Effects of post-disposal gas generation in a repository for low- and intermediate-level waste sited in the Opalinus Clay of Northern Switzerland

October 2008
Technical Report 08-07

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Abstract

Within the framework of Stage 1 of the "Sectoral Plan for Deep Geological Repositories" Nagra has proposed Opalinus Clay as a possible host rock for a repository for low- and intermediate-level waste (L/ILW). Opalinus Clay is characterised by a low permeability and is, therefore, an excellent barrier against radionuclide transport. Because significant amounts of gas are generated in a repository for L/ILW a demonstration is required that despite the low gas permeability of the Opalinus Clay the gas can escape without compromising long-term safety. The present study provides a comprehensive assessment of the question how gas generation and transport in a L/ILW repository affects system behaviour. For the purpose of the present study a geological repository for L/ILW in the Opalinus Clay of Northern Switzerland with a depth of about 300 – 400 m below the surface is assumed. The report provides relevant information regarding the layout and the operation of the L/ILW repository as well as a brief survey of the waste inventories and the expected amounts of gas generated. Furthermore the state of geoscientific understanding of gas transport processes in the underground structures of the repository and in the surrounding host rock is presented and the impact of gas generation on the isolation capacity of the repository is considered. The modelling activities described in the present report started in 2005 and were completed by the end of 2007. The results of the model calculations were used to optimise the layout of the L/ILW repository with respect to the effects of gas generation and transport. Specifically a design option was studied in which, by an appropriate choice of backfill and sealing materials, the gas can escape along the access ramp into the overlying rock formations without creating undue gas overpressures.

The estimates of the gas generation rates for the L/ILW repository are based on a waste inventory accounting for the existing nuclear power plants, with an assumed operation period of 50 years, and for wastes from medicine, industry and research with a collection period up to the year 2050. This inventory includes a total mass of approximately 40'000 tons of steel and other metals and about 2'200 tons of organic matter. Complete corrosion / degradation of all gas-generating materials yields a gas volume of approximately 20 to 30 million cubic meters (STP). The highest gas generation rates are expected in the early post-closure period up to several hundreds of years, followed by a steady decline. The expected total duration of the gas generation phase is in the order of 200'000 years.

The total pore volume in the backfilled repository is in the order of 58'000 m³ for the assumed waste inventory. If the total amount of corrosion and degradation gases were enclosed hermetically in this pore volume, a high gas pressure would result. In the real system, however, at least a part of the gas will be released through the host rock, resulting in much lower pressures. In order to keep the gas pressure low even in the case of a very low host rock permeability and / or an increased gas production, specially designed backfill and sealing materials could be used such as high porosity mortars as backfill materials for the emplacement caverns and sand/bentonite mixtures with a bentonite content of 20 – 30 % for backfilling other underground structures and for the seals ("engineered gas transport system" – EGTS). The EGTS is aimed at increasing the gas transport capacity of the backfilled underground structures without compromising the radionuclide retention capacity of the engineered barrier system. Sand/bentonite mixtures with a low bentonite content exhibit a low permeability for water and a relatively high permeability for gas due to their (micro)structure.

The development of gas overpressures in the backfilled emplacement caverns is unavoidable due to the large amount of corrosion and degradation gases. Numerical simulations show that, for the expected gas generation rate, the planned repository layout and a typical gas permeability of the host rock, the gas pressure in the emplacement caverns remains below the thresh-
old pressure for the onset of pathway dilation (approximately 6.5 MPa for the assumed site conditions). For such conditions, no additional design measures are needed to mitigate gas impacts. For the case of conservative gas generation rates, or the case of a very low gas permeability of the rock ($k_{opa} \leq 10^{-21} \text{ m}^2$), the gas pressure could rise above the critical threshold pressure for the onset of pathway dilation. Consequently, the use of appropriate backfill and sealing materials that ensure a release of a part of the gas along the access ramp would be a suitable design measure to limit gas pressure. Calculations indicate that such an approach could limit pressures in the emplacement caverns so that even in the case of a very low permeability host rock overpressures above hydrostatic pressure would remain within a range of 3 – 4 MPa.

As a result of the elevated gas pressures in the emplacement caverns, pore water containing dissolved radionuclides will be displaced into the geosphere. The gas pressure build-up as an additional driving force for mass transport also tends to increase the path length for radionuclide transport in the host rock, an effect which is further enhanced by the anisotropy of the intrinsic rock permeability. The displaced water is widely spread over the footprint area of the repository towards the adjacent rock formations above and below the host rock. The numerical simulations indicate specific water fluxes in the host rock of up to $10^{-11} \text{ m/s}$ in the very early gas generation phase (< 1'000 years after repository closure). The fluxes decline steadily with time until the regime of diffusion-dominated transport is reached in the late times of the gas production phase (specific water flux typically < $10^{-13} \text{ m/s}$ after several 10'000s of years). A comparison of these results with those from safety calculations using a wide range of specific water fluxes leads to the conclusion that pore water displacement caused by elevated gas pressures will not compromise the long-term safety of a L/ILW repository in Opalinus Clay.
Zusammenfassung


Résumé

Dans le cadre de la 1ère étape du plan sectoriel «Dépôts en couches géologiques profondes», la Nagra a proposé les Argiles à Opalinus comme roche d'accueil potentielle pour les déchets de faible et de moyenne activité (DFMA). Peu perméable, cette roche garantit un bon effet de barrière. Or, les émissions de gaz sont considérables dans un dépôt pour DFMA. Il s'agit par conséquent de démontrer qu'en dépit de cette faible perméabilité aux gaz, ces derniers peuvent néanmoins s'échapper sans compromettre la sûreté radiologique à long terme du dépôt en profondeur. La présente étude fournit une évaluation circonstanciée de la production et du transport des gaz dans un dépôt pour DFMA aménagé dans les Argiles à Opalinus du nord de la Suisse, à une profondeur de 300 à 400 mètres. Le rapport contient des informations-clés sur la conception et l'exploitation du dépôt pour DFMA ainsi qu'un bref aperçu de l'inventaire des déchets et des quantités d'émissions gazeuses escomptées. Il expose en outre les connaissances scientifiques relatives aux processus de transport des gaz dans des installations souterraines et les roches d'accueil environnantes, tout comme l'influence de la production de gaz sur l'efficacité du confinement par le système de barrières. Les calculs sur modèle cités à l'appui ont été entamés en 2005 et achevés à fin 2007. Les résultats de cette modélisation ont été utilisés pour optimiser la conception du dépôt pour DFMA eu égard à l'accumulation et au transport des émissions gazeuses. Une disposition en particulier a été étudiée, où des matériaux de comblement et de confinement spécifiquement choisis permettent aux gaz de s'échapper également par la galerie d'accès, et de là dans les formations rocheuses supérieures, sans qu'une pression gazeuse excessive ne puisse se créer.

Les estimations des émissions gazeuses dans le dépôt pour DFMA partent de l'inventaire des déchets, incluant ceux des centrales nucléaires existantes pour une durée d'exploitation présumée de 50 ans, et ceux de la médecine, de l'industrie et de la recherche jusqu'en 2050 ; on escompte une quantité totale de 40'000 t d'acier et d'autres métaux et de 2'200 t de matières organiques. Jusqu'à la corrosion ou dégradation intégrale de tous les déchets pertinents, le volume total de gaz produits devrait représenter 20 à 30 millions de mètres cubes normés. Les taux d'émission les plus élevés seront enregistrés dans la première phase qui suivra l'exploitation, à savoir durant les premiers siècles après le scellement du dépôt. La production de gaz diminuera ensuite constamment, pour atteindre un niveau 0 au bout de 200'000 ans environ.

Le volume interstitiel dans les installations d'entreposage comblées totalise quelque 58'000 m³. Si l'on enfermait hermétiquement l'ensemble des gaz de corrosion et de dégradation dégagés dans cet espace, il se formerait une pression gazeuse considérable. Dans le système réel toutefois, ces gaz sont libérés, du moins partiellement, par la roche d'accueil, réduisant ainsi nettement la pression. Pour limiter davantage encore cette dernière dans une roche peu perméable et/ou en cas d'émissions gazeuses accrues, il est possible de recourir à des matériaux de comblement et de scellement spéciaux, par exemple des mortiers très poreux pour combler les cavernes de stockage et des mélanges de sable/bentonite, avec une part de bentonite de 20 à 30 %, pour les ouvrages de fermeture et de scellement («Engineered Gas Transport System» – EGTS). L'EGTS a pour but d'augmenter la capacité de transport des gaz dans les installations souterraines comblées, sans pour autant compromettre la fonction de rétention des radionucléides par les barrières ouvragées. La (micro) structure des mélanges sable/bentonite avec une faible proportion de bentonite confère au matériau une faible perméabilité à l'eau, tout en garantissant une perméabilité aux gaz relativement élevée.

Etant donné la forte production de gaz de corrosion et de dégradation, les surpressions gazeuses sont inévitables dans les cavernes de stockage comblées. La présente étude démontre cependant, au moyen de modélisations mathématiques partant des taux d'émissions gazeuses attendus, que
la conception choisie du dépôt, pour une perméabilité aux gaz typique de la roche d'accueil considérée, permet de maintenir la surpression dans les cavernes en dessous de la pression seuil pour une propagation des gaz contrôlée par la dilatation (env. 6.5 MPa pour les conditions escomptées sur le site). Pour ces conditions, il n'est pas nécessaire de prévoir des mesures techniques supplémentaires pour l'évacuation des gaz. Dans l'hypothèse d'une valeur conservatrice de taux d'émissions gazeuses ou d'une roche très peu perméable ($k_{OPA} \leq 10^{-21} \text{ m}^2$), il se pourrait que la pression dépasse la valeur seuil précitée. Dans ce cas, l'utilisation de matériaux de comblement et de scellement spéciaux s'imposerait pour garantir l'évacuation des gaz par la galerie d'accès également. Les calculs sur modèle montrent qu'une telle conception limite la pression gazeuse dans les cavernes de stockage, permettant de la maintenir aux alentours de 3 à 4 MPa au-dessus la pression hydrostatique, même dans des roches très peu perméables.

Sous l'effet de la pression gazeuse accrue, l'eau interstitielle contenant des radionucléides dissous est refoulée des cavernes vers la roche d'accueil. Cette pression constitue une force motrice additionnelle, qui tend également à prolonger les voies d'écoulement dans la roche. Ce phénomène se trouve encore renforcé par l'anisotropie de la perméabilité de la roche d'accueil. L'eau chassée se répartit à large échelle sur la surface de base du dépôt et se répand dans les formations rocheuses adjacentes. Les modélisations indiquent des flux aqueux spécifiques dans la roche d'accueil de $10^{-11} \text{ m/s}$ au maximum durant la phase initiale de production de gaz (< 1'000 ans après le scellement du dépôt). Ces flux diminuent constamment jusqu'à ce que le transport de matières durant la phase ultime d'émissions gazeuses soit dominé par la diffusion (flux aqueux spécifiques typiques de $< 10^{-13} \text{ m/s}$ après plusieurs dizaines de milliers d'années). La comparaison de ces flux aqueux avec ceux qui ont été considérés dans les études techniques sur la sûreté indique que le refoulement de l'eau interstitielle sous l'effet des surpressions gazeuses ne compromet d'aucune manière la sûreté à long terme d'un dépôt pour DFMA aménagé dans les Argiles à Opalinus.
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1 Introduction

1.1 Background and scope

In underground repositories for radioactive waste, significant quantities of gases may be generated as a result of various processes, comprising anaerobic corrosion of metals and microbial degradation of organic substances. The most important gases generated are hydrogen, methane and carbon dioxide. The potential impact of gas generation, accumulation and migration on the performance of both the engineered barriers and the natural geological barrier is an important issue in the assessment of long-term radiological safety of a nuclear waste repository.

In the framework of the site selection process for geological repositories ("Sectoral Plan for Geological Repositories – Stage I"), Nagra had to submit proposals for siting regions for repositories for spent fuel (SF), vitrified high-level waste (HLW) and long-lived intermediate-level waste (ILW) and for low- and intermediate-level radioactive waste (L/ILW). The main aim of this study is to provide arguments that justify the proposal of siting regions in Opalinus Clay for a L/ILW repository despite the low permeability of the Opalinus Clay and the significant amounts of gas generated in the L/ILW repository.

