling effects of the seal and the host rock, in addition to the rock convergence, the EDZ may reseal with time and both the enhanced gas transport capacity and storage capacity could vanish as part of the long-term evolution of the EBS

A rough summary of gas related properties for the relevant host rock formations and the various buffer materials will be presented in the following chapters.

3.2. Basic gas transport mechanisms in geological material

This chapter sets the general framework of gas transport in crystalline and low permeability rock formations by introducing the basic transport mechanisms and highlighting special features of gas transport in the rock formations of interest. Marshallet al. (2008) illustrates the multitude of factors influencing the accumulation and release of the gases that have been generated in the waste emplacement tunnels of a nuclear waste repository while demonstrating fundamental differences between the various host rocks.

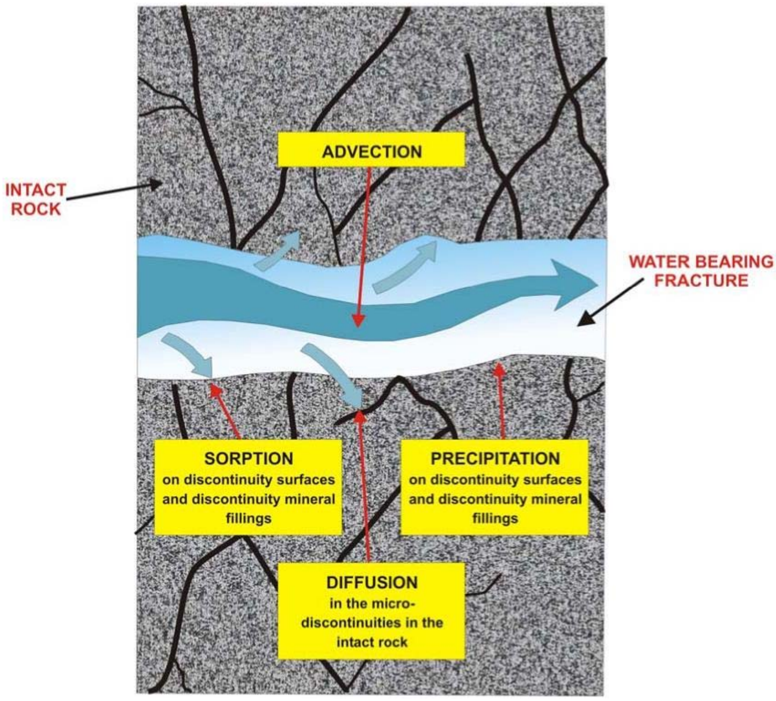


Figure 3-1. An illustration of the potential mechanisms in crystalline rocks that influence the transport of gas from a repository into the biosphere (after SKB, 2001).

Crystalline rock masses cannot be considered as impermeable barriers because their permeability is heterogeneous (average permeabilities range from 10^{-11} to 10^{-17} m^2) and, in addition, scale effects in permeability have to be considered (e.g. Clauser, 1992). Whereas the matrix permeability of these rocks is generally low their overall permeability and flowing porosity results from their discontinuity due tectonic forces that may have created discontinuities (faults and fractures) within the rock mass network (Rodwell et al., 1999).

In such fractured host rocks, gas transport occurs preferentially along discrete water-conducting features (fractures), whereas the low-porosity rock matrix remains saturated all time - sorption and diffusion processes may be of minor importance (Figure 3-1). Gas transport in a fracture network is focused along those connected channels with the widest apertures. Gas transport in the water-conducting rock matrix is a two-phase flow process; the interconnectedness of the fracture network together with the internal heterogeneity of the individual features have a significant influence on gas transport. Taking into account the highly heterogeneous nature of a discontinuous rock mass, flow paths are likely to be highly complex. It follows, that the nature of discontinuities and discontinuity networks need to be understood as they provide the bulk permeability of the rock, and help to understand the nature of flow.

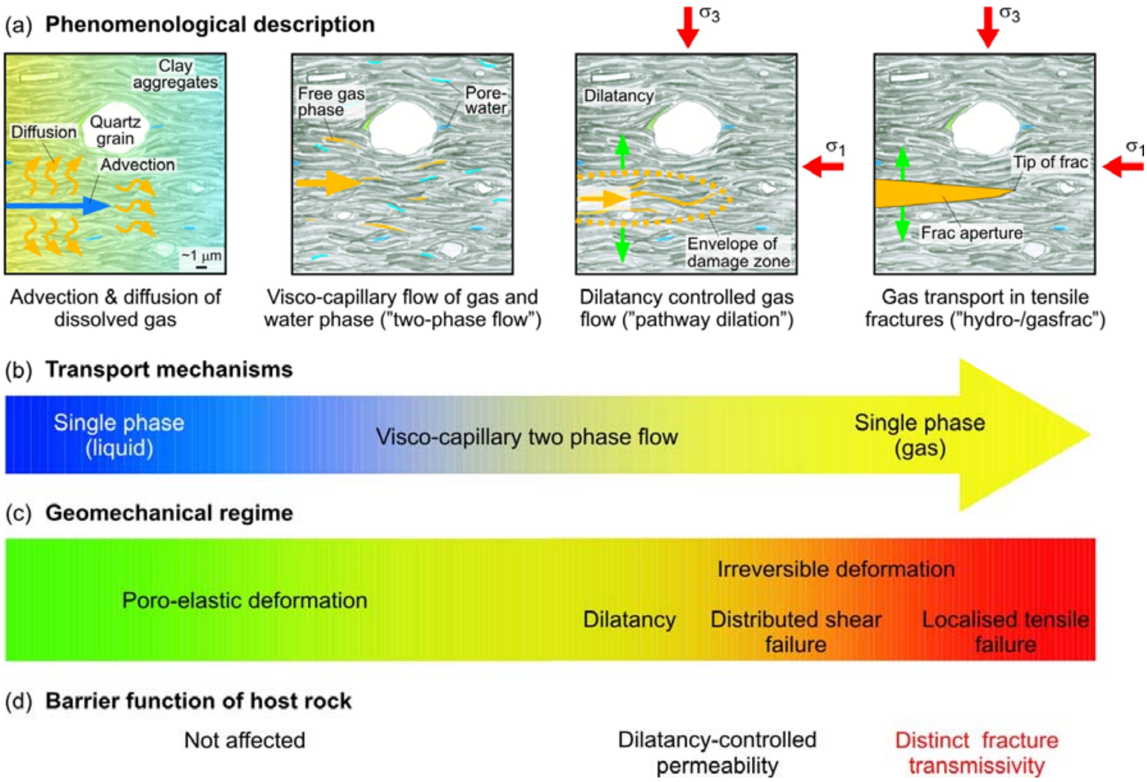


Figure 3-2: Classification and analysis of gas transport processes in low-permeability formations, exemplary applied for Opalinus Clay (after Marschall et al. 2008): (a) phenomenological description based on the microstructural model concept, (b) basic transport mechanisms, (c) geomechanical regime and (d) effect of gas transport on the barrier function of the host rock.

In low-permeability rock formations with a distinct matrix porosity (e.g. in clay formations) gas transport through the rock matrix is controlled not only by the hydraulic and mechanical rock properties (intrinsic permeability, porosity, rock strength), but also by the hydromechanical state of the rock mass (i.e. water saturation, porewater pressure, stress state). Phenomenological considerations suggest the following subdivision of the basic transport mechanisms (Figure 3-2):

- advective-diffusive transport of gas dissolved in the porewater;
- visco-capillary two-phase flow;
- dilatancy-controlled gas flow;
- gas transport along macroscopic tensile fractures (hydro- and/or gas-fracturing).

This process-oriented classification of gas transport mechanisms holds for a wide range of geomaterials, even though the actual governing processes could differ markedly, depending on the microstructural characteristics of the rock. Figure 3-2a is inspired by the microstructural conceptualisation of the Opalinus Clay (Nagra, 2002a). The complex hydromechanical processes are decomposed into a problem of transport of immiscible fluids (Figure 3-2b) and a geomechanical problem (Figure 3-2c).

The effect of gas transport on the hydraulic barrier function of the rock is highlighted in Figure 3-2d for each of the transport mechanisms: rock permeability remains practically unchanged for elastic rock deformation, whereas plastic deformation (dilatancy, fracturing) could enhance permeability significantly.

Table 3-1: Summary of distinct stages in gas migration. Stage I & II are characterized by single phase flow and transport; stage III & IV by two-phase flow and transport. Sl = liquid saturation, Sgr = residual gas saturation, Pl = liquid pressure, Pg = gas pressure (taken from Norris, 2009).

<table>
<tr><th colspan="2">Stage</th><th>Description</th><th>Gas migration</th><th>Conditions</th><th>Degree of liquid saturation S_l</th></tr>
<tr><td colspan="2">I</td><td>Gas can be dissolved in the liquid phase as soon as it is produced</td><td>Diffusive transport of dissolved gas</td><td>[gas] < solubility</td><td>S_l=1, saturated porous medium</td></tr>
<tr><td colspan="2">II</td><td>Formation of free gas phase, liquid starts to be expelled</td><td>Diffusive transport of dissolved gas</td><td>$P_l < P_g < (P_l$+gas entry value)</td><td>1- $S_{gr} < S_l < 1$ Desaturation of EBS and host clay</td></tr>
<tr><td colspan="2" rowspan="2">III</td><td>Pores have desaturated to allow gas to start flowing</td><td>Principally advective flow but diffusive transport continues</td><td>(P_l+gas entry value)<P_g < breakthrough pressure of clay</td><td>Desaturation of EBS and host clay continues</td></tr>
<tr><td colspan="4">Note: For some host rocks at limited depths or with higher air entry value, (Pl + gas entry value) could be greater than minimal component of the principal tensor of total stresses and the system could go abruptly from stage II to stage IV.</td></tr>
<tr><td rowspan="4">IV</td><td rowspan="2">1st Hypo-thesis</td><td>Gas breakthrough occurs in the EBS and host clay.</td><td>Non-darcian flow through preferential pathways</td><td>Pg ≥ breakthrough pressure of clay</td><td>Depends on the newly formed pore space, but further desaturation likely to be small</td></tr>
<tr><td colspan="4">Cyclic behaviour: Pg drops due to the release of gas after breakthrough. After the preferential pathways are closed owing to the self sealing capacity of the Boom Clay, Pg will build up again … The cyclic behaviour goes on until the gas production rate becomes small enough for that the dissolved gas to be evacuated via the pore system, which may be desaturated initially but gradually saturates again.</td></tr>
<tr><td rowspan="2">2nd Hypo-thesis</td><td>Microfractures will form to release gas</td><td>Advective flow with deformation dependent flow parameters</td><td>P_g ≥ breakthrough pressure of clay</td><td>Depends on the newly formed pore space</td></tr>
<tr><td>Propagation of macrofracture</td><td>Non-darcian flow through preferential pathways</td><td>When the combined effect of pore water displacement and formation of small-scale fractures no longer counterbalances the gas production rate and gas pressure.</td><td>Depends on the newly formed pore space</td></tr>
</table>

Related to time-dependent gas pressure build-up and the associated processes Norris (2009) presents a tabular summary of the current phenomenological understanding of the liquid-gas interaction due to gas generation and migration based on the conceptual model of Mallants et al. (2007).

As shown in Table 3-1 the whole sequence of gas-production induced processes can be subdivided into four distinct periods, whereas especially for the last period it is questionable which gas process will be dominant, i.e. if only visco-capillary gas flow along preferential flow paths occurs (without damage) or if pressure induced dilatancy accompanied with path way opening or fracture propagation may become likely.

3.3. Gas flow through the engineered barrier

A key purpose of the buffer is to serve as a diffusive barrier between the canister and the groundwater in the rock, but its efficiency is directly related to its gas transport properties (e.g. Sellin & Alheid, 2009). Gas build-up from corrosion of canister iron could potentially affect the buffer performance in four ways:

1. Permanent pathways in the buffer could form at gas break-through. This could potentially lead to a loss of the diffusive barrier.
2. If the buffer does not let the gas through, the pressure could lead to mechanical damage of the other barriers. The main concern is damages to the near field rock and the buffer itself.
3. The gas could dehydrate the buffer.
4. A gas phase could push water with radionuclides through the buffer along gas-generated pathways.

It's obvious that these potential scenarios are strongly related to the intrinsic gas transport properties of the various material of the plug, which will be shortly outlined.

3.3.1. Bentonite buffer matrix

A number of laboratory gas migration experiments in compacted bentonite samples, with different materials, geometries and boundary conditions, have been performed over the last 20 years. Several of these are summarized in Table 3-2 representing the state of knowledge until 2003.

As pointed out by Olivella & Alonso (2008) the table provides information on the type of compacted bentonite tested, its initial dry density, the flow imposed (either linear or radial in most cases), the controlling mechanism to impose a gas flow rate, and the confining conditions. Tests have been performed in a variety of cells (oedometric, isotropic, triaxial, constant volume).

The buffer material behaves quite similar to the natural low-permeability rocks described in the chapter before, i.e. the relevant gas mechanisms as graphically presented in Figure 3-2 are qualitatively the same.

A common finding is that gas begins to flow once it has reached some pressure (the breakthrough pressure) that forces it through the specimen (see phenomenological model in Figure 3-3). Breakthrough times, breakthrough pressures, the evolution of gas inflow rates, upstream gas pressure and downstream flow rates are commonly reported. A frequent finding is that gas pressure reaches a marked peak at the time of breakthrough and then decreases. This behaviour has been interpreted (Horseman et al., 1999; Harrington & Horseman, 2003) as an indication that, in these cases, gas essentially flows through preferential paths developed inside the matrix, induced by the gas pressure in a phenomenon similar to the more familiar hydraulic fracture mechanism.

Table 3-2. Gas migration tests in compacted bentonite - GAMBIT Workshop, Madrid, 2003 (taken from Olivella & Alonso, 2008 – for citied references see the latter paper).

Authors	Bentonite	Dry density: Mg/m^3	Flow geometry	Gas flow controls	Confining conditions
Pusch & Forsberg (1983)	MX80	~1·35–1·65	Linear	Constant pressure/pressure increments	Constant-volume oedometer
Pusch *et al.* (1985)	MX80	~1·1–1·78	Linear	Pressure increments	Constant-volume oedometer
Horseman & Harrington (1997)	MX80	1·5–1·7	Linear (axial) flor	Displacement of gas by water from upstream reservoir	Constant isotropic stress in flexible sleeve subject to external fluid pressure (8–22 MPa)
Horseman & Harrington (1997)	MX80 paste	1·3–1·4	Point source and sink	Displacement of gas by water from reservoir	Cylindrical pressure vessel with confining pressure (0·8–2·7 MPa) imposed on floating end cap
Tanai *et al.* (1997)	Kunigel VI, Fo-Ca Clay	1·4–1·8	Linear	Pressure increments	Constant-volume cylinder
Gallé (2000)	Fo-Ca Clay	1·6–1·9	Linear	Pressure increments	Constant-volume oedometer cell
Graham *et al.* (2002)	Avonlea	0·6–1·4	Linear	Pressure increments	Constant-volume oedometer cell
Harrington & Horseman (2003)	MX80	1·577–1·582	Radial, central source	Displacement of gas by water from upstream reservoir	Constant-volume cylindrical vessel
Harrington & Horseman (2003)	MX80	1·596	Linear	Displacement of gas by water from upstream reservoir	Cylindrical pressure vessel with confining pressure (10 MPa) applied to floating end caps

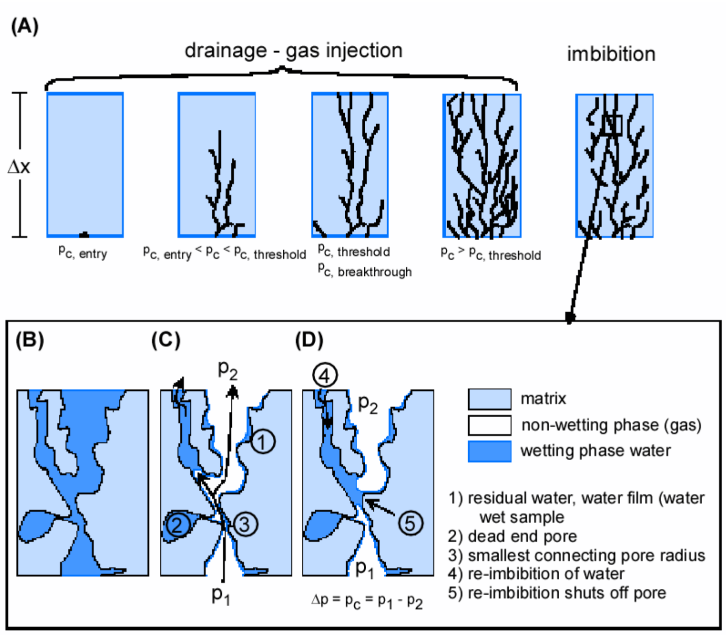


Figure 3-3. Schematics of gas transport in a water saturated bentonite matrix (after Hildenbrand, 2003).

However, no specific studies have been conducted for the purpose of studying how gas dissolves in the pore water in the bentonite. Due to different experiences from various water saturation tests it remains unclear if highly-compacted bentonite would achieve complete water-saturation and that no trapped gas remains (e.g. Figure 3-4). However a mechanistic assumption is that the suction of the bentonite compresses trapped gas (significantly reducing its volume), which is then dissolved in the pore water and this gas is ultimately transported away by diffusion.

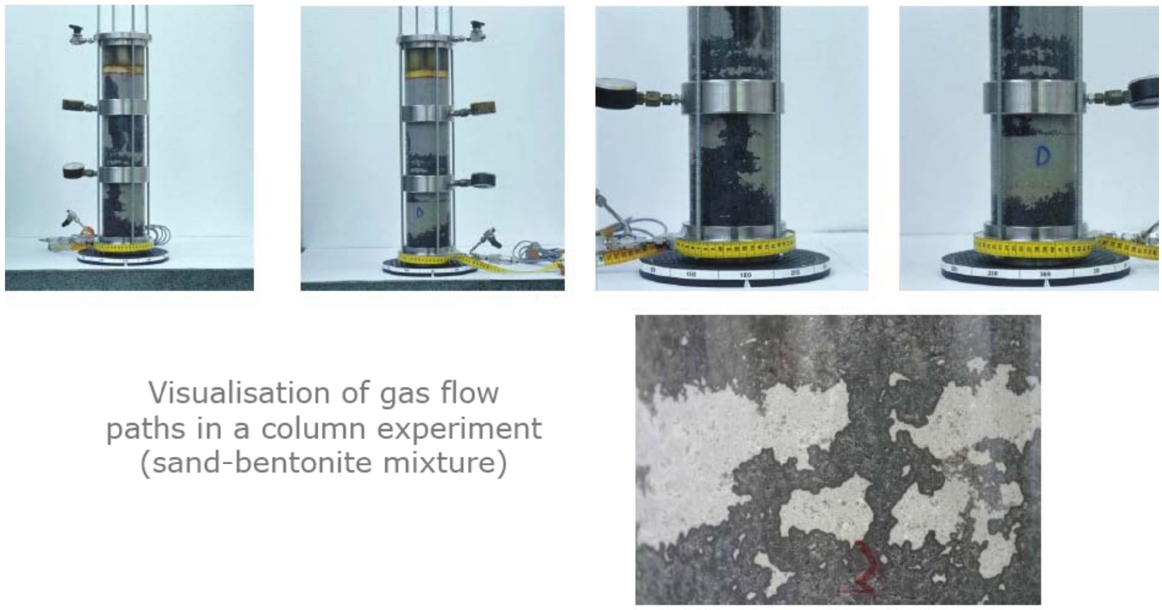


Figure 3-4. Inhomogenous water flow inside a column field with a bentonite/sand mixture (presented by P. MARSHALL „Water solute and gas transport in the EDZ for different disposal systems Cross-cutting topic 3“, NF-Pro's third workshop: 14-16 November, 2006, San Lorenzo de El Escorial, Spain.).