The present study thus provides a comprehensive assessment of the gas issue for a generic geological repository for L/ILW in the Opalinus Clay of Northern Switzerland, assuming a repository depth of about 300 – 400 m below the surface. A complete synopsis is given, comprising the state of geoscientific understanding of gas transport processes in and around the repository together with the consideration of the impact of gas generation on the isolation capacity of the repository. The modelling activities reported in this study started in 2005 and were completed by the end of 2007. During this period, the L/ILW disposal concept was subjected to various changes with respect to the waste inventory and the repository layout. These changes gave rise to successive model adaptations, which are reflected in slight modifications of the repository geometry and the model input parameters. In this context, modelling played an important role in the refinement and optimisation of the repository layout with respect to the gas release issue.

Basic geoscientific concepts and the corresponding performance assessment (PA) approaches dealing with the gas release from radioactive waste repositories were elaborated in the context of previous investigation programmes (e.g. Wiborgh et al. 1986, Zuidema et al. 1989, Nagra 1993, Nagra 1994, Nagra 1997). The present report draws on those former studies and in particular on the recent Project "Entsorgungsnachweis" (Nagra 2002a, b, c and d, Nagra 2004), which was aimed at demonstrating the feasibility of a SF/HLW/ILW repository, sited in the Opalinus Clay formation of the Zürcher Weinland in Northern Switzerland. The existing understanding of the relevant gas transport mechanisms has been confirmed by new empirical and experimental evidence and the existing data base on gas-related properties of the host rock formation is complemented. Furthermore, the scenarios for the evolution of the backfilled repository and the relevant gas paths are analysed in a similar way as in the SF/HLW/ILW programme. On the other hand, a specific assessment for a L/ILW repository is required to address adequately the waste-specific (e.g. gas generation), concept-specific (repository layout, size of underground structures) and site specific differences (lower burial depth). Of particular importance is the impact of the backfill and sealing materials which can be designed and optimised to allow a controlled transport of the gases along the backfilled and sealed underground structures. Figure 1-1 provides a schematic sketch of the different gas paths from the emplacement caverns through the geosphere and along the backfilled underground structures. The transport routes of interest are (i) the excavation-damaged zone around the backfilled and sealed underground structures, (ii) the engineered barrier system (EBS), comprising cavern plugs and seal sections...
and, (iii) the host rock formation. Reliable estimates of the transport capacities of the different gas paths are an important element of the comprehensive assessment of the gas issue for a generic geological repository for L/ILW in the Opalinus Clay of Northern Switzerland.

Important factors for gas build-up in the repository are the gas storage and transport capacities of the backfilled underground structures, comprising the cavern plugs, the backfilled branch, operation and access tunnels and the seals.

In the last decade the international community of nuclear waste management agencies has paid increasing attention to the production of gases and their transport from deep radioactive waste repositories, giving rise to numerous investigations of gas migration through engineered and geological barriers. A comprehensive review of the status of the basic understanding of the relevant gas-related topics was accomplished under the joint auspices of the European Commission (Rodwell et al. 1999, Rodwell & Norris 2003) and the OECD Nuclear Energy Agency (NEA 2001). In addition, several synopses of gas-related studies have been recently published (Schulze 2002, Rübel et al. 2004, Andra 2005).
1.2 Objectives

The assessment of gas release from the emplacement caverns of a L/ILW repository is a complex and interdisciplinary task with multiple interactions in the fields of engineering, geoscience and performance assessment (PA). A transparent and traceable assessment approach is therefore an important part of the gas-related safety arguments. The present summary of the gas-related studies is aimed at providing:

- A complete presentation of the gas-related requirements and project boundary conditions for ensuring long-term safety of a L/ILW repository in the Opalinus Clay formation. Requirements and project boundary conditions are formulated by the engineers and by the PA project team. This also includes an evaluation of the gas generation rates based on the Swiss model waste inventory.

- Traceable and transparent documentation of the overall assessment. The assessment is presented for a generic repository, i.e. the requirements, the project boundary conditions and the calculations are formulated in a way, which allows adaptation of the assessment to future site specific repository configurations.

- A complete presentation of the available geoscientific database and of the adopted simulation tools.

- A discussion of the key arguments, which confirm that gas production and gas release will not impair the long-term radiological safety of a L/ILW repository in the Opalinus Clay formation.

The efforts in summarising the gas-related studies for a L/ILW repository in the Opalinus Clay take also into account the feedback on Nagra's Project "Entsorgungsnachweis" which was received from various national and international review teams (NEA 2004, HSK 2005, KNE 2005, KSA 2005; cf. Nagra 2008b). A compilation of the comments and recommendations is found in Nagra (2008b).

1.3 Structuring the assessment

The assessment of the impact of gas generation, accumulation and migration on the performance of both the engineered barriers and the natural geological barrier requires a close collaboration between the disciplines of engineering, performance assessment and geoscience. The responsibilities of the different disciplines can be outlined as follows:

- Engineering (construction & operation): Definition of requirements and technical boundary conditions related to the site selection process, to the repository layout, to operational aspects and to the closure (backfilling and sealing) of the repository. The engineering aspects are covered mainly in chapter 2 (repository layout and operational aspects) and chapter 3 (backfill and sealing materials) of this report.

- Performance assessment: Definition of requirements and boundary conditions related to the radiological long-term safety of the repository, including the siting requirements, gas generation issues and gas-related design optimisation (chapter 2), and assessment of the effects of gas accumulation and gas release on the overall performance of the repository system (chapter 5).
- Geoscience: Development of a consolidated understanding of gas transport mechanisms and compilation of consistent databases of gas-related properties for both the host rock and the backfill and sealing materials (chapter 3). Development of a mature understanding of the long-term evolution of the closed repository system concerning the impact of continuous gas production in the emplacement caverns by the use of detailed numerical models (chapter 4).

The assessment can be broken down into a number of work packages with well-defined interfaces. A close link between the geoscientific studies and the PA-related activities is maintained by the so-called "geodata set" interface, ensuring a traceable exchange of information through a formalised data clearance procedure. The main elements of the overall assessment and the interfaces between geoscience, engineering and performance assessment are presented in Figure 1-2 and discussed in the following sections.

Fig. 1-2: Structure of the synthesis of gas-related studies in support of the L/ILW repository in Opalinus Clay.
The role of geoscience

The geoscientific understanding of gas transport processes and of the gas-related evolution of the disposal system is developed as a staged procedure, consisting of four major categories:

- Compilation of gas-related parameters for both the host rock and the backfill and sealing materials. The in-situ data on gas-related host rock properties refer to investigations in the Benken borehole and in the Mont Terri Underground Laboratory (URL). The studies comprise laboratory tests on rock samples and in-situ tests in boreholes and underground facilities, respectively. The in-situ investigations are complemented by desk studies on gas-related research in other geoscientific disciplines (oil & gas exploration, natural gas storage, CO₂ sequestration).

- Development of a conceptual understanding of gas transport mechanisms in the near-field and in the host rock. The conceptual description of gas transport mechanisms builds on well-established geoscientific theories, in particular on the theoretical framework of multiphase flow in porous media. The spectrum of relevant gas transport mechanisms can be reduced by the fact that ranges for the gas generation rates and for the total volumes of produced gas can be bounded. Thus, processes such as hydro- and gas-fracturing can be excluded from the start due to the low gas production rates of the L/ILW. The other gas transport mechanisms such as visco-capillary flow and dilatancy controlled gas flow are investigated by dedicated laboratory and in-situ experiments.

- Development of an integrated system understanding. Elaboration of a detailed system understanding requires a close interaction with the PA project team, because the design of the disposal system has a significant impact on the potential gas transport paths and the corresponding release scenarios. The task comprises (i) a detailed analysis of the composite gas path from the locus of gas generation through the near-field and the geosphere, (ii) the assessment of the most likely gas release scenarios and (iii) detailed modelling of gas transport through and around the backfilled repository structures, aimed at bounding the gas pressure evolution in the emplacement caverns. Figure 1-1 shows a schematic sketch of the considered gas flow paths considered and highlights their role both as potential transport paths and storage volumes.

- Compilation of a "gas geodata set" according to the needs of PA. Elaboration of the so-called "geodata set" is a joint effort between the geosynthesis group and the PA project team. For this purpose the end-users (PA project team) specify their needs with respect to the generation, accumulation and transport of repository gas. The geosynthesis group delivers the corresponding model abstractions, provides relevant information in a format that can be directly used by the PA project team (safety case). The gas-related geodata set comprises a set of qualitative statements about the relevant gas transport mechanisms, the most likely gas release pathways, and, last but not least, simplified quantitative process and system models. In this context, relevant scenarios and conceptual uncertainties of gas transport in the vicinity of the repository are discussed and a table of representative gas transport parameters is compiled, complemented by alternative parameters which describe the parameter uncertainty.

The role of performance assessment and engineering

From the viewpoint of performance assessment and engineering the gas issue is broken down into the following work packages:

- Assessment of gas generation in the L/ILW emplacement tunnels. Gas generation in the backfilled and sealed disposal tunnels is largely determined by the waste inventory and those gas-producing engineering materials which cannot be removed when closing the
repository. A comprehensive survey of the total amount of corroding and degradable material was accomplished for the Swiss L/ILW repository concept which led to well-founded estimates of the total amount of gas produced and the gas species to be expected. Furthermore, the temporal evolution of gas production was assessed. Time-dependent gas generation rates were calculated by summing up all relevant fractions of gas species.

- Impact of the repository layout and detailed EBS design on gas accumulation and transport. The repository layout and EBS design are determining factors for the definition of the gas transport paths (cf. Fig. 1-1) and the corresponding release scenarios. Each potential gas transport path can be characterised by a transport length, a transport capacity and a storage volume as defined by the detailed design of the EBS (geometry, porosity, permeability, swelling pressure, etc.). Gas storage capacity of the different repository components was estimated and design options for an engineered gas transport path were developed.

1.4 Report outline

This report provides a comprehensive assessment of the gas issue for a generic geological repository for low- and intermediate-level radioactive waste (L/ILW) in the Opalinus Clay of Northern Switzerland.

Chapter 1 describes the motivation and scope of the gas-related investigations. References are given to previous studies, both for the SF/HLW and the L/ILW repository. Last, but not least, the main components of the interdisciplinary assessment approach are presented and the authors of the report are acknowledged.

Chapter 2 is dedicated to the description of the L/ILW repository, including the waste inventory and gas production. Northern Aargau (siting region Bözberg) is used for this study as a typical geological setting for the L/ILW repository in the Opalinus Clay formation. This choice is somewhat arbitrary and should in no way imply that this region is preferred above the other siting regions for the L/ILW repository proposed by Nagra. The generic layout of a L/ILW repository is presented and a detailed review of the relevant project boundary conditions and engineering and safety requirements is given. The main repository components are described at an appropriate level of detail for these gas-related studies. A simplified timeline of the construction, operation and closure phases of a repository is given. Based on the reference concept of the L/ILW repository, a systematic appraisal is conducted of design options for the gas-related optimisation of the repository layout. The optimisation includes the design of individual repository components, the selection of appropriate backfill and sealing materials and the use of appropriate techniques for emplacement of the backfill and sealing materials. As an outcome of the optimisation process, an adapted reference concept with an engineered gas transport path (EGTS) is presented. Chapter 2 closes with an overview of the inventory of gas-generating wastes.

Chapter 3 summarises the current understanding of gas transport mechanisms and the associated coupled hydromechanical and hydrochemical processes. Furthermore, reference parameters of gas-related properties are given for the host rock and the engineered barriers. This chapter concludes with an overall evaluation of the state of knowledge on gas transport phenomena. An outlook on upcoming projects on gas-related issues is also given.

Chapter 4 contains the assessment of the effects of post-closure gas generation on the long-term performance of the L/ILW repository. Conventional hydrodynamic simulations of the repository resaturation are conducted. This includes also the evaluation of the possibility of quick resaturation of the backfilled and sealed underground structures, which provides less favourable starting
conditions for the release of gas from the repository system. Then, the gas release through the host rock is evaluated. Furthermore, the performance of the engineered gas transport system is investigated by the means of numerical two-phase flow simulations for a variety of evolution scenarios and configuration parameters. The integrated model interpretation forms the basis for drawing an overall picture of the repository evolution with special focus on the safety-relevant issues, namely gas pressure build-up in the backfilled and sealed emplacement caverns, displacement of contaminated porewater and the state of saturation in the repository near-field.

Chapter 5 summarises the state of knowledge and evaluates the relevance of gas generation and transport for a L/ILW repository in the Opalinus Clay.

1.5 Authors and acknowledgements

The present study was produced by an interdisciplinary team of geoscientists and engineers of Nagra's science and technology division together with associated contractors. The teams of authors of the different chapters are given in alphabetical order in Table 1-1 (responsible authors in italics).

Tab. 1-1: Report outline and list of authors.

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<tr>
<td>Chapter 5: Summary and conclusions</td>
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The authors would like to acknowledge the contributions of further individuals. Particularly, the team benefited greatly from fruitful discussions with Piet Zuidema, who showed indefatigable dedication to this work. A group of external advisors pursued closely the development of the gas-related studies and provided comprehensive technical contributions (Prof. Eduardo Alonso/UPC Barcelona, Prof. Wolfgang Kinzelbach/ETH Zürich, Dr. Roland Lenormand/IPF/CYDAREX Paris and Prof. Günther Pusch/TU Clausthal-Zellerfeld). Detailed technical reviews were conducted by Dr. P. Gribi and Mr. G.W. Lanyon. Special thanks are due to the head of the drawing office Bruno Kunz and his co-workers.
2 Description of the L/ILW repository and wastes

2.1 Introduction
This chapter provides basic information on the geological setting of a L/ILW repository in the Opalinus Clay formation in Northern Switzerland (chapter 2.2). Furthermore, the general layout and details of the repository are presented, concerning the design and materials aspects that influence gas release (chapter 2.3). In this context, the evolution of the repository structures during the operational phase is of special relevance, because this defines the initial conditions for the post-closure phase (chapter 2.4). Design options for mitigating gas-related effects are discussed in chapter 2.5, comprising various design options for engineered gas transport along the backfilled and sealed underground structures. The result of the gas-related design optimisation, called "reference repository project with an engineered gas release system" is described in chapter 2.6. The description of the L/ILW repository system is completed by a brief survey of the quantities of waste and the gas-generating materials (chapter 2.7). Finally, the approach for calculating representative gas generation rates is described in chapter 2.8 and the results of the calculations are presented.

2.2 Geological setting
The region of Northern Aargau (Fig. 2-1) has been proposed as one of the siting regions for a L/ILW geological repository in Opalinus Clay (Nagra 2008c). This region in the Tabular Jura is well documented from reflection seismic lines and from the surface geology (maps in 1:25'000 scale). In the vicinity of the potential repository area (Fig. 2-1b) there is one investigation borehole, the Riniken borehole (Nagra 1989). The basic geometrical data on geology used in the present report have been taken from the Nagra geographic information system.

The Bözberg region belongs geologically to the so-called Precursory Folding Zone ("Vorfaltenzone") of the Tabular Jura. The Precursory Folding Zone has been sheared off from its underlying formations and has been slightly transported to the north, as can be witnessed from the Mandach thrust fault. The shear horizon is located in a series of Triassic evaporites. The sediments above the Triassic formations have been slightly deformed by this northern thrust but do not exhibit distinct compressive structures or significant faults. Figure 2-1c shows the slightly SE dipping layers.

The relief of the reference region (Fig. 2-1c) is relatively flat with a ground surface that varies between approx. 400 and 650 m asl (reference value 500 m asl). The SE dipping Opalinus Clay has an average thickness of approx. 100 to 110 m; its base is between 80 and 135 m asl (reference value: 125 m asl). The information regarding the thickness of the Lias/Keuper layers (reference value 170 m) and the depth of the Muschelkalk (reference value for the top of the Muschelkalk: -45 m asl) have been derived from the results of the Riniken borehole.
Fig. 2-1: Siting Region Bözberg for a L/ILW repository in Opalinus Clay (from Nagra 2008c): (a) lithostratigraphical profile, (b) sitting region, (c) cross sections.
The formations of the Middle and Upper Dogger (Passwang formation, Hauptrogenstein formation, Upper Dogger) above the Opalinus Clay have a thickness in the reference region of approx. 140 to 160 m. The basis of the Malm lies between 335 – 395 m asl. The Hauptrogenstein formation in the Middle Dogger represents a potential aquifer; for this reason the base of the Hauptrogenstein formation has been used in the present study as the upper boundary of the model (reference value for the base of the Hauptrogenstein formation: 300 m asl).

The porewater pressures in the relevant hydrogeological units are estimated from the level of the local discharge area. Under the assumption that the hydraulic conditions in the aquifer systems are controlled by the local discharge areas, the altitude of the discharge area at Sissle in Bözen (403 m asl) can be assumed as the formation pressure. Alternatively one can also assume a hydrostatic pressure corresponding to the average ground surface level of 500 m asl.

Fig. 2-2: Geological longitudinal section along the access ramp, operation tunnel and shaft.
2.3 Layout of the L/ILW Repository

This report draws on a generic repository concept which is the basis for developing proposals for siting regions for the L/ILW repository (Nagra 2008c,d) and is also documented in the "Entsorgungsprogramm 2008" (Nagra 2008a). Several elements of the facility and operation concept are based on the Wellenberg Project (GNW 1994, GNW 2000) as well as on Project "Entsorgungsnachweis" (Nagra 2002b). The repository concept used is generic in the sense that the corresponding repository configuration data can be easily adapted to future project requirements, such as site specific modifications of the repository layout and updated waste inventories.

2.3.1 Components of the repository system

The following layout description draws on the current base concept for L/ILW. The options for gas-related design optimisation are presented in chapter 2.6.

Figure 2-3 shows a plan view of the repository, which would be excavated at an altitude of 160 m asl within the Opalinus Clay formation. This corresponds with an overburden at the level of the repository between 300 and 400 m. The main elements of the repository layout include:

- Surface facilities (entrance facility, head of shaft)
- Access ramp and a shaft as well as a central area and operation tunnel at repository level
- Pilot facility and test area with dedicated tunnels and a pilot cavern
- An array of seven L/ILW caverns of approximately 200 m length, spaced 80 m apart. This corresponds to a waste volume (conditioned and packaged) of approximately 75'000 m³ (scenario with wastes from the existing nuclear power plants with an assumed operation time of 50 years)\(^1\); a design variant for an enlarged waste volume ("umhüllendes Abfallinventar" with 200'000 m³ of L/ILW, in this report referenced as "bounding inventory"; cf. also chapter 2.7) as used for the evaluation of siting regions is described in Nagra (2008e). Each cavern is linked to the operation tunnel by a branch tunnel. The branch tunnel is enlarged at the beginning of the cavern in order to facilitate reloading operation.

Those components of the repository system, which are of special relevance for the assessment of gas release, are discussed in the subsequent chapters.

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\(^1\) This inventory corresponds to that presented in "Entsorgungsprogramm 2008" (Nagra 2008a, see Tab. 2-5 for details).
Fig. 2-3: Plan view of the repository for L/ILW in Opalinus Clay for the waste inventory from the existing nuclear power plants with an assumed operation time of 50 years.

2.3.2 Disposal Containers for L/ILW

A large variety of different waste types are produced as a result of operation and decommissioning of nuclear power plants and from use of nuclear materials in medicine, industry or research. These wastes include metals, organics and inorganic materials. The treatment and conditioning of the radioactive waste involves mixing with either cementitious materials or bitumen in steel drums or fibre-cement waste packages as shown in Figure 2-4. For the decommissioning waste that will arise in the future, concepts for the treatment exist.
In the entrance facility of the repository the waste drums are placed into prefabricated reinforced concrete disposal containers and the void spaces within the containers are filled with cementitious mortar M2 (cf. chapter 2.5). Figure 2-5 shows the various types of disposal containers for L/ILW.

Fig. 2-4: The various waste packages containing L/ILW (dimension in mm).
Waste packages of type KC-T12/30 (PSI) and GC-T24 (PSI) according to Figure 2-4 will be placed directly into the emplacement caverns without being packaged into disposal containers.

### 2.3.3 Emplacement caverns

The disposal containers are emplaced in caverns with a cross section$^2$ of approximately 11.0 × 13.2 m as shown in Figure 2-6. The length of the caverns is approximately 200 m. The caverns need to be supported with rock bolts and sprayed concrete lining including reinforcement (steel wire mesh). Each cavern is connected to the operation tunnel with a branch tunnel. The emplacement containers are to be transported through both of these tunnels. At the transition to the emplacement cavern, the branch tunnel is enlarged to provide for sufficient space for the transfer of the disposal containers from the railway wagon to the deposition overhead crane.

---

$^2$ This cross section is chosen as the reference case. Depending upon the host rock and the depth of the caverns, other cross sections will be chosen (see Appendix 2 of Nagra 2008e).
The lower part of the cavern ("cavity") will be partitioned into disposal sections of approx. 28 m length by reinforced concrete walls ("bulkhead"). The void space between the disposal containers is filled with low-viscosity cementitious mortar (M2); the void space between the crane columns and between the disposal containers in the upper part of the cavern ("top heading") is filled with mono-grain cementitious mortar (M1, high viscosity mortar). The reference design for the caverns is shown in Figure 2-6.

Fig. 2-6: Cross sections of L/ILW emplacement cavern after closure.
2.3.4 Access tunnel and shaft

The access tunnel provides the connection between the entrance facility at the surface and the underground facilities during both construction and operation. For operation and ventilation a clearance cross section of approx. 31.8 m² has been chosen, which corresponds to an excavation cross-sectional area of approx. 42.2 m². With an average inclination of approx. 11.1 %, the total length is assumed to be about 2.4 km of which approx. 650 m lie within the Opalinus Clay. The ventilation shaft, which has an inner diameter of 4 m, reaches a depth of approx. 320 m, of which approx. 47 m cross through the Opalinus Clay. For the access tunnel and the ventilation shaft a liner with shotcrete (reinforced with steel fibres or wire mesh) and rock bolts (from steel or fibreglass reinforced plastic) are used.

2.3.5 Pilot facility and test area

The test area (rock laboratory) consists of various tunnels, niches and boreholes, which will be used for different experiments and measurements and will also be utilised for the long-term monitoring of the pilot facility. The observation tunnel is assumed to have a clearance cross section of approx. 20.5 m² and an excavation cross section of approx. 26.5 m². The pilot facility consists of a shortened emplacement cavern of 30 m but with the same cross section. The layout will be such that it can be monitored over a long period of time.

Fig. 2-7: Longitudinal section of L/ILW emplacement cavern after closure.

2.3.6 Backfilling and sealing systems

As soon as the emplacement of wastes into one disposal section of a cavern cavity is completed, the voids between the containers and the cavern lining are backfilled with cementitious mortar. When all sections of the cavern cavity and the top heading are backfilled the enlarged section of the branch tunnel at the caverns entrance is also backfilled with mono-grain mortar (M1). Each cavern is closed with a concrete plug (see Fig. 2-7).

At the end of the operational phase, both the operation tunnel and the access tunnel are backfilled; it is intended to use processed excavated Opalinus Clay as backfill material. Also at this stage, a seal will be placed within the access tunnel at the intersection of Opalinus Clay to the adjacent geological formation. The seal is approximately 40 m long and consists of highly compacted bentonite blocks (seal type V4 according to Nagra 2002a). Furthermore, a concrete plug will be placed at repository level at the end of the operation tunnel adjacent to the ventilation shaft. Final closure of the facility involves the emplacement of a seal within the shaft, also made of highly compacted bentonite (seal type V1 according to Nagra 2002a).
Both long-term seals V1 and V4 are designed to limit the water flow in the access tunnel and the shaft as far as required. This will be achieved by the following steps:

1. The sprayed concrete (shotcrete) liner of tunnel/shaft is removed within the seal section.
2. A ring of Opalinus Clay is excavated to a depth of approx. 1 m to remove the excavation-damaged zone, which may have been altered by contact with the concrete and with air.
3. An abutment is installed across the tunnel.
4. An approximately 40 m section of highly-compacted bentonite blocks is installed, keyed into the Opalinus Clay.
5. The second abutment is emplaced; the remaining parts in the adjacent rock formations above the host rock are then backfilled with processed excavated rock.

The design of the seals is described in more detail in Nagra (2002a).

2.4 Phases of repository operation and closure

The concept of repository operation and closure envisages backfilling and sealing of an individual cavern once the cavern is completely filled. When all caverns are filled, both the branch tunnels and the operation and access tunnel including the central area are backfilled and sealed and the observation phase starts. When the observation phase is terminated, the entire underground facility will be closed; this involves backfilling of the remaining openings and placement of the necessary seals. With this concept, for each of the caverns backfilled and sealed a significant level of passive safety is achieved already during the operational phase while maintaining an adequate level of retrieveability of the wastes emplaced, until final closure of the repository. With final closure of the repository no further maintenance and observation is needed, although monitoring from the surface can continue as long as wanted.

Fig. 2-8: Status of the repository during the operation phase, during the observation phase (with all caverns backfilled and sealed) and after final sealing and closure.

Green: accessible; red: not accessible; yellow: seal.