3.3.2. Clay/sand mixtures

As alternative to compacted bentonite appropriate clay/sand mixtures may be used as buffer and/or as sealing backfill in disposal boreholes or disposal drifts. In contrast to highly compacted buffers, clay/sand mixtures exhibit a high permeability to gas in the unsaturated state and a comparably low gas entry/break-through pressure in the saturated state while providing an adequate self-sealing potential due to swelling of the clay minerals after water uptake from the host rock. By using optimized material mixtures, the evolution of high gas pressure in the repository near field due to corrosion of the waste containers will be avoided and possible migration of radionuclides from the waste matrix in the liquid phase through the buffer will be diffusion controlled just like in the host rock.

The sealing properties of clay/sand mixtures have been investigated in detail by GRS within the “Two-Phase Flow” Project (Jockwer et al., 2000), the KENTON project (Miehe et al., 2003) and the SB (**S**elf-sealing Clay/Sand-**B**arriers) project in the framework of ESDRED (Rothfuchs et al., 2007). Seal properties such as permeability to water and gas, gas entry and breakthrough pressure, and swelling pressure have been determined for different mixing ratios and different degrees of compaction.

Table 3-3 summarizes the ranges and the mean values (in parentheses) of the determined properties for the investigated clay/sand mixtures and compares them to the requirements deduced in the ESDRED-project. It can be expected as pointed out by the GRS that the gas break-through pressure may reduce further in the case of significantly lower gas generation rates which are to be considered in a real repository.

Table 3-3. Comparison of the measured parameters to the requirements (averages in parentheses) – The sample number refers to the clay/sand-ratio (taken from Rothfuchs et al., 2007).

Measured parameters at installation conditions					
Sample	Gas permeability under dry conditions	Initial water permeability at full saturation	Gas break-through pressure	Gas permeability after gas break-through	Swelling pressure
	m^2	m^2	MPa	m^2	MPa
35/65	1.2E-13	3.3E-17 - 9E-18 (5.2E-18)	0.4 - 1.1 (0.75)	1.1E-17 - 1.6E-17 (1.4E-17)	0.2 - 0.4 (0.28)
50/50	7.5E-14	1.1E-18 - 4.3E-18 (2.2E-18)	0.4 - 2.8 (1.83)	5.5E-18 - 6.2E-18 (5,9E-18)	0.3 - 0.5 (0.35)
70/30	1.2E-15	5.5E-19	1	n.d.	0.4-?
Requirements					
	Gas permeability under dry conditions	Initial water permeability at full saturation	Gas break-through pressure	Gas permeability after gas break-through	Swelling pressure
	high	1E-17 - 1E-18	2	high	2

3.3.3. Cementitious materials

According to Reeves et al. (2006) cements more closely resemble a porous medium than clay buffers, since the pore structure is defined by a relative rigid solid phase. Cementitious materials are complicated reactive microporous materials with complex pore structures in which pore sizes are distributed between 1nm and 1 µm (or larger if unconnected voids are included). Cements are also reactive with certain gases such as carbon dioxide (CO_2). The connectivity of the pore space is complicated and commonly larger pores are linked by finer pores. The gas migration properties of cementitious materials depends on the formulation of the material. Recorded gas permeability values cover a range of at least eight orders of magnitude between 10^{-20} and 10^{-12} m^2 (Rodwell et al., 1999). The basic features of observed two-phase flow behaviour in cements are generally described by conventional models of two-phase flow in porous media (see chapter 5.).

4. Experimental investigation of gas transport and interface properties

4.1. Key properties to be investigated

The nature of the internal EBS interfaces and discontinuity networks associated with the surrounding host rocks need to be understood as they provide the bulk permeability of the EBS, and help to understand the nature of acting gas flow mechanisms. Due the highly heterogeneous nature of a discontinuous rock mass associated with EBS, potential flow paths along the various interfaces are likely to be highly complex. In addition the random conditions will change with time (see chapter 2.1.3).

Table 4-1 separates the key aspects related to various group of required information, i.e. structural, hydraulic and geotechnical data according to the different constituents of an EBS, i.e. the host rock around the EBS, the buffer and the complex interfaces inside the buffer (see chapter 3.1). However, because the various processes are strongly coupled a necessary separation into various discrete investigation steps facilitating a precise determination of a single parameter is not an easy task.

Table 4-1. The key physical properties of various information groups that need to be assessed to help develop a conceptual model of the gas transport behaviour along interfaces (modified after Reeves et al., 2006) – to be completed.

	Property / Parameter	**Description or examples**
Structural Data	Geometrical properties of the interface	• Spacing between discontinuities / Length • Aperture of the interfaces • Shape of discontinuity surface • Nature of discontinuity surface / JCR index (“ Joint roughness coefficient”) • Relative movement along discontinuity / Direction of movement including extension
	Normal stress across fracture	• The normal stress that is acting across on the interface, i.e. due to host rock convergence or swelling
	Shear stress along the interface	• The shear stress that is acting along an identified interface, , i.e. due to host rock convergence, swelling or acting gas or fluid pressures
	EBS layout / geometry	• Block masonry / block size / arrangement • Measure of tunnel respectively plug length and diameter
	EDZ thickness	• Measure of depth / extension of disturbance into the wall-rock • Discontinuity density / Expression of connection of fracture network / Number of fractures per unit volume of rock
	Host rock properties	• This family of parameters describe rock complexity; including heterogeneities, bedding, purity of clay (i.e. does it include silt, nodules, etc)

Hydraulic Data	**2-phase-Flow properties** (matrix flow) • Host rock • EDZ • Buffer	• Intrinsic permeability: property of the geological medium and is not affected by the nature and properties of the fluid. • Capillary pressure: The difference in the pressure between two immiscible fluid phases separated by a curved meniscus and occupying the pores of a solid rock. • Diffusivity coefficient: Measure of the diffusion properties of pore fluids • Total porosity: ratio of the total pore volume to the bulk volume • Effective/kinetic porosity: amount of porosity that is available for fluid flow. This will be less than the total porosity as isolated/disconnected pores are not part of the transport network • Relative permeability: The permeability of a rock, gas, or water with respect to each other when more than two are present • Entry pressure: The pore fluid pressure for which fluid flow initiates. Below this pressure, the rock behaves impermeably
	2-phase-Flow properties • Interface	• Relative permeability: The permeability of a rock, gas, or water with respect to each other when more than two are present • Entry pressure: The pore fluid pressure for which fluid flow initiates. Below this pressure, the discrete pathways are tight against gas
Geomechanical data	**Effects due to mechanical interactions (stress / strain)** "Matrix response" • Host rock • EDZ • Buffer	• Stress field characterisation: Deviatoric stress, effective stress, mean stress, octahedral stress, normal stress, shear stress, load path / stress path coefficient etc. • Modulus of elasticity (E) • Bulk modulus (K) • Poisson's ratio (ν) • Uniaxial and triaxial strength properties (e.g. Mohr Coulomb parameters: cohesion/friction angle) • Anisotropy effects (Many of the mechanical and hydraulic parameters listed in this table are directional and have strong anisotropy. For a thorough understanding, each parameter should be quantified for anisotropy) • Tensile strength • Ratio of average horizontal to vertical stress • Pore pressure effects (i.e. Biot-parameter α / effective stress concept - Description of whether a rock perfectly obeys the law of effective stress, which states that effective stress = total stress – pore pressure. Perfect conditions occur for $\alpha = 1$) ➢ **Effect of confining pressure/deviatoric stresses on porosity and permeability**
	Interface properties	• Shear strength properties (The internal resistance of a body to shear stress, typically including a frictional component and cohesion) • Tensile strength (mechanical cohesion between buffer and host rock) • Anisotropy effects • Pore pressure effects (mechanical opening of path ways) ➢ **Effect of shearing (strain/stress) and normal stresses (e.g. sealing due to swelling pressures or convergence) on the interface permeability**

4.2. Major Field tests

In order to understand fully the transport properties of a rock mass and discontinuities that occur in an EBS it is necessary to conduct field tests at a realistic scale in the Underground Research Laboratories (URL). For interpretation respectively numerical simulation of the results field tests however require support from laboratory or smaller scale borehole measurements. Only under well-controlled random conditions specific material properties (e.g. matrix or interface properties) can be determined. Ideally, matrix properties (bulk porosity and permeability) and interface properties can then be extrapolated to the entire EBS (SKB, 2001).

Back analysis of previous in situ sealing experiments (e.g. TSX at the AECL, Canada; FEBEX and GMT at Grimsel, Switzerland; EB at the Mont Terri, Switzerland; RESEAL at Hades URL, Belgium; KEY at the LSMHM, France, LASGITE at Äspö, Sweden) demonstrates that, in addition to losses of injected water/gas either from inflow into the sealing plug or from direct intake by the host-rock gas, existing interfaces were identified as pronounced flow paths channelling significant fluid flow through the EBS.

Exemplarily, results from the (1) TSX-experiment (horizontal repository type) and (2) from the GMT-experiment (vertical silo type option) will be presented in more detail.

4.2.1. TSX - Tunnel Sealing Experiment

The Tunnel Sealing Experiment (TSX) operated between 1998 and 2004 on the 420-m-level of AECL's (Atomic Energy of Canada Limited) Underground Research Laboratory (URL) in a tunnel 3.5 m in height by 4.254 m width (Figure 4-1). The rock mass was unfractured granite and granodiorite. Details are described in Dixon et al. (2002) or Martino et al. (2007). The objectives of the TSX were:

- to assess the applicability of technologies for construction of practicable concrete and clay bulkheads
- to evaluate the performance of each bulkhead
- to identify and document the parameters that affect that performance.

Because the drift was excavated in granitic rock with high differential in situ stresses the rock surrounding the openings was supposed to a considerable post-excavation stress-relief which developed an Excavation Damaged Zone (EDZ). In consequence, this provided an opportunity to demonstrate technologies to predict the extent of EDZ development in crystalline host rock and how seals can be designed and installed that will effectively deal with the EDZ, the interface between the rock and the seal as well as maintain their effectiveness under conditions of rising temperatures.

The clay bulkhead portion of the TSX was a 2.5-m long assembly of approximately 9000 densely compacted clay blocks. In the central two metres of his length the bulkhead was keyed 1 m deep into the surrounding rock. There were also 0.25 m unkeyed sections of bulkhead upstream and downstream of the key. The stress, strain, thermal, hydraulic conditions in and around the clay bulkhead and the adjacent rock mass were monitored via several hundred sensors. This provided a continuous record of system evolution and performance under changing hydraulic and thermal conditions. The concrete bulkhead was a mass poured as an un-reinforced mass of low pH, high performance concrete that was also partially keyed into the surrounding rock.

The first phase of the TSX was conducted at ambient temperature (15°C) while a second phase involved heating the pressurized water between the bulkheads with temperatures ultimately reaching 65 °C near the upstream face of both bulkheads. Instrumentation in the experiment monitored parameters that are important indicators for bulkhead performance. By keying the bulkheads into the rock, flow along the EDZ was minimized making the interface the key pathway.

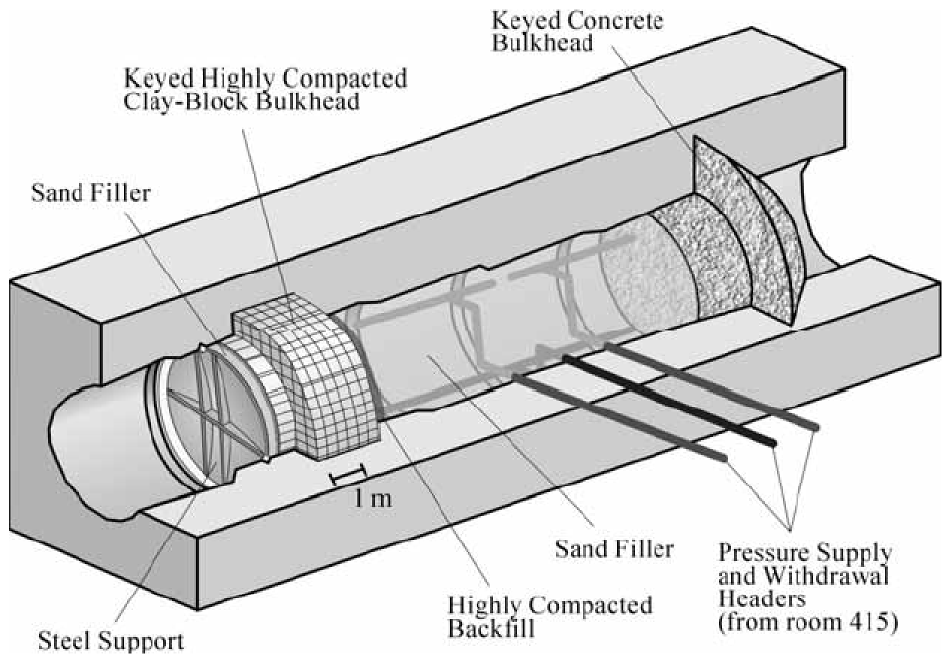


Figure 4-1. Configuration of the TSX. Clay Bulkhead is 2.6 m thick; Concrete Bulkhead is 3.5 m thick.

For the clay bulkhead, a low hydraulic conductivity was achieved by placing material with a high density and sufficient bentonite content to ensure swelling to reduce hydraulic conductivity. Tightly fit construction joints inside the clay bulkhead minimized potential flow paths and allowed hydration to quickly seal the joints.

As much as a 5 cm layer of pneumatically placed bentonite-sand mixture (shotclay) was applied to the rock surface prior to installation of the clay blocks. Use of this material allowed the clay blocks to be placed tightly without large gaps or voids between them and the surrounding rock perimeter. This shotclay gradually increased in density due to compression by the swelling clay blocks and mechanical loading induced by hydraulic pressure in the adjacent tunnel. Increase in shotclay density resulted in a decrease the hydraulic conductivity along the clay-rock interface. By the end of the test, saturation of the clay blocks and compression of the shotclay along the interface produced a bulkhead seal with a very low hydraulic gradient.

During the test, there were initially high flows passing the clay bulkhead, however, hydration and subsequent swelling of the clay reduced the seepage rate. Flow was primarily at the shotclay and clay-rock interface for the clay and at the interface for the concrete bulkhead. High seepage also occurred at the concrete-rock interface, requiring remedial cement grouting. Ultimately, at 4 MPa hydraulic pressure across these bulkheads, the grouted concrete bulkhead and the saturated clay block bulkhead had effective hydraulic conductivities of 10^{-10} m/s (~10 ml/min seepage) and 10^{-11} m/s (~1 ml/min seepage) respectively.

As one of the highlights of test results it was demonstrated for both bulkheads that **the treatment of the interfaces** inside the bentonite abutment and the plug/host rock interface was a key issue for controlling water movement through the EBS because flow through the EDZ was minimized by technical measures.

4.2.2. GMT-Gas Migration Test

The Gas Migration Test (GMT) at the Grimsel Test Site underground laboratory in central Switzerland was designed to investigate gas migration through an engineered barrier system (EBS). The EBS consists of a concrete silo embedded in a sand/bentonite buffer emplaced in a silo cavern that intersects a shear zone in the surrounding granite host rock (Figure 4-2). The sand/bentonite buffer material consisting of 20% bentonite (Kunigel V1) and 80% sand (by weight) was emplaced as a series of lifts, typically 6-9 cm thick after compaction by using “stamper” machines at an in-situ density of about 1.8 g/cm^2 and a water content of 11% (water saturation of about 70%).

Besides the practical demonstration of a silo-type disposal concept the main test objectives are:

- Assess the function of the system EBS and adjacent geosphere as a whole with respect to migration of waste-generated gas;
- Evaluate models (conceptual and numerical) applicable to gas migration through barriers under realistic in-situ conditions;
- Provide data for further improvement of the EBS design with respect to gas.

The GMT was initiated in 1997 and field testing was completed in December 2004 (Fujiwara et al., 2006).

The experiment was performed in a series of stages: (a) excavation of the access drift and silo cavern, (b) construction and instrumentation, (c) saturation of the EBS, (d) water tests, (e) long-term gas injection at different rates, (f) post gas water testing, (g) gas injection with a "cocktail" of gas tracers, and (h) depressurization and dismantling.

After dismantling measurements of bentonite/sand density indicated a relatively uniform high dry density (~1.9 g/cm^3), low porosity buffer. In-situ permeability measurements demonstrated hydraulic conductivity of <10^{-11} m/s for the untraced bentonite/sand and about 10^{-10} m/s for the bentonite/sand traced with lead nitrate. No indications of any macroscopic fracture or opening could be identified within the buffer. Tracer pads placed in the buffer at construction typically indicated diffuse water flow paths, with the exception of some pads located on the top of Layer 8 where some of the flow was concentrated in horizontal channels.

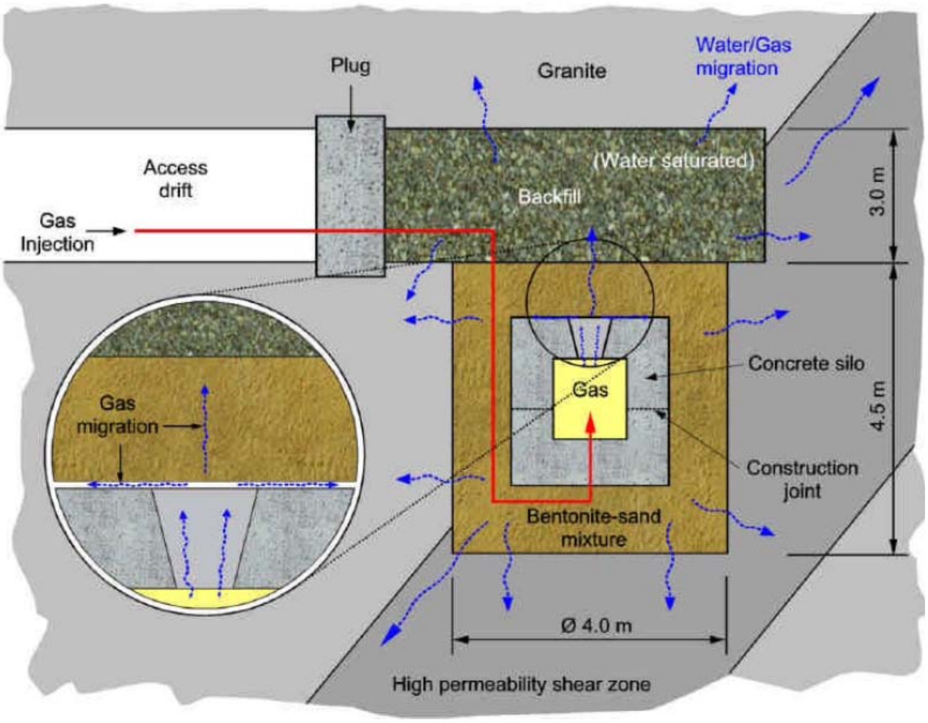


Figure 4-2. Overall concept of the Gas-Migration-Test (GMT) showing the simplified layout and components of composite system – dimensions in m (Fujiwara et al., 2006).

Based on the measured data various numerical models were developed for the design and analysis of the different stages and to describe the relevant phenomena associated with saturation of the buffer and subsequent gas migration (e. g. Senger et al., 2008, Olivella et al., 2005). The different stages of the experiment were simulated in sequence using the results of the previous stage as initial conditions for the subsequent stage.