This concept thus foresees phases as follows:

- **Operation phase**: when the emplacement of the waste of a disposal section of a cavern is completed, the remaining voids are backfilled with cementitious grout (M2) and mortar (M1). When all disposal sections are backfilled, waste packages are emplaced at the upper
part (top heading) of the cavern and backfilled with mortar (M1). The direct access to the cavern is plugged with concrete (V5) at the cavern entrance.

- **Observation phase and closure of the main repository (direct access to caverns):** when all caverns are filled, both the branch tunnels to the caverns and the operation and access tunnel are backfilled. A long-term seal is placed within the access tunnel (V4) at the transition of Opalinus Clay with the adjacent geological formation. A concrete plug (V2) separates the backfilled underground facilities from the shaft, the pilot facility and the test area.
- **Final closure:** Once the observation period is terminated, all remaining open underground facilities are backfilled and sealed. A long-term seal (V1) is installed in the Opalinus Clay within the shaft.

### 2.5 Design options for gas-related optimisation of the repository layout

#### 2.5.1 Design options for gas release

Scoping calculations were conducted for the L/ILW repository layout given in chapter 2.3 (see Appendix C). The calculations indicate that the total amount of the produced gas (20 – 30 million m³, cf. chapter 2.8) cannot be contained in the pore space of the repository structures (58'000 m³, cf. chapter 2.6) at acceptable gas pressures. This chapter addresses engineering measures, which can mitigate excessive gas overpressures in the emplacement caverns if release of gas through the host rock is not sufficiently effective. With the gas production rates taken as fixed, the measures that are primarily considered are associated either with an increase in the gas storage volume and/or an increase in the gas transport capacity. The build-up of gas overpressures can be reduced by means of the following measures:

- through the design of the underground components of the facility (size, configuration, length)
- through the selection of backfill and sealing materials
- through the application of suitable layout and methods for emplacement of backfill and sealing materials

**Size of the underground facility components**

The gas storage volume can be enhanced by expanding the cross section of repository caverns, by not fully loading the caverns with disposal containers and thus by extending the length of caverns or by excavating additional caverns. The key factors for the gas-related optimisation of the size of the caverns are: (i) the prevailing geomechanical site conditions as they determine the acceptable diameter of the cavern for ensuring the mechanical stability of the underground structures during the operational phase, (ii) the lateral extent of the body of host rock, suitable for constructing caverns and (iii) economic considerations, as the ratio between waste volume and excavation volume affects the repositories economic efficiency. For the generic reference project described in chapter 2.3, doubling the cavern length (combined with a less efficient loading of the caverns with disposal containers) would increase the total gas storage volume by approximately 40'000 m³.

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3 Currently, studies are underway to investigate the possibilities to reduce gas generation rates by alternative waste conditioning methods.
In addition, approximately 40'000 m$^3$ gas storage volume is gained without any increase of the excavation volume when the storage volume of the adjacent underground facilities within the host rock is accessible for gas (i.e. access tunnel, operation tunnels, central area, test facility)\textsuperscript{4}. As a prerequisite, the plugs at the cavern's entrance need to have sufficient gas transport capacity to allow the gas to escape slowly to the adjacent branch tunnel for the time needed.

Gas storage in the adjacent underground structures is also desirable because the resulting increase in contact area between the gas phase and the host rock formation increases the dissipation of the accumulated gases through the host rock by processes such as dissolution in the pore-water, diffusion and advection. Assuming a constant specific gas flow rate per square meter at the surface area between the gas front and Opalinus Clay, the gas release capacity would be enhanced proportionally to the increased surface area.

**Selection of backfill and sealing materials**

Additional gas storage can be acquired if the porosity of the backfill material is increased. Typical porosities of the cementitious backfill mortars range from 0.2 to 0.3. Special high permeability/high porosity mortars have been developed and tested in the past in Nagra's RD&D programme (Jacobs et al. 1994a, and b, Mayer et al. 1998). These provide porosities as high as 50%. Doubling of the existing porosity to 50% would provide an additional gas storage volume of around 24'000 m$^3$.

Backfill and sealing materials, which have a significantly lower gas entry pressure than the surrounding host rock help to safely release the gas along the access pathways from the caverns to the operation tunnel. Sand/bentonite mixtures exhibit a significantly lower gas entry pressure than, for example, construction concrete or compacted bentonite, and still provide sufficiently low hydraulic conductivity.

**Application of suitable layout and of techniques for emplacement of backfill and sealing materials**

The gas-relevant properties of the backfill and the plugs and seals can be adjusted to meet the requirements for gas storage and release capacity through the application of suitable layout and emplacement techniques, for example the compaction methods, the gravimetric water content, the sequence of emplacement and the length of the sealed sections. In addition, the gas-relevant properties can be adjusted through an optimisation of the specific material parameters, for example, mixing ratio of sand and bentonite and particle size distribution for the backfill mortar. The optimisation of the emplacement techniques is especially important for the design of the seal systems.

The possibilities of adjusting the gas-relevant properties of the emplaced materials with respect to the functional requirements of the engineered system elements (e.g. seal systems) are demonstrated in the following using as an example the sand/bentonite backfill. Thus, design-specific adjustments of the hydraulic conductivity, or the intrinsic permeability, of the sand/bentonite mixtures can be obtained through:

- appropriate choice of the mixing ratio of the sand/bentonite
- appropriate choice of the emplacement density

\textsuperscript{4} Assuming a porosity of 40% for the processed Opalinus Clay.
Comprehensive fundamental databases for the geotechnical characterisation of sand/bentonite mixtures have been obtained in the past in various national programmes (e.g. JAEA 1999, Tashiro et al. 1998, Graham et al. 1997; see also Lanyon & Rüedi 2008, Lanyon et al. 2001); this data shows the dependency of the hydraulic conductivity of sand/bentonite mixtures on bentonite contents from 0 % to 80 % (weight %). A typical characteristic is the significant decrease of the hydraulic conductivity between 0 % to 20 % bentonite content of approx. 6 orders of magnitude, followed by a moderate decrease of approx. half to 1 order of magnitude from bentonite contents between 20 % and 80 %. Figure 2-9 shows experiments performed with the Japanese bentonite Kunigel. Comparable experiments with other bentonites (e.g. Serrata/ Febex, MX-80, Avonlea) exhibit a similar behaviour (see Graham et al. 1997). The characteristic relationship between the hydraulic conductivity and the bentonite content can be explained by considering the micro-structural arrangement of the sand/bentonite mixture (see also chapter 3.3.4). For sand/bentonite mixtures with low bentonite content, the actual structural framework of the medium is determined by the sand because of the direct contact of the sand grains. A distinct microstructural variability is observed, which is expressed by the multi-modal pore size distribution of the material (see also Fig. 3-7). The very fine bentonite particles are distributed in the void space between the sand grains; when water invades they swell at these locations and the hydraulic conductivity of the sand/bentonite mixture is drastically reduced. As a result, sand/bentonite mixtures with low bentonite content are characterised by a high compressive strength, a limited swelling capacity and a high sensitivity of the hydraulic conductivity to the sand/bentonite ratio. When compared to pure bentonites, the gas entry pressure of sand/bentonite mixtures is reduced. This is attributed to the fraction of the large pore sizes in the multi-modal pore size distribution and leads to a strong enhancement of the gas transport capacity. With increasing bentonite content the geomechanical properties of the sand/bentonite mixture change significantly, because the bentonite not only occupies the pore space between the grains, but increasingly interrupts the contact between the sand grains. Thus, the swelling capacity of the material increases and the stiffness decreases. The hydraulic properties of the sand/bentonite mixture approach those of pure bentonite.

Fig. 2-9: Dependence of the hydraulic conductivity of sand/bentonite mixtures on the bentonite content (from JAEA 1999).

The experiments were performed for the HLW programme (H12 report).
The mixing ratio between sand and bentonite determines, however, not only the average hydraulic conductivity of the sand/bentonite mixture, but also the homogeneity and consequently the possibility of developing preferential flow paths. Figure 2-10 (from Tashiro et al. 1998) shows the results of a series of experiments performed in the framework of the Kodoka Project of RWMC (Japan). Permeameter tests were performed for three different ratios of sand/bentonite mixtures (10 %, 20 %, 30 % bentonite content) with different dry densities varying between 1.65 and 2.0 g/cm$^3$. The bentonite used was Kunigel. It is shown that the permeabilities for bentonite contents of 10 % vary strongly over a range of approx. 2 orders of magnitude and even for high dry density values between $1 \times 10^{-10}$ m/s and $1 \times 10^{-11}$ m/s are observed. For values of bentonite content of 20 %, the range of variability corresponds to approx. one order of magnitude, whereas even smaller variations are observed for a bentonite content of 30 %. For the entire spectrum of dry densities from 1.65 g/cm$^3$ to 2.0 g/cm$^3$, the hydraulic conductivity varies between $2 \times 10^{-12}$ and $7 \times 10^{-13}$ m/s, less than half an order of magnitude. Furthermore, mixtures with higher bentonite content allow higher densities to be reached, because through appropriate compaction measures the fine particles of the bentonite part can be better distributed within the sand part; additionally, at such a high bentonite content the exact mixing and compaction procedures are less critical.

Fig. 2-10: Dependence of the hydraulic conductivity on the dry density of sand/bentonite mixtures for bentonite contents of 10 % (left), 20 % (middle) and 30 % (right) and different compaction methods (after Tashiro et al. 1998).

Open symbols represent compaction by "combined roller" and full symbols represent compaction by vibratory plate compactor.

The dry densities of individual backfill and sealing materials can be adjusted through appropriate emplacement techniques, and thus, the required hydraulic permeabilities can be achieved. The dry density can either be achieved by the compaction method or through controlling the water content of the sand/bentonite mixture at emplacement. Tests to achieve the desired dry density have been systematically performed within the framework of the GMT experiment$^5$ in the geotechnical laboratory of CIEMAT (Madrid) (Villar et al. 1999). Focus was on the determination of the emplacement density which corresponds to the maximum dry density ("optimum emplacement density"). The bentonite content of the sand/bentonite mixtures was fixed at around 20 wt% and for comparison three different types of bentonite were used (Serrata, MX-80, Kunigel). Optimum emplacement densities were determined for 4 different compaction methods (modified Proctor, special Proctor and uniaxial compaction at 17 MPa and 60 MPa). In these experiments the water content during the mixing process of the sand/

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$^5$ GMT – Gas Migration Test, initiated in 1997 under the leadership of the Radioactive Waste Management Funding and Research Center (RWMC) in Japan. The in-situ experiment was carried out at the Grimsel Test Site (GTS).
bentonite mixture was fixed very precisely. The samples were compacted and the dry density of the compacted samples was then determined. Figure 2-11 shows the results of the laboratory experiments for MX-80 for the aforementioned compaction methods. The results indicate that depending on the compaction method and the water content the dry density of the sand/bentonite mixture can reach values between 1.85 and 2.1 g/cm³. The hydraulic conductivity was determined each time for the optimum point (highest density) for the samples compacted with the modified Proctor and the 60 MPa uniaxial compression. The values for the samples compacted with the modified Proctor for Kunigel, MX-80 and Serrata bentonite lie in a similar range of $4 - 8 \times 10^{-11}$ m/s.

![Graph showing dependence of dry density on gravimetric water content of sand/bentonite mixtures.]

The optimum water content depends on various compaction methods (Villar et al. 1999; mixing ratio 80/20; Bentonite: MX-80).

Practical experience with the emplacement of sand/bentonite mixtures at a larger scale under relevant construction conditions was obtained in the framework of the GMT in-situ experiment at the Grimsel Test Site (Kickmaier et al. 2001, Nagra 2001c; cf. Fig. 2-12). In this experiment, a sand/bentonite mixture with a bentonite content of 20 % (Kunigel) was emplaced in a specially constructed cavern (Fig. 2-12c) in order to test its behaviour in relation to gas release. The material was prepared in an industrial mixer (Fig. 2-12a) and was then emplaced in layers of approx. 15 cm thickness and subsequently compacted (Fig. 2-12b). An important component of the experiment was the application of clearly defined quality assurance methods, to demonstrate that sand/bentonite mixtures can be managed reliably not only in the laboratory but also at a larger scale. The mixing as well as the compaction methods were tested in advance through application of the same methods at a smaller scale (a concrete box $0.8 \times 2$ m) and the quality and homogeneity of the mixing and the compaction was verified through dedicated tests (Fig. 2-12d).
The GMT experiment provided further evidence for the high gas transport capacity of sand/bentonite mixtures both on the laboratory scale (Romero et al. 2003) and on the in-situ scale (Olivella & Alonso 2005, Senger 2005). Typical gas entry pressures of the mixtures with a sand/bentonite ratio 80/20 were in the order of 10 to 40 kPa. The corresponding intrinsic permeabilities ranged between $10^{-16}$ and $10^{-19}$ m².