Olivella et al. (2005) focused on the numerical simulation of interfaces which is achieved by means of special continuum elements to simulate gas flow through planar openings. The sand/bentonite mixture was described by means of an elasto-plastic model (BBM). Model parameters were found by means of a back analysis of suction controlled oedometer experiments on the sand/bentonite compacted samples. Two-phase-flow parameters for the EBS were derived from laboratory experiments on core samples of the different materials that comprise the EBS, while hydraulic properties of the sand/bentonite and of relevant interface zones were calibrated to the pressure responses in the silo and selected piezometers in the sand/bentonite.

Based on the experimental data the outcome of supporting modelling results was summarized by Olivella et al. (2005) as follows:

- Water pressurization induces changes of interface permeability.
- Gas flow paths develop along surfaces which experience an increase of intrinsic permeability.
- Correlation between zones that undergo irreversible deformations and preferential gas flow paths could be established. It was also found that the established water flow largely controls the paths of gas flow.

- The coupling of the two phase flow of water and gas with the mechanical problem was found to be a crucial aspect in the test simulation, especially because the intrinsic permeability variations induced by deformations (and processes along interfaces).

4.2.3. Conclusions from field testing

The primary outcome of field tests (e.g. Martino et al., 2007) was that testing of candidate repository materials at full scale demonstrates that it is possible to construct functional clay and concrete bulkheads to seal tunnel or silo-type seals with limited axial flow. Referring to the concrete bulkhead this was found to be able to withstand the loading from hydraulic pressure with minimal offset and once grouted provided considerable hydraulic resistance. This suggests concrete would make a suitable restraint for a swelling clay component of a seal.

However, especially prior to the TSX-experiment it was believed that the EDZ would be the primary pathway for water flow around the bulkheads but the keyed seals were found to be powerful tool for cut-off or at least reduction of flow through the EDZ (for more details, see Ozanam & Su, 2003). Instead of that **interfaces, i.e. between various contacts of concrete / rock or bentonite components / rock and technical discontinuities inside the bentonite element** were identified as primary pathways

Table 4-2. Technical solutions to control and limit the EDZ hydraulic effects (taken from Ozanam & Su, 2003)

Group of actions	Studied technical solution	Feasibility and efficiency of the technical solution
Avoid or limit the EDZ extension and amplitude during excavation	Put rigid lining close to the front-end	Not suitable if used alone *To be used in combination with other technical solution*
	Grout the rock before excavation	Technically impossible to increase sufficiently (2 times) the rock cohesion
	Overexcavation with various gallery supports	Not suitable: support unable to avoid EDZ propagation
	Rock reinforcement with prestressed or passive rockbolts	Technically impossible
Close the existing fractures	Prestressed lining to applied a confining pressure	Technically very difficult to apply a prestress of some MPa and long term durability not demonstrated
Interrupt hydraulic continuity of EDZ	Circular cut-off with or without confining pressure	Not suitable. Cut-off form unable to avoid the propagation of EDZ
	Cone-shape cut-off with concrete support placed before cut-off excavation	Possible solution for concrete seals – *To be improved in terms of global permeability*
	'Cross-cut' trench back-filled by bricks of highly compacted swelling clay	Possible solution for clay seals (and perhaps for concrete seals – not studied yet)
Limit EDZ permeability	Grouting of EDZ after excavation	Not suitable : long term durability of grout materials not demonstrated

Thus it can be concluded that the essential boundary conditions for gas transport are the geometries of the conducting features at the internal plug interfaces of the block masonry, the buffer material and the rock around the EBS. The main geometric aspects of these boundaries are the number, location and geometry of interfaces intersecting the bentonite plug and the efficiency of discontinuities inside the excavation damaged zones around the EBS.

However, referring to the role of the EDZ the experiments also showed that the development of the EDZ can be minimized through selection of appropriate tunnel geometries and orientations that reduce the near-field compressive stress concentrations and tangential stress gradient, and avoid tensile regimes in the sidewalls. In addition, technical measures exist to interrupt existing flow paths inside the EDZ (Table 4-2).

Thus the development of design criteria for design of repository seals can be used to assist in design of seals for a range of host rock types. However, every location will have unique features, and design criteria should be developed to address important site-specific features that could potentially affect seal performance.

Fortunately, the swelling clay bulkhead of the TSX also demonstrated the ability of the bentonite plug for self sealing/healing and to adjust to differential displacements in its own mass without developing leaks. Nevertheless, especially the knowledge about gas flow along interfaces was found not to be sufficient. There are a number of issues that are not generally covered, such as:

- How to deal with viscous and capillary instabilities during gas flow;
- How to determine suitable two-phase flow parameters on an appropriate scale;
- How to provide macroscopic conceptual models that will bridge the gap between microscopic understanding and the prediction of scale behaviour (Rodwell *et al.*, 1999).

4.3. Laboratory scale

Laboratory test results are important to deduce the THM parameters for numerical calculations evaluating the long term integrity of EBS. Referring to interface properties the main objectives of the laboratory work are:

- to perform long term laboratory tests (duration of several months up to two years) on artificial contact interfaces between sealing material bricks (i.e. bentonite) and to the host rock under well controlled stress and swelling conditions with water injection and subsequent gas injection
- to provide data for time dependent interface “permeability” changes (i.e. sealing) during long term compaction and fluid injection
- to provide data about gas entry pressures and relative gas permeability changes during pressure dependent gas injection
- to provide experimental data from short term tests in a direct shear apparatus with measuring of gas transport and mechanical contact properties for the various interface configurations undergoing shear deformation at defined normal stresses

4.3.1. Random conditions and experimental layout

Laboratory and field tests should be performed under representative conditions, with the test procedure carefully designed to prevent inducing a material response which is non-representative of the natural behaviour. The selection of test methodology for investigating gas transport properties and subsequent design of the experimental programme should be appropriate for the formation under investigation in order to provide quantify data suitable for the purposes of the study (for details see Cuss et al., 2006). The following constraints have to be considered:

- Sufficient sample size: Due to the small grain size of the buffer respectively an argillaceous host rocks sample sizes of several centimetres should be large enough to ensure representative sample conditions. However due the sample recovery and preparation significant sample damage should be taken in mind. In addition, with respect to crystalline rocks larger geometries may be adequate;
- Proper layout of the triaxial cell to ensure measurements of swelling pressure / application of controlled stress conditions simultaneously with fluid flow: A circular geometry ensures uniform stress and flow conditions in a triaxial cell. In addition, hydrostatic or deviatoric loading can be used in order to ascertain the changes in transport properties during deformation. However, an oedometric cell layout with a stiff confinement is preferred to ensure realistic in-situ conditions with minimized lateral strain. Otherwise the change of volumetric strain, i.e. due to swelling, should be measured.

  Various interface geometries can be realized (Figure 4-3):

  - o Circular interface with a hollow cylinder geometry, i.e. a bentonite plug in the hole and an argillaceous clay simulating the surrounding host rock – small scale mock up test of an circular EBS-drift plug (for details see Davy et al., 2009). A radial stiff confinement equipped with DMS-bridges ensures measurement of the radial stress build-up. Fluid-flow tests can be performed in axial direction.
  - o Axial interface between two half-sheets of bentonite/host rock respectively bentonite/bentonite specimens – simple axial flow geometry but requires measurement of the radial stress
  - o Axial flow geometry with two cylindrical specimens as described before with an gas inlet in the centre of the interface – radial flow geometry.
- The swelling pressure P_s is the contribution of the total stresses and the pore pressure P_w:

$$P_s = \frac{\sigma_v + 2 \cdot \sigma_r}{3} - P_w \qquad (4\text{-}1)$$

  where : σ_v total vertical stress (MPa)
  σ_r total radial stress, i.e. = σ_3 (MPa)
  P_w pore pressure, i.e. gas or water (MPa)

  Because in most experimental setups the development of the swelling pressure is only measured in a preferred direction and not spatial, it is assumed, as simplification, that the overall stress field in the buffer is isotropic.

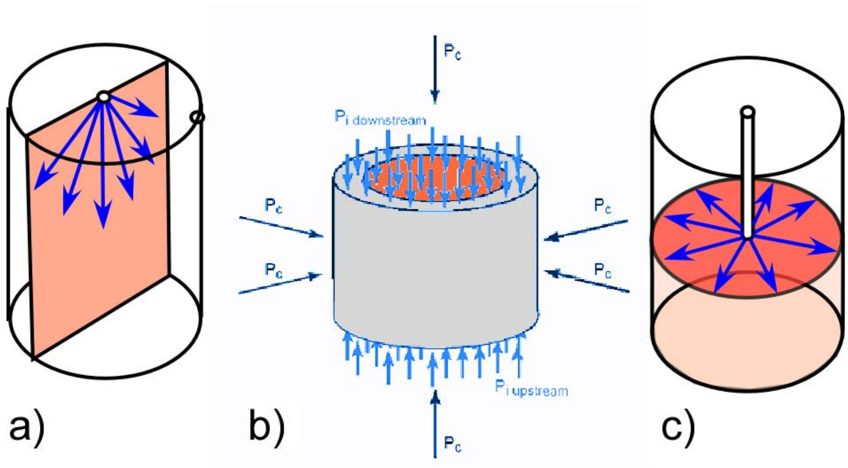


Figure 4-3. Geometries for flow measurements along interfaces. Axial symmetry: a) plane interface between two-half-shells; b) circular interface with a hollow cylinder geometry. Radial geometry: c) two cylindrical specimens with central injection through the common end faces.

- Various experimental techniques are available for investigating gas transport properties:
  - In **constant pressure gas testing**, the injection pressure of the permeant is raised in a series of steps until gas entry occurs. Subsequent steps in gas pressure are used to define the gas permeability function.
  - In **constant flow rate tests**, the gas permeant is pumped into the upstream reservoir of the injection system, gradually raising its pressure until it overcomes the resistance for flow within the laboratory specimen. Once gas movement within a specimen occurs, flow rate into the injection system can be varied to examine the transport characteristics of the material, thereby defining the permeability function.
  - In **pressure decay tests**, the gas pressure is increased rapidly to a value exceeding that of sum of capillary entry and porewater pressures, so that gas flow begins at the start of the test. Pressure in the injection system is then allowed to decay with time. The shape and asymptote of the pressure decay curve can be analysed to yield both permeability and capillary pressure data.

However, constant pressure and constant flow rate tests result in a progressive desaturation of the material as gas pressure and saturation increases (i.e. a drainage response). In contrast, pressure decay tests result in a progressive reduction in gas saturation as gas pressure decreases (i.e. an imbibition response). The hysteresis between these two types of behaviour and the time dependency of some of the processes under investigation may result in a range of values depending on the test methodology selected. A comparative study of the different testing techniques has yet to be undertaken. However, given the unique physico-chemical properties of argillaceous rocks and diversity and complexity of their behaviour, a rigorous and complete appraisal may take considerable time.

When determining intrinsic permeability in chemically reactive formations such as clays, mudrocks and shales, drill fluids and aqueous permeants should be matched, where appropriate, to the properties of the interstitial fluid.

4.3.2. Experimental observations on buffer interfaces during isostatic conditions

Unfortunately, only some few studies have been conducted by various institutions (e.g. CIEMAT, CEA, CERMES and SKB) on rock-bentonite interfaces, but preferable in order to examine the hydration process of the buffer (Gens et al., 2002) or to investigate the evolution of the voids between the buffer and the rock due to bentonite swelling (Grindrod et al., 1999; Pusch, 1983; Marcial et al., 2001). However, gas-flow measurements along interfaces are still rarer (e.g. Davy et al., 2009).

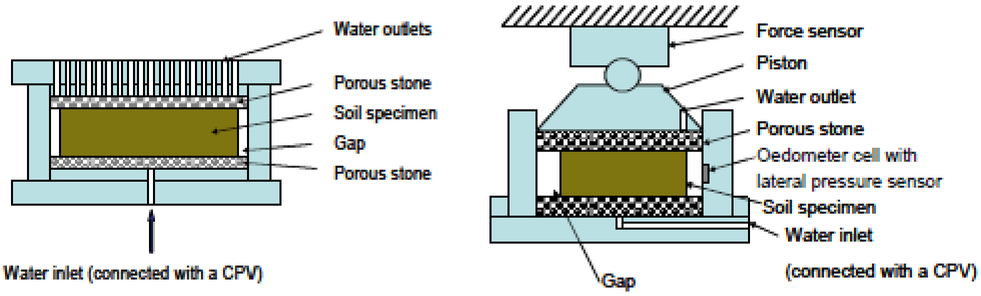


Figure 4-4. Percolation cell (left) and oedometer cell (right)

In order to verify interface effects on the performance of the annular seal system and more specifically on the hydraulic resistance and the gas migration properties through a bentonite / argillite interface (e.g. indurated clay), laboratory percolation tests at 20°C and 80°C were performed at the French CERMES institute and the Lille university (for details see ESRDED, 2009).

Compacted samples of MX-80 bentonite with an initial water content of 10% and a dry density of 1750 kg/m^3 were investigated in two devices: The first one (Figure 4-4 - left) was a percolation cell of 50-mm inner diameter. The soil specimen (5 mm high) was confined between two porous stones. The diameter of the soil specimen was smaller than the inner diameter of the cell, defining a gap between the soil and the cell wall. The water inlet of the cell was connected to a controller of pressure/volume (CPV).

The second device used (Figure 4-4 - right) was a constant-volume oedometer of 50-mm inner diameter equipped with vertical and horizontal stress sensors. The diameter of the soil specimen was also smaller than the inner diameter of the cell and a CPV was connected to the lower base of the cell. The gap between the soil specimen and the cell wall represented the technical gap existing, in real conditions, between the bentonite ring and the gallery wall (Boom Clay).

Injection tests were performed in these two different cells in which a cylindrical gap of controlled thickness was prepared between the soil specimen and the cell wall. When starting injection tests, water appeared to flow freely through the gap, keeping the water pressure equal to zero for some time. When the soil was put in contact with water, it swelled rapidly and reduced the gap, thus increasing the water injection pressure. The drop-down of pressure was observed during the first hours when the water injection pressure reached the hydraulic resistance of the soil/wall interface. The evolution of the radial stress applied by the swelling soil on the inner wall of the cell evidenced a rapid swelling rate.

Because it is believed that in the real situation of the seal/host rock interface the performance of a seal highly depends on the interface characteristic, several tests have been carried out in the percolation cell with three gap thicknesses (2.0, 1.8, and 1.6 mm) and at two temperatures (20°C and 80°C). In addition, several tests have been performed in an oedometer cell at 20°C. All tests show that the hydraulic resistance of the soil/wall interface is higher than 5 MPa after completion of soil swelling, confirming the performance of the compacted bentonite seal under the foreseen hydraulic and thermal conditions.

A multi-step mock-up experiment which was designed in order to reproduce an interface between bentonite and a surrounding material was performed by Davy et al. (2009). As shown in Figure 4-3b the experiment consists of placing a specimen inside a triaxial cell and subject it to both confining pressure (p_c) and interstitial gas or liquid upstream and downstream pressures ($Pi_{upstream}$ and $Pi_{downstream}$). The specimen is sealed by a ductile tube made of a ductile material and instrumented with four strain gauges which provide an evaluation of the pressure sustained by its inner surface, viz. the bentonite swelling pressure and then let to swell in presence of water. During all tests, applied pressure levels are taken as determined by experimental *in situ* investigations: 4 MPa interstitial pressure for bentonite and 12 MPa confinement (also named lithostatic pressure) of the whole specimen.

Simulation of the swelling plug inside an argillite host rock due to saturation of the bentonite resulted subsequent in sealing of the argillite/bentonite interface, i.e. establishing of a hydraulic tight EBS. In the next step, an increase in storage tunnel gas pressure was simulated and the interface gas migration pressure (or gas critical pressure) was evaluated. The gas injection pressures overlapped the apparent swelling pressure which was interpreted as a (pore fluid/solid matrix) mechanical coupling, combined with a structural effect, which provides an upper bound for in situ swelling pressure. Hence, the authors concluded that when bentonite-argillite mock-up gas critical pressures are identified, the coupling has to be taken into account, and a correction to the associated effective swelling pressure has to be performed.

4.3.3. Hydromechanical behaviour rock-plug interfaces under shearing

The "shear failure" of a sealing plug due to fluid pressurisation or swelling phenomena is governed by hydromechanical characteristics of the confined plug / host rock interface. If shear slip occurs on a critically stressed interface, it can raise the permeability of the fracture through several mechanisms, including brecciation, surface roughness, and breakdown of seals (Barton et al., 1995). However, increased pore pressures acting in the interface may also lower the acting minimal stress, thus initiating the shear failure.

The most fundamental criterion for fault (shear) slip is derived from the effective stress law and a Coulomb criterion, rewritten as:

$$\tau = C + \mu\,(\sigma_n - p) \qquad (4\text{-}2)$$

where τ is the shear stress, C is cohesion, μ is the coefficient of friction, σ_n is the normal stress, and p is the fluid pressure (Scholz, 1990). Equation 4-2 indicates that increasing fluid pressure during a gas pressure build-up (for example) may induce shear slip (see Figure 4-5).

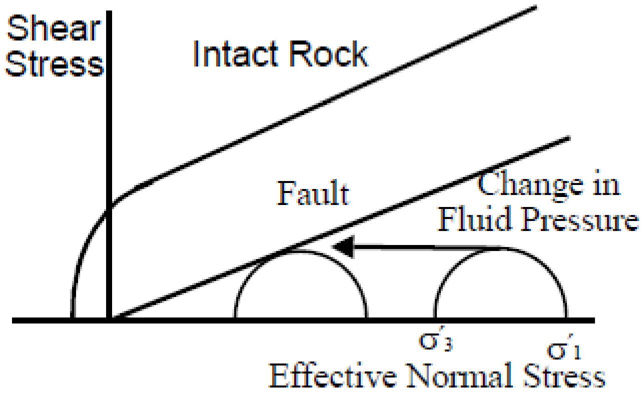


Figure 4-5. Shear slip along a pre-existing fault (or interface) as a result of increased fluid pressure

An improved model for hydromechanical coupling during shearing in rock joints is presented by Olsson & Barton (2001) focusing on fluid flow in fractured rocks, mainly in the context of water flow. The model consists in a relationship between the actual aperture of the joint, which is referred to as the mechanical aperture, and the hydraulic aperture. The hydraulic aperture makes it possible to use a cubic law to determine the flow rate under a hydraulic gradient (compare chapter 5.2). According to experimental observations, the mechanical aperture is larger than the 'hydraulic' aperture (back-calculated from permeability measurements). This is motivated by the effect of roughness, which provides a reduction of permeability that, in the case of the cubic law, is ignored because a planar surface is assumed. The Olsson & Barton model provides a relationship between the hydraulic conductivity and mechanical apertures via the JCR (joint roughness coefficient).

In this context, coupling means that a hydraulic parameter is obtained from a mechanical parameter via a constitutive equation. Following this work, Lee & Chou (2002) applied the model to investigate the hydraulic characteristics of rough fractures under normal and shear deformations of fractured granite and marble. Under normal loading, fracture permeability can be modelled through empirical relationships between normal stress and permeability. Under shear loading, variations of permeability of two orders of magnitude were observed, which were attributed to aperture changes induced by dilation and to roughness variations due to gouge production.

The hydromechanical behaviour of rock-bentonite Interfaces under compression and defined shear conditions was investigated by Buzzi et al. (2006) using the direct shear box BCR3D and the associated hydraulic device available at the University Grenoble. The results show that there is no major influence of the bentonite fraction or the nature of the additive as long as the additive is inert (sand or crushed rock): all the interfaces are closed for low values of normal stress (about 4 MPa). On the other hand, the hydromechanical behaviour of the interfaces changes when a high fraction of cement is used. Moreover, it has been shown that bentonite is very sensitive to hydraulic erosion, producing flow channels within the interface zone. The importance of erosion for the hydromechanical behaviour of the interface was confirmed by a numerical study.