The experiments described above demonstrate, using the example of sand/bentonite mixture, the possibility of designing backfill and sealing materials for the L/ILW deep geologic repository in such a way that they meet the safety-relevant requirements. For cement-based backfill of emplacement caverns (M1 and M2 mortar), methods for producing the materials and their emplacement have also been successfully tested (Jacobs et al. 1994b, Mayer & Wittmann 1996, Mayer et al. 1998).

Fig. 2-12: Emplacement of the sand/bentonite buffer (mixing ratio 80/20) in the GMT field experiment at the Grimsel Test Site under conditions close to reality.
2.5.2 Evaluation of design options for gas release

If the gas generated in the repository cannot escape through the host rock and/or the access tunnel/shaft, a possible technical solution is to increase the gas storage volume through engineering measures. However, the total volume of gas produced amounts to a multiple of the available storage volume (cf. chapter 2.8 and Appendix C). Thus, providing additional storage volume alone is not a feasible option for avoiding excessive gas overpressures. A complementary engineering solution is based on the choice of suitable backfill and sealing materials that allow the gas to be released into more permeable adjacent rocks along the access tunnel and/or shaft. The design target for the gas dissipation rate along such a 'gas transport paths' has to correspond to the maximum expected gas production rate in the unfavourable case that the host rock has negligible gas transport capacity. The additional gas storage volume reduces the gas pressure build-up resulting from the expected initial high gas production rates.

2.6 Reference project with engineered gas transport system (EGTS)

2.6.1 Design concept for engineered gas transport system (EGTS)

For this study, it is assumed that the formation above the upper confining units (Hauptrogenstein formation, cf. Fig. 2-2) exhibits a sufficiently high gas transport capacity and can accommodate the resulting gas fluxes without major pressure build-up. From the engineering perspective a technical solution is foreseen which allows the release of gas directly from the emplacement caverns into the overlying more permeable rock formations (in particular the Hauptrogenstein formation). The obvious gas path follows from the caverns through the branch tunnels into the operation tunnel and then along the access tunnel into the more permeable units. Figure 2-13 shows the concept with the expected engineered gas transport path on the basis of the reference project.

The gas transport properties of the seals and plugs are relevant for calculating the gas transport rate for the given cross sections of the underground structures. To ensure a sufficient gas transport capacity, the materials used for plugs (concrete) and the seals (compacted bentonite) are replaced with alternative materials that combine long-term stability with higher gas permeability and/or lower gas entry pressure so as to function like a "gas valve". Sand/bentonite mixtures are materials that possess such properties.
Fig. 2-13: Concept of the designed gas path (red arrows) for the L/ILW repository in Opalinus Clay for the waste inventory from the existing nuclear power plants with an assumed operation time of 50 years.

2.6.2 Adapted repository layout

The concept of the engineered gas transport system has to allow the release of the gas produced in the emplacement caverns, through the branch and operation tunnels to the adjacent rocks, as well as along the access tunnel. For the design of the system it is required that the gas pressure in the emplacement caverns remains at any time below the frac pressure of the host rock at repository level. Favourably, the system is designed such that visco-capillary two-phase flow is the prevailing gas transport mechanism in the engineered gas transport system.

Both the layout of the L/ILW repository and the operation and closure phases remain the same as for the concept described in chapter 2.3. However, for the envisaged engineered gas transport system, the closure system (especially the use of alternative backfill and sealing materials) has to be adjusted (see Fig. 2-14).

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6 Including pilot facility (cavern).
Fig. 2-14: Plan view of the repository layout for L/ILW in the Opalinus Clay with the engineered gas transport system (waste inventory from the existing nuclear power plants with an assumed operation time of 50 years).

A temporary reinforced concrete wall ("bulkhead") of approximately 50 cm thickness at the intersection with the branch tunnel forms the temporary seal (V5) until the end of the operational phase. Prior to the final backfilling and sealing of the repository, the temporary concrete wall has to be removed.

The data for L/ILW emplacement caverns and for the engineered gas transport system as used in the model calculations (see chapter 4) are summarised in Table 2-1.
Tab. 2-1: Summary of data related to gas storage and transport in the L/ILW repository system.

<table>
<thead>
<tr>
<th>Repository Element</th>
<th>Tunnel length [m]</th>
<th>Excavated cross-section area [m²]</th>
<th>Clearance cross-section area²) [m²]</th>
<th>Excavated volume [m³]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Access tunnel (host rock only)</td>
<td>653</td>
<td>42.2</td>
<td>31.8</td>
<td>27557</td>
</tr>
<tr>
<td>Central area</td>
<td>100</td>
<td>85.4</td>
<td>64.1</td>
<td>8'540</td>
</tr>
<tr>
<td>Operation tunnel L/ILW</td>
<td>945</td>
<td>42.2</td>
<td>31.8</td>
<td>39'879</td>
</tr>
<tr>
<td>Observation tunnel</td>
<td>600</td>
<td>26.5</td>
<td>20.5</td>
<td>15'900</td>
</tr>
<tr>
<td>Niches</td>
<td>-</td>
<td>1'250</td>
<td>938.0</td>
<td>1'250</td>
</tr>
<tr>
<td>Test area (access)</td>
<td>50</td>
<td>26.5</td>
<td>20.5</td>
<td>1'325</td>
</tr>
<tr>
<td>Test area (tunnel)</td>
<td>160</td>
<td>12.0</td>
<td>9.0</td>
<td>1'920</td>
</tr>
<tr>
<td>Test area (cavern)</td>
<td>30</td>
<td>80.0</td>
<td>60.0</td>
<td>2'400</td>
</tr>
<tr>
<td>Ventilation shaft</td>
<td>123</td>
<td>20.4</td>
<td>12.6</td>
<td>2'509</td>
</tr>
<tr>
<td>Branch tunnels</td>
<td>960</td>
<td>26.5</td>
<td>20.5</td>
<td>25'440</td>
</tr>
<tr>
<td>Unloading area</td>
<td>72</td>
<td>46.9</td>
<td>36.0</td>
<td>3'377</td>
</tr>
<tr>
<td>Transfer area</td>
<td>88</td>
<td>80.4</td>
<td>55.3</td>
<td>7'075</td>
</tr>
<tr>
<td>Pilot facility (cavern)</td>
<td>29</td>
<td>123.6</td>
<td>102.3</td>
<td>3'584</td>
</tr>
<tr>
<td>Emplacement caverns 1 – 7</td>
<td>1'351</td>
<td>123.6</td>
<td>102.3</td>
<td>166'984</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>5'161</strong></td>
<td></td>
<td><strong>307'740</strong></td>
<td></td>
</tr>
</tbody>
</table>

¹) The clearance cross-section is the reference cross-section of the underground structures, when tunnel construction is completed.

### 2.6.3 Design of engineered gas transport system

The engineered gas transport system involves modifications of the backfilling and sealing systems. The sealing concepts described below are based on concepts that have been developed within the framework of Project "Entsorgungsnachweis" (c.f. Nagra 2002a and b). For this report no detailed dimensioning of the individual construction elements was made. The lengths of the sealing and/or static elements were rather derived on the basis of analogies from the Project Opalinus Clay. The individual sealing systems are described in the following paragraphs.

Instead of the concrete plugs at the entrance of each emplacement cavern or pilot cavern, two modification options are proposed. Option 1 consists of a temporary reinforced concrete wall ("bulkhead") of approximately 50 cm thickness at the intersection with the branch tunnel (V5; Fig. 2-15). Prior to the final backfilling and sealing of the repository, this temporary concrete wall will be removed.
The transitional layer consists of varying gravel and sand layers in order to fulfill filter criteria.

As an alternative to option 1 (the temporary concrete wall, V5), a final seal according to Figure 2-16 can be installed (option 2), consisting of a compacted sand/bentonite mixture (80/20 wt%) and an abutment formed by gravel (and stones). In contrast to the concrete wall, this seal will not be removed.
At the end of the operational phase, both the operation tunnel and the access tunnel are backfilled with sand/bentonite mixture (80/20 wt%) instead of processed excavated Opalinus Clay material. They are sealed with two different seals (V2 and V4.mod), one type being approximately 40 m long (V4.mod). Figure 2-17 illustrates this type of seal, incorporating highly compacted sand/bentonite mixture (70/30 wt%), placed at the boundary of Opalinus Clay and the upper confining unit within the access ramp.

The other seal (V2), shown in Figure 2-18, comprises approximately 30 m of compacted bentonite supported by approximately 30 m of concrete and would be placed at repository horizon at the end of the operation tunnel adjacent to the ventilation shaft instead of the concrete plug.

Final closure of the facility would involve emplacement of the main seal, made of highly compacted bentonite (V3), within the shaft. The implementation of both long-term seals V3 and V4.mod can be carried out in a similar manner to that described in chapter 2.3.6.

2.6.4 Excavation volumes and backfill materials

Gas-related design specifications of backfill material

It is foreseen to backfill the emplacement caverns with special mortar with high hydraulic conductivity and high porosity. Two types of mortar have been developed for this purpose, namely mono-grain (Mortar 1) and low-viscosity mortars (Mortar 2). Comprehensive characterisation
programmes were conducted for these backfill materials as described in more detail in chapter 3.3.3. In the following paragraphs, back-of-the-envelope estimations of the total pore volume of the emplacement caverns are given.

The emplacement of the disposal containers into the caverns takes place in two phases: In the first phase, the disposal containers are stacked on top of each other at the base of the cavern with the aid of an overhead travelling crane. Disposal sections with a length of approx. 28 m facilitate the emplacement of the backfill in the lower part of the cavern. These sections will be created by reinforced concrete walls ("bulkhead") perpendicular to the cavern axis. After the whole lower part of the cavern has been filled with disposal containers and backfilled, the overhead crane will be removed and the remaining space in the roof of the cavern will be filled with further disposal containers. Backfilling will occur alternating with emplacement of disposal containers. This ensures that the mortar backfill can be properly emplaced.

Tab. 2-2: Backfilling of emplacement cavern: Backfill materials and respective volumes (incl. pilot facility).

<table>
<thead>
<tr>
<th>Solid material</th>
<th>Total volume [m³]</th>
<th>Volume per emplacement cavern metre [m³]</th>
<th>Typical porosity</th>
<th>Pore volume [m³]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mortar M1</td>
<td>40'515</td>
<td>29.4</td>
<td>30 %</td>
<td>12'155</td>
</tr>
<tr>
<td>Mortar M2</td>
<td>33'426</td>
<td>24.2</td>
<td>35 %</td>
<td>11'699</td>
</tr>
<tr>
<td>Shotcrete</td>
<td>16'988</td>
<td>12.3</td>
<td>25 %</td>
<td>4'247</td>
</tr>
<tr>
<td>Filling concrete</td>
<td>12'406</td>
<td>9.0</td>
<td>20 %</td>
<td>2'481</td>
</tr>
<tr>
<td>Bulkhead (walls)</td>
<td>3'135</td>
<td>2.3</td>
<td>20 %</td>
<td>627</td>
</tr>
<tr>
<td>Concrete bedding</td>
<td>1'490</td>
<td>1.1</td>
<td>20 %</td>
<td>298</td>
</tr>
<tr>
<td>Disposal container</td>
<td>10'804</td>
<td>7.8</td>
<td>20 %</td>
<td>2'161</td>
</tr>
<tr>
<td>Waste matrix</td>
<td>51'804</td>
<td>37.5</td>
<td>20 %</td>
<td>10'361</td>
</tr>
<tr>
<td><strong>Total volume</strong></td>
<td><strong>170'568</strong></td>
<td><strong>123.6</strong></td>
<td><strong>25.8 %</strong></td>
<td><strong>44'028</strong></td>
</tr>
<tr>
<td>Total volume excluding shotcrete and filling concrete</td>
<td>141'174</td>
<td>102.3</td>
<td>26.4 %</td>
<td>37'300</td>
</tr>
</tbody>
</table>

Materials and respective volumes for the backfilling of the emplacement cavern are summarised in Table 2-2. Using typical porosities of the construction concrete (disposal containers and cavern lining) and of the backfill mortar M1 (mono-grain) and M2 (viscous), the total pore volume of the emplacement caverns can be inferred and an average backfill porosity can be determined. The bounding calculations in Table 2-2 exhibit an upper bound of the pore volume of approx. 44'000 m³, including the contributions of the shotcrete and the filling concrete. A lower pore volume of approx. 37'000 m³ is calculated, when the estimates are based on the clearance cross-sectional area according to Table 2-1. The corresponding average backfill porosity ranges between 25.8 and 26.4 %.