5. Modelling approaches of gas transport

5.1. Basics

5.1.1. Two phase flow

If in a porous rock gas is generated faster than it can be dissolved and advected and/or diffused away from the source zone then it may form a separate phase. Transport of the gas will then be affected by its interaction with the aqueous phase. A generalisation of the single phase Darcy's law is usually assumed with the form

$$\overline{q}_f = -\frac{k_{rf}(S_f)}{\mu_f}(\nabla p_f - \rho \overline{g}) \qquad f = w, g \qquad (5\text{-}1)$$

where *f* is the phase, water (*w*) or gas (*g*), ∇p_f is the pressure gradient, μ_f are the viscosities of the fluids (Pa · s), k_{rf} is the relative permeability of phase *f* (m^2), and S_f is the saturation of phase *f*, or fraction of the pore space occupied by the phase, $\overline{q}$ is the Darcy velocity, i.e. specific discharge, or rate of transmission of the fluid/gas through the medium ($m \cdot s^{-1}$) and $\overline{g}$ is the acceleration due to the gravity ($m \cdot s^2$), ρ is the fluid density ($kg \cdot m^{-3}$).

Gas and water pressures are related by the capillary pressure, p_c, which is a function of the gas saturation:

$$p_g - p_w = p_c(S_g) \qquad (5\text{-}2)$$

Gas and water saturations are related by

$$S_g + S_w = 1 \qquad (5\text{-}3)$$

The functional dependencies of k_{rf} and p_c on the phase saturations cannot in general be determined from first principles and many parameterised functions have been introduced in the literature. Amongst those most commonly applied to granular porous media are the Brooks-Corey (Brooks & Corey, 1964) and the van Genuchten (van Genuchten, 1980, Luckner et al., 1989) functions which are described in more detail below. It should be noted, however, that all such functions are necessarily approximations and ideally explicit data for permeability versus saturation etc. for specific rocks should be used where possible.

The full transport equations are obtained by combining the above flow law equations with continuity equations for fluid and solid components. The formulation is completed with additional constitutive relations that describe the compressibility of solid and fluid phases, usually combined with an assumption that solid phase displacements are small.

➢ ***Brooks-Corey functions***

The Brooks-Corey relative permeability for the aqueous phase is defined in terms of an effective saturation, S_e, given by

$$S_e = \frac{S_w - S_{wr}}{1 - S_{wr} - S_{gr}} \qquad (5\text{-}4)$$

where S_{wr} is the residual water saturation, below which the water is immobile, and S_{gr} is the residual gas saturation. The aqueous phase relative permeability is then given by

$$k_{rw} = S_e^{(2+3m)/m} \qquad (5\text{-}5)$$

where m is a fitting parameter, which may be set to $m = 2$ to give the simpler equations of Corey(1954). The gas phase relative permeability is given by

$$k_{rg} = (1 - S_e)^2 (1 - S_e^{(2+3m)/m}) \qquad (5\text{-}6)$$

The dependence of the capillary pressure on the effective water saturation is given by

$$p_c = \frac{p_d}{S_e^{1/m}} \qquad (5\text{-}7)$$

where p_d is the air entry pressure.

➢ ***van Genuchten functions***

The aqueous and gas phase relative permeabilities are given by

$$k_{rw} = S_e^{\eta} \left[1 - (1 - S_e^{1/n})^n\right]^2 \qquad (5\text{-}8)$$

and

$$k_{rg} = (1 - S_e)^{\xi} \left[1 - S_e^{1/n}\right]^{2n} \qquad (5\text{-}9)$$

where S_e is given by Eq. 5.4, n is a parameter related to the pore-size distribution of the porous medium and η and ξ are pore connectivity parameters, often taken to be equal to 0.5. The capillary pressure function is given by

$$p_c = \frac{1}{\alpha} (1 - S_e^{-1/n})^{(1-n)} \qquad (5\text{-}10)$$

where α is the reciprocal of the air entry pressure. An important difference between the Brooks-Corey & van Genuchten models is that in the latter the capillary pressure goes to zero as saturation approaches unity. It may be noted that neither of these models include any hysteretic effects, but other authors have suggested modifications to accommodate this (e.g. Parker & Lenhard, 1987).

5.1.2. Discrete fracture network models

The formulations for two-phase flow, presented before, were originally developed for and applied to granular porous rocks for which they have been found to provide good approximations of the processes involved. When gas and water flow mainly in networks of fractures or discrete interfaces the application of these equations becomes more questionable. In particular, the scale of the fractures and their interconnections may be such that the averaging implicit in the derivation of continuum models becomes inappropriate in that the size of a representative volume is no longer small compared to size of the total region being modelled.

Fracture network models provide an alternative approach for simulating fluid flow and gas transport along the EDZ of a backfilled disposal system. It is assumed, that the hydromechanical behaviour of the complex fracture network can be determined, when the hydromechanical coupled processes of a single fracture are well understood.

Consequently, the discrete approach starts with the assessment of basic fracture mechanisms in a single fracture (Figure 5-1). The cubic law describes the relationship between the fracture aperture and the fracture transmissivity for an ideal parallel plate configuration (e.g. Bear et al. 1991):

$$T_r = \frac{\rho_w \cdot g \cdot a_h^3}{12 \cdot \eta_w} \tag{5-11}$$

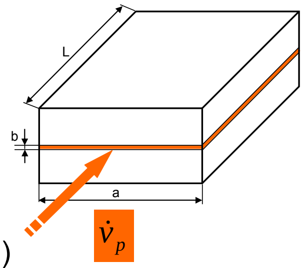
T_r	- Fracture transmissivity of, [m^2/s]
a_h	- Fracture aperture, [m]
ρ_w	- Density of pore water, [g/m^3]
η_w	- Dynamic viscosity of pore water, [g/(m×s)]
g -	gravity constant [m/s^2]

With the approximate cubic law assuming laminar flow transmissivity of a single fracture can be calculated in a simplified way where a_b is the aperture of the single fracture for different geometries (Figure 5-1). However using a fluid mechanics software enables a more sophisticated method to calculate a number of relevant flow parameters useful for understanding the experimental results.

Real fractures are characterised by a certain spatial variability of the geometric fracture aperture $a_g = a_g(\underline{x})$. The equivalent hydraulic fracture aperture a_h used in the cubic law is a parameter, which has to be determined by dedicated experiments (hydraulic tests) or by using empirical relationships between geometric and hydraulic aperture (e.g. Bear et al., 1991).

The simulation of fluid flow in non-deformable fracture networks is a well-established scientific area in hydrogeology. Mature numerical codes are available to simulate flow and transport processes even for huge fracture networks with millions of fractures (e.g. www.fracman.com; www.connectflow.com). However, discrete networks of 'fracs' or discontinuities (e.g. interfaces) undergoing deformation required consideration of coupled HM-processes, as described in the following chapter.

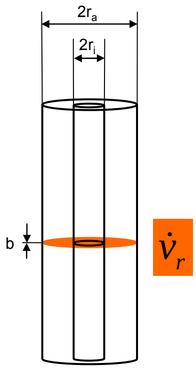
Stress changes acting on the fracture plane can either increase or decrease the fracture transmissivity, corresponding to an opening and closing of the fracture, respectively (for details see Marshall et al., 2008). In rocks with low rock strength, fracture closure due to a stress increase is most likely associated with crushing of the fracture asperities (Figure 5-2). Consequently, the closure process is not fully reversible and a subsequent reduction of the stress would not necessarily result in the restoration of the initial fracture transmissivity.



$$K = \frac{b^2}{12} \qquad A = a \cdot b$$

$$\dot{v}_p = \frac{b^2}{12\mu} \cdot ab \cdot \frac{\Delta p}{L} \qquad \dot{v}_p = \frac{b^3}{12\mu} \cdot a \cdot \frac{\Delta p}{L}$$

a)



$$K = \frac{b^2}{12} \qquad H = b$$

$$\dot{v}_r = \frac{b^2}{12\mu} \cdot 2\pi b \cdot \frac{\Delta p}{\ln(\frac{r_a}{r_i})} \qquad \dot{v}_r = \frac{b^3}{12\mu} \cdot 2\pi \cdot \frac{\Delta p}{\ln(\frac{r_a}{r_i})}$$

b)

Figure 5-1. Representation of discrete water flow with the cubic flow law: a) parallel flow through a single fracture; b) radial flow from a bore hole through a cross section perpendicular to the hole.

In order to formulate such hydromechanical fracture closure laws, the effective stress on the fracture plane has to be decomposed in a normal effective stress component p' (normal effective stress: p'= S_n - p_w) and a shear stress q (Figure 5-2). Various aperture-stress relationships have been proposed in the past for different types of rock. For the relationship between effective normal stress and hydraulic aperture, the following laws are frequently used:

Linear:
$$a_h = \max\left(a_{h0} - \frac{p_n' - p_{n0}'}{\kappa_n}, a_{res}\right) \tag{5-12}$$

Exponential:
$$a_h = a_{h0}\left(\frac{p_n'}{p_{n0}'}\right)^{Exponent/3} \tag{5-13}$$

Hyperbolic:
$$a_h = a_{ho} \cdot (1 - \frac{p_n'}{a_{ho} \cdot K_{no} + p_n'}) \tag{5-14}$$

K_{no} - Normal fracture stiffness for p_n'=0, [Pa/m]

a_{res} - Fracture aperture for $p_n' = \infty$, [m]

a_{ho} - Fracture aperture for p_n'=0, [m]

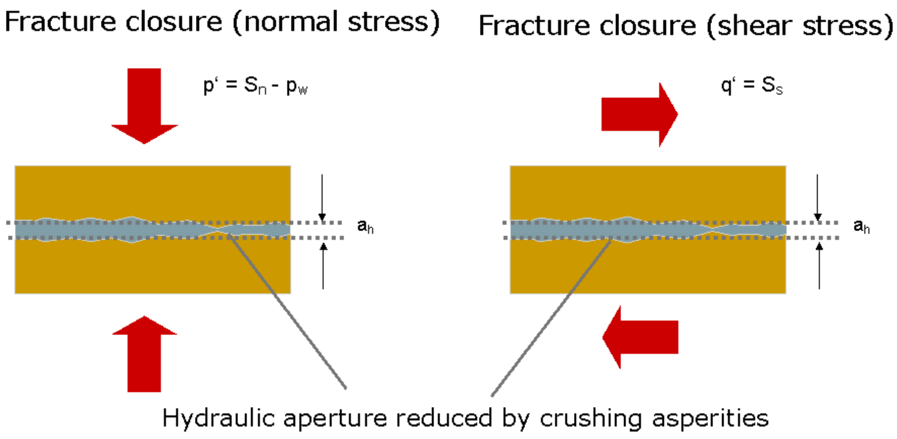


Figure 5-2. Fracture closure mechanisms – schematic sketch (taken from Marshallet al., 2007).

The formulation of stress-aperture laws for shear stress is more sophisticated, because an increase in shear stress could result either in an increase ("dilatancy") or a decrease ("shear compaction") of fracture transmissivity. Therefore, the corresponding stress-aperture laws are strongly rock specific and depend in a distinct manner on the associated stress path (e.g. Esaki et al., 1998; Lee & Cho, 2002; Makurat et al., 1990; Olsson & Barton, 2001; Pyrak-Nolte et al., 1987). In this context, a study by Guiterrez et al. (2000) is worth mentioning, describing experiments on stress-dependent permeability of shales. In the general formulation the hydraulic fracture aperture can be expressed as the sum of two components, according to the actual stress path (p',q):

$$a_h(p',q) = a_{h0} - \Delta a_{normal}(p') + \Delta a_{shear}(p',q) \qquad (5\text{-}15)$$

However, as described in chapter 4.3.3, the permeability of existing voids or fractures may change as a result of dilation caused by over-pressuring or shearing processes. The fracture dilation and consequent increase in permeability will depend upon the fractures characteristics. Long, thin fractures will show greater proportional dilation and permeability increases than short, thick fractures.

5.2. Numerical tools for modelling of HM-properties in geological media

As pointed out by Marshall et al. (2008) numerical gas transport model provides a quantitative estimate of flow and the transport behaviour of a system based on the description by a conceptual model. However, the hydraulic properties of a discontinuous rock mass are likely to be highly heterogeneous even within a single lithological unit, e.g. the buffer. In addition, hydraulic/mechanical coupled processes have to be considered if a realistic description of time and stress dependent changes around EBS should be performed. Numerical methods have been in use for some decades and there have been considerable recent improvements in terms of efficiency, accuracy and computational time. Nonetheless, the accuracy of the results is highly dependent on the use of realistic constitutive models and material parameters and accurate modelling of the problem geometry.

The main difficulty in modelling gas flow in a discontinuous rock is to describe this heterogeneity. Flow paths are controlled by the geometry of discontinuities and their open void spaces (Anon, 1996). The characterization level should give enough detail to enable specific mass transfer models, i.e. gas transport for different major types of interfaces (e.g. single discontinuity between bentonite blocks or discontinuity zones – transition between plug contact and EBS) within a EBS to be used for modelling (Widestrand et al., 2003).

The conceptual approaches for the description of HM-processes (e.g. for pressure induced pathway dilation processes) in complex engineered barrier systems can be divided in three major categories:

(1) *Continuum approaches*, describing the deformable medium in the framework of classical continuum mechanics. The range of applicability of continuum approaches is given by the condition, that the material inhomogeneities (e.g. fractures) are small when compared to the scale of observation (i.e. stresses and deformations can be treated as continuous functions in the entire domain).

(2) *Discrete approaches*, describing the medium as a large system of distinct interacting general shaped (deformable or rigid) bodies or particles that are subject to gross motion.

(3) *Micro-mechanics approaches*, analysing HM-properties at the particle scale allowing a physically based description of inelastic, non-linear and time-dependent deformation processes coupled with pore space processes, e.g. pore pressures, transport.

It is obvious that the choice of the most suitable approach depends on the considered problem. This includes in particular the scale of interest (borehole / tunnel / repository scale) and the rock type (plastic / indurated clay, crystalline). Further aspects are the general environmental conditions (porewater pressure, stress, excavation history). As a prerequisite the necessary input parameters for modelling should be obtained from site specific data for safety assessment.

However, as demonstrated by Javeri (2008) the results depend substantially on the coupling functions of HM-processes, which describe the hydrological properties such as porosity, permeability and capillary pressure as a function of stress or strain. The numerical results can be applied to quantify safety margin related to hydro-fracturing and dilatancy due to fluid or gas pressure build-up and can help to define bounding analyses, if the main hydrological properties depending on volumetric strain, mean effective stress or minimum compressive principal stress are employed.

The subsequent sections are dedicated to a brief review of the fundamentals for the various approaches.

➢ Continuum models for coupled THMC-processes

Continuum models of flow and transport in porous medium have been used to provide predictions for the performance assessment of underground radioactive waste disposal for many years.

Various codes are available, e.g.:

(1) *CODE_BRIGHT (CIMNE, Enresa (ES))* – Olivella et al., 2008 ; Olivella et Alonso, 2008

A porous medium composed by solid grains, water and gas is considered. Thermal, hydraulic and mechanical aspects are taken into account, including coupling between them in all possible directions. The problem is formulated in a multiphase and multispecies approach.

The resulting system of partial differential equations is solved numerically dividing the operation into spatial and temporal discretisations. The finite element method is used for the spatial discretisation while finite differences are used for the temporal one.

The mechanical stress-strain relationship of the buffer clay is defined by means of an elasto-plastic model specially designed for unsaturated soil and known as the "Barcelona Basic Model". The early difference in physical state between the zone with pellets and the blocks of bentonite is considered by using different parameters but maintaining the same model. Rock is considered elastic in all the analyses.

(2) COMPASS (Cardiff University (UK)) – Metcalf et al., 2008

Partly saturated soil is considered as a three-phase porous medium consisting of solids, liquid and gas. The liquid phase is the buffer pore water containing multiple chemical solutes and the gas phase is pore air. A set of coupled governing differential equations has been developed to describe the flow and deformation behaviour of the soil.

A numerical solution of the governing differential equations is achieved by a combination of the finite element method for the spatial discretisation and a finite difference time stepping scheme for temporal discretisation. The Galerkin weighted residual method is employed to formulate the finite element discretisation. For the flow and stress/strain equations shape functions are used to define approximation polynomials. The software package, COMPASS, has been developed to implement the numerical approach detailed above. The package has a modular structure to aid the implementation of suitable code and documentation management systems. It has two main components, i.e. a pre and post processor and an analysis 'engine'. Evaluation of integrals is achieved via Gaussian integration. For the elasto-plastic based stress equilibrium equations a stress return algorithm is used.

(3) Coupling of TOUGH2 and FLAC3D – Rutqvist et al., 2002, Javeri, 2008

The previous codes are integrated codes to model the coupled thermo-hydraulic-geomechanical processes and their influence on gas and nuclide transport in a two phase flow through the porous medium. To analyze the coupled thermo-hydromechanical (THM) processes and their influence on gas and nuclide transport in a two phase flow configuration in porous media, a sequential coupling of the thermo-hydrodynamic code TOUGH2 (Pruess, 1990) and the thermo-mechanic code FLAC3D (Itasca, 2002) at each time step is suggested by Javeri (2008) according to (Rutqvist et al., 2002). Linkage of these two codes facilitates to utilize the advanced multiphase fluid-flow capabilities in TOUGH2, as well as the advanced mechanical feature in FLAC3D.

- **Discrete or discontinuum codes**

For many rock engineering problems, it is more important to account for the particular behavioural characteristics associated with natural rock fractures. In this instance discontinuum or discrete element (DEM) codes are required (e.g. Hart et al., 2000). As opposed to continuum packages commonly used, the discontinuous medium is treated as an assemblage of discrete polygonal blocks, and the blocks themselves can be modelled as rigid or deformable. Various two- and three-dimensional numerical codes, such as UDEC (Universal Distinct Element Code) and its three-dimensional counterpart 3DEC (Cundall, 1988; Hart et al., 1988) are commercially available and widely used for study of the deformation of blocky and jointed rock. Both, UDEC and 3DEC consist of libraries of

- material models for discontinuities (e.g., Coulomb slip, continuously-yielding),

respectively tools for

- Thermal and thermal-mechanical calculation
- Excavation and backfill simulation
- Coupled fluid flow in joints and pressure in cavities

➢ **Micro-mechanical models**

As argued by Fairhurst (1997) taking a micro-mechanics approach, analysing a large number “elements” but at the particle scale may be more realistic where inelastic, non-linear and time-dependent deformation processes are likely to dominate. The ‘microparticle’ codes assume that forces and deformations are transmitted through the solid via particle to particle interface contacts. Frictional slip and tensions can occur, and cementitious bonding around the contacts can be included. The appropriate properties of the contacts are deduced by calibrating the response of a simulated particulate specimen against laboratory compression tests results.

Micro-mechanical numerical models such as Itasca’s Particle Flow Code (PFC, Itasca, 2002) have recently been developed in order to provide the means to accurately model deformation behaviour in a rock mass which cannot be captured using continuum techniques (e.g. Walter et al., in press). 2D - and 3D codes are available.

PFC can simulate processes associated with crack propagation, joint dilation, or block toppling at increasing scales of analysis. PFC2D has been employed to obtain a clearer understanding of the variation of joint dilation angle with shear deformation, confinement and thermal effects for the proposed nuclear waste repository at Yucca Mountain, Nevada, USA (Hart & Fairhurst, 2000).

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