**Excavation and gas storage volume**

The gas storage volume of the backfilled underground structures depends on the volume, the porosity and the initial saturation of the backfill and construction materials (see Tab. 2-3). In addition, and especially for the cement-based backfill materials, the microscopic pore structure
and the bonding state of the water in the microscopic pore space plays a central role (residual water saturation). An overview of the gas-related properties of the backfill materials can be found in chapter 3.3. For estimating the gas storage capacity gross reference values for the average porosity are used.

In the subsequent overall estimation of the gas storage volume of the underground structures (Tab. 2-3), an average porosity of 25 % is used for the cementitious backfill and the total volume of the emplacement caverns is based on the clearance cross-sectional area according to Table 2-1. Consequently, for all emplacement caverns a gas storage volume of approx. 37'000 m³ would be available. If one considers in addition the gas storage volume of the remaining underground structures within the Opalinus Clay host rock, the total gas storage volume is further increased by 57 % to a total of 58'000 m³. Here it is assumed that the remaining underground structures are backfilled with a sand/bentonite mixture (average porosity of 27 %).

Tab. 2-3: Summary of gas storage volume.
S/B: Sand/Bentonite.

<table>
<thead>
<tr>
<th>Profile</th>
<th>Access to gas</th>
<th>Total volume [m³]</th>
<th>Backfill</th>
<th>Porosity [-]</th>
<th>Gas storage volume [m³]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Access tunnel</td>
<td>yes</td>
<td>20'765</td>
<td>S/B</td>
<td>0.27</td>
<td>5'607</td>
</tr>
<tr>
<td>Central area</td>
<td>yes</td>
<td>6'410</td>
<td></td>
<td>1'731</td>
<td></td>
</tr>
<tr>
<td>Operation tunnel</td>
<td>yes</td>
<td>30'051</td>
<td></td>
<td>8'114</td>
<td></td>
</tr>
<tr>
<td>Observation tunnel</td>
<td>no</td>
<td>12'300</td>
<td></td>
<td>3'321</td>
<td></td>
</tr>
<tr>
<td>Niches</td>
<td>no</td>
<td>938</td>
<td></td>
<td>253</td>
<td></td>
</tr>
<tr>
<td>Test area (access)</td>
<td>no</td>
<td>1'025</td>
<td></td>
<td>277</td>
<td></td>
</tr>
<tr>
<td>Test area (tunnel)</td>
<td>no</td>
<td>1'440</td>
<td></td>
<td>389</td>
<td></td>
</tr>
<tr>
<td>Test area (cavern)</td>
<td>no</td>
<td>1'800</td>
<td></td>
<td>486</td>
<td></td>
</tr>
<tr>
<td>Ventilation shaft</td>
<td>no</td>
<td>1'550</td>
<td></td>
<td>418</td>
<td></td>
</tr>
<tr>
<td>Branch tunnel</td>
<td>yes</td>
<td>19'680</td>
<td>S/B 0.27</td>
<td>5'314</td>
<td></td>
</tr>
<tr>
<td>Unloading area</td>
<td>yes</td>
<td>2'592</td>
<td>Mortar M1 0.25</td>
<td>648</td>
<td></td>
</tr>
<tr>
<td>Transfer area</td>
<td>yes</td>
<td>4'866</td>
<td>Mortar M1 &amp; M2</td>
<td>1'217</td>
<td></td>
</tr>
<tr>
<td>Pilot facility (cavern)</td>
<td>yes</td>
<td>2'967</td>
<td></td>
<td>742</td>
<td></td>
</tr>
<tr>
<td>Emplacement caverns 1 – 7</td>
<td>yes</td>
<td>138'207</td>
<td>Mortar M1 &amp; M2</td>
<td>34'552</td>
<td></td>
</tr>
<tr>
<td><strong>Total volumes (potential)</strong></td>
<td></td>
<td>244'591</td>
<td></td>
<td>63'069</td>
<td></td>
</tr>
<tr>
<td><strong>Gas storage volume</strong></td>
<td></td>
<td>148'632</td>
<td>Mortar M1 &amp; M2</td>
<td>37'158</td>
<td></td>
</tr>
<tr>
<td><strong>Gas storage volume of remaining facilities in Opalinus Clay with access to gas</strong></td>
<td></td>
<td>76'906</td>
<td>S/B 0.27</td>
<td>20'766</td>
<td></td>
</tr>
<tr>
<td><strong>Total gas storage volume (Opalinus Clay only)</strong></td>
<td></td>
<td></td>
<td></td>
<td>57'924</td>
<td></td>
</tr>
</tbody>
</table>
2.6.5 **Sealing material**

Materials are chosen which either serve as a seal or as an abutment material to transmit loads into the rock. These materials must have the required long-term durability. For the concrete plugs, the requirements on durability are less stringent.

As sealing materials, both clay/bentonite and sand/bentonite mixtures have the necessary long-term durability. Because of the very low intrinsic permeability of pure clay/bentonite, sand/bentonite mixtures are foreseen for those seals through which gas transport must be possible at reasonably low overpressures. The geotechnical specifications for the engineering design of the design option "gas valve", described below, are given in Table 2-4.

Well compacted gravel and stones (e.g. Diabas gravel and stones) are primarily considered as a load-bearing material to form the abutment with long-term stability with regard to gas permeability. Load bearing is accomplished through grain contact and the hydraulic conductivity is higher by many orders of magnitude than other plug and seal materials. The porosity is comparable to that of the other materials.

Indicative porosity and hydraulic conductivity values are given in Table 2-4 for various EBS materials, considered for the L/ILW repository.

Tab. 2-4: Summary of data for the backfill and sealing materials.

<table>
<thead>
<tr>
<th>Underground structures</th>
<th>Parameter</th>
<th>Parameter Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Backfill of branch, operation</td>
<td>Hydraulic conductivity</td>
<td>$1 \times 10^{-10} - 1 \times 10^{-11}$ m/s</td>
</tr>
<tr>
<td>and access tunnels (S/B 80/20, low</td>
<td>Porosity</td>
<td>$0.25 - 0.30$</td>
</tr>
<tr>
<td>compaction)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Seal sections</td>
<td>Hydraulic conductivity</td>
<td>$1 \times 10^{-11} - 1 \times 10^{-12}$ m/s</td>
</tr>
<tr>
<td>(S/B 70/30 or S/B 80/20, high</td>
<td>Porosity</td>
<td>$0.25 - 0.30$</td>
</tr>
<tr>
<td>compaction)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Concrete plugs</td>
<td>Hydraulic conductivity</td>
<td>$1 \times 10^{-10} - 1 \times 10^{-11}$ m/s</td>
</tr>
<tr>
<td></td>
<td>Porosity</td>
<td>$0.25 - 0.35$</td>
</tr>
</tbody>
</table>

2.7 **Quantities of waste and gas-generating materials**

The modelling activities reported in this synopsis started in 2005 and were completed by the end of 2007. In this period, the model waste inventory of the L/ILW repository was further developed for several reasons: (i) The work to develop the basis for allocation of the waste to the L/ILW and the HLW repositories as required by the Sectoral Plan was also performed in this period, resulting in the waste allocation described in Nagra (2008e). (ii) The description of the materials (including gas-generating materials) was further refined in the context of the periodic updating of the model waste inventory MIRAM. (iii) New scenarios had to be evaluated as part of the procedure set out by the Sectoral Plan, taking into account the possibility for additional wastes from new nuclear power plants (Nagra 2008e). An overview of the waste inventories considered is given in Table 2-5, including the corresponding volumes of waste and the key references. The inventory MIRAM 2008 (Nagra 2008f) was not available for the gas-related modelling activities at the time they were performed, and thus, the MIRAM 2005 inventory was
used to define a reference source term (cf. chapter 4.3.1). It is beyond the scope of this synopsis to determine gas source terms and to perform gas pressure build-up calculations for the different waste inventories in detail. Instead, a discussion of the calculation of the gas source term based on the MIRAM 2008 inventory is given in the subsequent paragraphs as this represents the current understanding of the basis for performing such calculations. A comparison of the gas production rates based on the inventories MIRAM 2005 and MIRAM 2008 is given in Figure 2-19.

Tab. 2-5: Overview of recent L/ILW waste inventories.

<table>
<thead>
<tr>
<th>Inventory ID</th>
<th>Volume of waste [m$^3$]</th>
<th>Remarks and references</th>
</tr>
</thead>
<tbody>
<tr>
<td>MIRAM (2005)</td>
<td>85'500</td>
<td>Assumptions: wastes from existing nuclear power plants (NPPs), 50 years of operation of NPPs; allocation of waste to L/ILW repository based on Nagra (2001b)</td>
</tr>
<tr>
<td>MIRAM (2008)</td>
<td>74'760</td>
<td>Assumptions: wastes from existing NPPs, 50 years of operation of NPPs; allocation of waste to L/ILW repository according to Nagra (2008e) / &quot;Referenzzuteilung&quot; RZ. Not included in this figure are reserves for wastes from medicine, industry and research of 12'000 m$^3$ and 2'220 m$^3$ of wastes from the SF/HLW encapsulation facility (Nagra 2008f)</td>
</tr>
<tr>
<td>Enlarged waste volume (&quot;umhüllendes Abfallinventar&quot; or bounding inventory)</td>
<td>200'000</td>
<td>Assumptions: Wastes from existing NPPs and from 3 new NPPs with 5 GWe, 60 years of operation of NPPs (rounded values); allocation of waste to L/ILW repository according to Nagra (2008e)</td>
</tr>
</tbody>
</table>

As discussed above, the gas generation calculations described here are based on Nagra's waste inventory MIRAM 2008 (Nagra 2008f). The types and quantities of gas-generating materials are shown in Table 2-6. This model inventory is based on the assumption of 50 years of operation of the existing nuclear power plants (NPPs) and a collection period for wastes from medicine, industry and research until the year 2050. Current planning also considers a variant with a waste volume that is approx. twice as large (enlarged waste volume ("umhüllendes Abfallinventar") with 200'000 m$^3$ instead of 74'760 m$^3$, see Nagra 2008e) that also takes into account the wastes from new NPPs and a prolonged collection period for wastes from medicine, industry and research. However, the inventory used here is considered to be a suitable starting point to draw conclusions also for this larger waste volume.

The following estimates of the total gas volume produced are based on the discussion of the gas generation processes in chapter 2.8. Assuming complete corrosion of the metals the volume of hydrogen produced would correspond to a volume of $2.1 \times 10^7$ m$^3$ ($2.5 \times 10^7$ m$^3$ according to the MIRAM 2005 inventory). The complete degradation of organics would produce a methane volume of $9.2 \times 10^5$ m$^3$ ($1.30 \times 10^6$ m$^3$ according to the MIRAM 2005 inventory). Carbon dioxide is very soluble in the alkaline cement porewater of the repository and precipitates as calcite. For this reason only methane is considered for further gas calculation. Thus, a maximum gas volume of $2.2 \times 10^7$ m$^3$ (methane CH$_4$ and hydrogen H$_2$) is expected ($2.6 \times 10^7$ m$^3$ according to the MIRAM 2005 inventory).
Tab. 2-6: Total inventories of gas-generating materials in the L/ILW repository (MIRAM 2008).

<table>
<thead>
<tr>
<th>Metals</th>
<th>Mass [kg]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steels</td>
<td>$3.8 \times 10^7$</td>
</tr>
<tr>
<td>Aluminium / Zinc</td>
<td>$3.7 \times 10^5$</td>
</tr>
<tr>
<td>Zircaloy</td>
<td>$9.6 \times 10^4$</td>
</tr>
<tr>
<td>Organics</td>
<td></td>
</tr>
<tr>
<td>High molecular weight organics</td>
<td>$1.9 \times 10^6$</td>
</tr>
<tr>
<td>Cellulose and low molecular weight organics</td>
<td>$2.8 \times 10^5$</td>
</tr>
</tbody>
</table>

2.8 Gas generation: processes and rates

2.8.1 Earlier work on gas generation
The gas generation calculations are based on earlier studies for L/ILW repositories in Switzerland. The basic processes (incl. stoichiometry) and data have been published by Wiborgh et al. (1986). Similar data have been used for the safety analysis of the Wellenberg L/ILW repository project (Nagra 1994) taking into account new results from the literature. Also for Project "Entsorgungsnachweis" the published data were reviewed and gas production has been calculated for a repository for spent fuel, high-level waste and long-lived intermediate level waste sited in Opalinus Clay (Nagra 2002d, Nagra 2004).

2.8.2 Gas-generation processes
The low hydraulic conductivity of the Opalinus Clay will result in slow saturation of the cementitious grout of the emplacement caverns and of the infill of the disposal containers with the waste drums. Oxygen is expected to be consumed relatively quickly (within decades) leading to anaerobic corrosion of metals. Corrosion processes are assumed to start immediately after emplacement of the waste drums when the emplacement caverns are backfilled. Due to the amount of concrete in the near-field, the porewater pH is calculated to lie between 12.5 and 13 (Neall 1994). The main processes leading to gas production (anaerobic corrosion of metals, microbial degradation of organic matter, and radiolysis of porewater) are discussed in detail below.

Anaerobic corrosion of metals
A variety of metals is present in the waste and some steel is also used as construction material (reinforcement). The following metals are considered as corrodbile: iron (including carbon steel and various stainless steels), "Inconel", aluminium, zinc, magnesium, Zircaloy, lead, and the alloy "Ag80/In15/Cd5" (from NPP control rods), whereas metallic copper is considered not to corrode under repository conditions. In estimating the molar quantities of hydrogen produced by anaerobic corrosion, it is assumed that the alloys are entirely composed of the predominant metal (e.g. Fe for all steels and Zr for Zircaloy, exception: Ag80/In15/Cd5).
**Carbon steel:** Fujisawa et al. (1997) determined the corrosion rate of carbon steel by measuring H$_2$ evolution in mortar-equilibrated water at pH 12.6 over the temperature range from 15°C to 45°C. Based on their data, the rate at ~ 40°C, the expected long-term ambient temperature of the ILW tunnels, is estimated to be 0.1 μm a$^{-1}$. Kreis (1991) measured rates of corrosion of iron wire at 21°C in NaOH, KOH and Ca(OH)$_2$ solutions at a pH of 12.8, as well as in cement porewaters. Long-term corrosion rates ranged from 1 to 30 nm a$^{-1}$, and Kreis (1991) recommended a conservative value of 70 nm a$^{-1}$ to allow for uncertainties in the evolution of the porewater composition. Naish et al. (1990) observed a decrease in corrosion rate of carbon steel by a factor of four in cement porewater as the H$_2$ partial pressure was increased from 0.1 to 10 MPa. There are some indications that elevated Cl$^-$ concentrations may increase the rate somewhat (Naish et al. 1990), but the effect is unlikely to be large, based on the small effect of Cl$^-$ on corrosion rates observed by Kreis (1991) at pH 8.5. It is reasonable to conclude from all these studies that in a cementitious environment a realistic corrosion rate for iron, carbon steel and various mild steels is 0.1 μm a$^{-1}$. A comprehensive discussion on how the corrosion rate is related to the partial pressure of hydrogen is found in King (2008). The study indicates that the effect can be neglected.

**Stainless steels:** The anaerobic corrosion rate of 304 stainless steels has been measured by Wada et al. (1999) at 30 and 50°C at pH 12.5. Rates were < 1 nm a$^{-1}$ at both temperatures. A more pessimistic value of 10 nm a$^{-1}$ is adopted here for all stainless steels and Inconel.

**Zircaloy:** The measurements of Kurashige et al. (1999) and Wada et al. (1999), both performed at a pH of 12.5 to 13, gave rates of about 1 nm a$^{-1}$. A more pessimistic value of 10 nm a$^{-1}$ is selected, allowing for the fact that there are no reported corrosion rate measurements under alkaline conditions for irradiated Zircaloy. The thickness of Zircaloy cladding is about 600 μm.

**Aluminium and zinc:** Hydrogen production due to corrosion of Al and Zn occurs even under oxidising conditions. Fujisawa et al. (1997) observed that aluminium corrosion rates in mortar decreased from ~ 1 mm a$^{-1}$ to ~ 1 μm a$^{-1}$ after several thousand hours. However, the aluminium in the containers may be in contact with steel wastes, which may lead to galvanic coupling, thus sustaining a higher rate until the aluminium has completely corroded. For example, Smart & Blackwood (1998) performed galvanic coupling measurements that gave rates of up to 10 μm a$^{-1}$. It is concluded that it is prudent to adopt a corrosion rate for Al (and Zn, for which little data is available) of 0.1 mm a$^{-1}$ although this may considerably overestimate the rate. As can be seen from the values recommended above, these reference case rates are pessimistic, ranging from 3 to 10 times higher than experimentally measured steady-state values.

**Degradation of organic matter**

Two broad categories of organic wastes have been defined: these are easily degradable organics such as cellulose, and organics such as plastics, resins and bitumen that may be resistant to complete degradation. Degradation of organic waste materials (most likely catalysed by microbes) will produce approximately equimolar amounts of methane (CH$_4$) and carbon dioxide (CO$_2$), for which a simplified reaction can be written as (Stumm & Morgan 1996):

\[ 2\{\text{CH}_2\text{O}\} \rightarrow \text{CH}_4 + \text{CO}_2 \]  
(Eq. 2-1)

where {CH$_2$O} represents an average composition of organic materials. Carbon dioxide would dissolve in the alkaline porewater and precipitate as calcite. The rate of microbial degradation of organic matter depends on the nature of the material, with cellulose more susceptible to rapid degradation, and is uncertain because the environment, in particular the high pH, is considered
poor for optimum microbial activity, although it is unlikely to prevent it from occurring. The maximum rates of degradation of organic matter to CH\(_4\) and CO\(_2\) in the tunnels have been estimated based on values given by Wiborgh et al. (1986) and are 0.7 mol kg\(^{-1}\) a\(^{-1}\) of cellulose and 0.05 mol kg\(^{-1}\) a\(^{-1}\) of other organic material. These rates have been used as the basis of gas production calculations for SKB's SFL3-5 repository (SKB 1999) and in Nagra studies for a L/ILW repository (Grogan et al. 1992). Studies of gas generation rates of actual mixed wastes in both brine and cementitious water (Kannen & Müller 1999) indicate rates that are more than an order of magnitude lower than the reference values of Wiborgh et al. (1986).

### Radiolysis of water

Due to the very low \(\alpha\)-activity in L/ILW and in accordance with international practice (see, e.g., Rodwell & Norris 2003) the gas generation from the radiolysis of water is not considered in calculating gas generating rates.

#### 2.8.3 Gas generation rates: calculations and results

The first calculations of gas generation were based on a preliminary radioactive waste inventory (MIRAM 2005). The compilation and publication of the new radioactive waste inventory MIRAM 2008 (Nagra 2008f) allowed an update of these earlier gas generation calculations based on the new input data. Figure 2-19 shows the results for both inventories.

The gas generation rates were calculated as the sum of the hydrogen gas produced by the anaerobic corrosion of the metals and the methane produced by the microbial degradation of the organic components of the waste. Carbon dioxide is very soluble in the alkaline cement pore-water of the repository and precipitates as calcite. For this reason only methane is considered for further gas calculation. The degradation of the organic material is calculated using a first order equation. For low molecular weight organics and easily degradable high molecular organics like cellulose (organics type 1), a higher degradation rate is assumed. For other high molecular organics (organics type 2) a lower degradation rate is used.

Corrosion processes are assumed to occur only at the surface of the metal. Thus an average surface-to-mass ratio is given in the model inventory for the different metal types in each waste type to take into account the reaction interface for metallic waste pieces. For the metal corrosion calculations, it is assumed that each metal piece has the shape of a flat sheet, which is corroding from both sides with a constant rate.

The rate of the hydrogen gas production is proportional to the corroding metal surfaces. The surface area \(O\) [m\(^2\)] of a metal component can be calculated from the mass \(m\) [kg] per container and the surface-to-mass ratio \(k_{OM}\) [m\(^2\)/kg] of a piece of metal with the formula:

\[
O = m \cdot k_{OM} \tag{Eq. 2-2}
\]

The surface area is corroded with the given corrosion rate \(r\) [m/a]. During one year, the corroded mass \(m_m\) [kg/a] for a piece of metal with the density \(\rho_m\) [kg/m\(^3\)] can be calculated as:

\[
m_m = O \cdot r \cdot \rho_m \tag{Eq. 2-3}
\]
The resulting hydrogen gas volume can be calculated from the stoichiometry of the corrosion reaction and the molar mass of the metal $M_m$ [kg/mol]. The stoichiometry factor of the corrosion reaction depends on the reaction product. For the calculations the most stable corrosion product under the given chemical conditions in the repository is assumed to be the final reaction product. For the corrosion of iron the reaction is:

$$3 \text{Fe} + 4 \text{H}_2\text{O} \rightarrow \text{Fe}_3\text{O}_4 + 4 \text{H}_2 \quad (\text{Eq. 2-4})$$

The resulting stoichiometry factor is $4/3$, which means that 1.33 mol of hydrogen per mol of corroded iron are formed.

The annual hydrogen gas volume $V_H$ [m$^3$/a] generation is calculated from the metal mass $m_m$ [kg/a] corroded per year and the molecular mass of the metal $M_m$ [kg/mol]:

$$V_H = \frac{m_m}{M_m} \cdot V^0 \quad (\text{Eq. 2-5})$$

where $V^0$ [m$^3$/mol] is the molar gas volume.

The duration of the corrosion reaction for a particular metal piece is calculated from its thickness $d$ [m]. Assuming that the metal component with the thickness $d$ [m] (derived from the surface-to-mass ratio $k^{\text{OM}}$ [m$^2$/kg]) is corroded from two sides with the corrosion rate $r$ [m/a], the reaction time $t$ [a] is:

$$t = \frac{d}{2 \cdot r} \quad (\text{Eq. 2-6})$$

The gas generation model assumes that the organic components of the waste are degraded to a mixture of equal amounts of methane and carbon dioxide (see Eq. 2-1).

**Results**

Results for the gas generation calculations are shown in Figure 2-19. They include calculations based on Nagra's waste inventories MIRAM 2008 (Nagra 2008f) as well as those based on an earlier version of the inventory, MIRAM 2005, which was used for the gas release calculations ("realistic" gas source term, see below).

Figure 2-19 shows that the updates of the waste mass data and the surface-to-mass ratios of the metals resulted in some differences of the evolution of the gas generation over time. The total amount of gas generated and the general trend of the gas generation curve are however comparable. Note that the initial gas generation rate calculated with MIRAM 2005 is more than a factor of five higher than the value based on the updated MIRAM 2008 inventory. This can be traced back to a revised (i.e. lower) estimate of the total amount of zinc in the inventory in MIRAM 2008 compared to MIRAM 2005. For the gas transport calculations in chapter 4.3 a sensitivity analysis with a "realistic" and a "conservative" gas source term is performed. The realistic source term is based on MIRAM 2005 (the only data available at the time the gas transport calculations were performed). The conservative case which assumes an increase of the rate by a factor of 10 for steels is an arbitrary sensitivity case to explore how the system behaves with gas production rates that are far above the measured values. This case bounds the gas production rates based on MIRAM 2005 and MIRAM 2008.
Fig. 2-19: Comparison of the gas production rates based on the MIRAM 2005 and MIRAM 2008 waste inventories.
3  Gas transport – processes, phenomena and gas-related parameters

3.1  Rationale

The release of the gases produced in the backfilled emplacement caverns of the repository can occur by a variety of transport mechanisms. Gases will be dissolved in the porewater and eventually, when the solubility limit is exceeded, a separate phase may form. At elevated gas pressures the porous medium (host rock and backfill material, respectively) could undergo mechanical deformation. Last but not least, chemical interactions within the 3-phase system (gas, water, solid) could change with time the gas storage and transport capacity of the porous medium.

The prevailing gas transport mechanisms are controlled by the hydrodynamic properties of the fluids and by the environmental conditions, such as in-situ pore pressure, rock stress and water saturation in the porous medium. For the hydrodynamic properties the microstructural and macroscopic characteristics of the porous medium, including the pore size distribution, the pore connectivity, spatial variability of porosity and the mineralogical composition of the solid phase (wettability) are important. Consequently, the mechanisms of gas transfer are strongly related to the individual gas paths (intact rock, EDZ, sand/bentonite) and the specific features of gas transport need to be addressed for the different paths (e.g. scale effects).

It is the purpose of this chapter to provide a systematic overview of the main gas transport processes, the gas-related parameters and the coupled processes which may be associated with the transport of the gas through the Opalinus Clay and the backfilled underground structures. The chapter is structured as follows:

- Gas transport mechanisms: the relevant gas transport mechanisms are specified and their characteristic features are discussed (chapter 3.2).
- Gas transport parameters: databases of gas-related parameters are given for the host rock and for all relevant backfill and sealing materials (chapter 3.3).
- Coupled phenomena and interactions: a systematic review is given for the relevant hydro-mechanical and hydrochemical couplings associated with gas transfer through the host rock and the backfilled underground structures, respectively (chapter 3.4).
- Evaluation of process understanding: transport capacity of the different gas transport mechanisms and impact on the evolution of the L/ILW repository are assessed (chapter 3.5).

3.2  Gas transport mechanisms: phenomenology and modelling concepts

Gas transport through low-permeability rock formations is controlled not only by the hydraulic and mechanical properties of the rock mass (intrinsic permeability, porosity, rock strength), but also by the gas pressure at the place of gas entry and the hydromechanical state of the rock (i.e. water saturation, porewater pressure, stress state). Phenomenological considerations suggest the following subdivision of the basic transport mechanisms (Fig. 3-1):

- 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 gas-fracturing)
As seen in Figure 3-1a, the phenomenological description is related to the microstructural conceptualisation of the Opalinus Clay (Nagra 2002a). The complex hydromechanical processes are decomposed into transport of immiscible fluids (Fig. 3-1b) and geomechanics (Fig. 3-1c). The effect of gas transport on the hydraulic barrier properties of the rock is highlighted for each of the transport mechanisms (Fig. 3-1d).

The different gas transport mechanisms are discussed in the following chapters. A key issue in the quantitative description of two-phase flow processes is addressed in chapter 3.2.5, dealing with the definition of a representative elementary volume of combined gas/water flow and with the up-scaling of two-phase flow parameters.

It is worth mentioning that different terminologies for the description of gas transport processes are found in the geoscientific literature. The term "capillary failure" is often used in oil & gas industry to describe the two-phase flow regime in cap rocks (e.g. Clayton & Hay 1994). "Membrane seal failure" describes gas transport through the pre-existing pore system of the caprock (i.e. advection/diffusion of dissolved gas and two-phase flow), whereas "hydraulic seal failure" is used to describe gas leakage due to hydromechanical processes in the seal (microfracturing, reopening of existing faults, hydro/gas fracturing). A comprehensive literature study on gas storage and gas transport phenomena is given in Evans (2008).

![Classification and analysis of gas transport processes in Opalinus Clay.](image-url)
3.2.1 Transport of gas dissolved in the porewater

Advective and diffusive transport of gas dissolved in porewater is characterised by three fundamental laws (Helmig 1997):

- Darcy's law, describing advective groundwater flow under the impact of pressure and gravitational forces
- Fick's law represents the diffusion of dissolved gas due to concentration gradients in the porewater
- Henry's law describes the solubility of gas in porewater

Darcy's law represents the general basis for quantitative descriptions of groundwater flow. It denotes the linear correlation between the specific discharge \( v_f \) (Darcy velocity) through a representative elementary volume and the hydraulic gradient. The proportionality constant for the relationship is provided by the hydraulic conductivity \( K \). Darcy's law is applicable only within certain limitations. For geomaterials with ultra-low permeability, such as the Opalinus Clay and bentonite, deviations from the linear flow law may be expected for low hydraulic gradients. The small pore radii cause electro-molecular rock-water interactions to gain significance in comparison to the viscous fluid properties, i.e. friction. In response, the formation water no longer behaves like a Newtonian fluid when exposed to a low hydraulic gradient. A comprehensive discussion of possible causes for non-linear porewater flow in clay-rich materials is found in Horseman et al. (1996). In empirical terms, this situation may be accounted for by introducing a hydraulic threshold gradient \( i_c \), (see, e.g. Bear 1972, de Marsily 1986). For the Opalinus Clay the threshold gradient necessary to establish Darcy flow was assessed by laboratory and in-situ experiments; the investigations indicated that Darcy's law holds for hydraulic gradients \( > 10 \) m/m (Marschall et al. 2003). For bentonites the validity of the linear relationship between flow and hydraulic gradient has been demonstrated down to gradients of about 100 m/m (Lloret et al. 2005).

Diffusion is a process induced by the random thermal motion of molecules and ions. Diffusion in a porous medium in its simplest form can be described by Fick's law (Domenico & Schwartz 1990):

\[
J = -D_d \text{grad}(C)
\]  
(Eq. 3-1)

with \( J \) being the diffusional flux [mol/L\(^2\)T]; \( D_d \) the effective diffusion coefficient [L\(^2\)/T] and \( C \) the concentration [mol/L\(^3\)] of a species.

In this equation the flux of each species is related to the concentration gradient by a diffusion coefficient that is specific for that species. The value of the diffusion coefficient of a species in water depends on the type of species, the temperature and pressure and its interaction with other species (Felmy & Weare 1991). Diffusion coefficients for up to 30 species in a wide temperature and pressure range are given in Oelkers & Helgeson (1988). Table 3-1 gives the diffusion coefficients in free water for a selection of gases, which are relevant for the assessment of gas release.

In the case of diffusion in a porous medium, the diffusion rate is further defined by the structure and the properties of the porous medium such as the effective porosity, describing the total pore space available for the diffusion of the species and the tortuosity, accounting for the pore space geometry. Among various definitions, one of the most cited is Greenkorn & Kessler (1972) expressing \( D_d \) as a function of porosity and tortuosity (Greenkorn & Kessler 1972):
where $\phi$ is the porosity, $d_w$ is the diffusion coefficient in free solution, and the tortuosity is defined as the ratio of the length of a flow channel for a fluid particle $L_e$, to the length of a porous medium sample $L$. These parameters are to some extent also species dependent. It is clear that cations, anions and neutral species have unequal pore diffusion coefficients. The higher diffusivity of cations is generally attributed to surface diffusion (Cole et al. 2000) or to the diffuse double layer, where the concentrations of cations are increased (Bourg et al. 2003).

The diffusion coefficient for a two-phase system with porosity $\phi$ is defined as:

\[
D_\beta^* = \phi \cdot \tau_o \cdot \tau_\beta \cdot d_\beta^* \tag{Eq. 3-3}
\]

where $d_\beta^*$ is the molecular diffusion coefficient for component $\kappa$ in phase $\beta$, $\tau_o$, $\tau_\beta$ is the tortuosity which includes a porous medium-dependent factor $\tau_o$ and a coefficient that depends on phase saturation $S_\beta$, $\tau_\beta = \tau_\beta (S_\beta)$. The diffusion coefficients for gases depend on pressure and temperature, as defined in Vargaftik (1975) and Walker et al. (1981). The saturation dependence of tortuosity can be described as parametric relationships, such as that by Millington & Quirk (1961).

Gas dissolution and exsolution can transfer significant quantities of mass between the gas phase and the porewater in a porous medium. According to Henry's law the partial pressure of an ideal gas in the gas phase is proportional to the concentration of the gas in the aqueous phase (Domenico & Schwartz 1990):

\[
K_H = \frac{(\text{gas})_{aq}}{P_{\text{gas}}} \tag{Eq. 3-4}
\]

Where $K_H$ is the Henry's law constant [mol Pa$^{-1}$], $P_{\text{gas}}$ is the partial pressure of the gas in the gas phase [Pa] and $(\text{gas})_{aq}$ is the molar concentration of the gas in solution. Table 3-1 provides the solubilities of various gases in water.

Tab. 3-1: Solubilities and diffusion coefficients of a selection of gases in water at standard conditions (25°C, 1 atm) (Lide 2000).

<table>
<thead>
<tr>
<th>Gas</th>
<th>Formula</th>
<th>Solubility (25°C, 1 atm) [mg l$^{-1}$]</th>
<th>Diffusion (25°C) [$\times 10^{-9}$ m$^2$ s$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>H$_2$</td>
<td>1.58</td>
<td>5.11</td>
</tr>
<tr>
<td>Helium</td>
<td>He</td>
<td>1.56</td>
<td>7.28</td>
</tr>
<tr>
<td>Oxygen</td>
<td>O$_2$</td>
<td>40.76</td>
<td>2.42</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>N$_2$</td>
<td>18.41</td>
<td>2.00</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>CO$_2$</td>
<td>1503.52</td>
<td>1.91</td>
</tr>
<tr>
<td>Methane</td>
<td>CH$_4$</td>
<td>22.74</td>
<td>1.84</td>
</tr>
</tbody>
</table>
This law is valid for ideal gases and very dilute porewaters only. In the case of real gases the fugacity should be taken into account instead of the partial pressure. The fugacity is a function of the temperature, the pressure and the composition of the gaseous phase. Equally, in the case of more realistic porewater compositions, activities should be used instead of concentrations. Activities are influenced by the pressure, the temperature and the composition of the solution and are significantly lower than the equivalent concentrations in cases where porewaters consist of concentrated brines at higher temperatures and pressures (Kervévan et al. 2005).

The transport of dissolved gas occurs even at low (total) gas pressures; the pressure-dependent dissolution of gas in porewater and the increased groundwater flux cause the specific flux of the dissolved gas to increase with an increase in the gas pressure. The low hydraulic conductivity of argillaceous rock significantly restricts the efficiency of this transport mechanism. Thus, scoping calculations were conducted as part of the SF/HLW programme, indicating that the gas transport capacity of diffusion and advection (of dissolved gases) is several orders of magnitudes lower than the transport capacity of two-phase flow. Further back-of-the-envelope calculations on the efficiency of this transport mechanism are given in Appendix C. Nevertheless, the general importance of diffusion and advection as slow background processes in all types of cap rock formations is beyond question and has been addressed in the context of many hydrocarbon exploration and reservoir engineering studies (Clayton & Hay 1994, Krooss et al. 1992, Schlömer & Krooss 1997).

3.2.2 Visco-capillary two-phase flow

In its conventional form, visco-capillary two-phase flow is described as a transport process whereby porewater in the pore volume of a rock formation is displaced by gas under the influence of viscous and capillary forces (e.g. Bear 1972). Visco-capillary two-phase flow accounts for the individual phase fluxes, given by the multiphase version of Darcy's law:

\[ v_\beta = -k \cdot \frac{k_{r\beta}}{\mu_\beta} \left( \nabla p_\beta - \rho_\beta \cdot g \right) \]  
(Eq. 3-5)

where \( v_\beta \) is the Darcy velocity (volume flux) in phase \( \beta \), \( k \) is the intrinsic permeability, \( k_{r\beta} \) is the relative permeability to phase \( \beta \), \( \mu_\beta \) is the viscosity, and \( p_\beta = p + p_{c\beta} \) the fluid pressure in phase, and the capillary pressure \( p_{c\beta} \). The coefficient \( g \) is the gravitational acceleration.

In a geomechanical sense, the rock mass behaves like an elastic medium, characterised by the porosity and the rock compressibility. The controlling factor for the two-phase flow characteristics of a porous medium is the gas entry pressure \( p_{ae} \), also known as the capillary threshold pressure, which represents the difference between gas pressure and water pressure needed to displace the porewater from the initially fully saturated medium. For a capillary tube, the Young-Laplace's equation gives the relationship between the gas entry pressure (capillary threshold pressure) and the pore radius:

\[ p_{ae} = \frac{2 \cdot \sigma_{gw}}{r} \cdot \cos \alpha \]  
(Eq. 3-6)

where \( p_{ae} \) is the gas entry pressure, \( \sigma_{gw} \) is the surface tension gas/water (ca. 0.073 N m\(^{-1}\) at 20°C), \( r \) represents the radius of the capillary tube and \( \alpha \) is the wetting angle. In porous media, Young-Laplace's equation can be adapted to define an equivalent pore radius of the medium by measuring the entry pressure with a non-wetting fluid (e.g. mercury porosimetry).
Once the gas entry pressure has been exceeded, the gas mobility is controlled mostly by the intrinsic permeability $k$ of the formation, the permeability-saturation relationship (relative permeability), and the relationship between the capillary pressure and the water saturation (suction or water retention curve). The functional dependency between the pore space saturation and the relative permeability or the capillary pressure is commonly described with parametric models. According to van Genuchten (1980), the parametric relationship between water saturation and capillary pressure is given as:

$$p_c = p_g - p_w = \frac{1}{\alpha} \left( S_w^{\frac{n}{n-1}} - 1 \right)$$  \hspace{1cm} (Eq. 3-7)

where $p_c$, $p_g$, and $p_w$ represent the capillary pressure, gas pressure and water pressure, respectively. $1/\alpha$, the inverse of van Genuchten’s $\alpha$ parameter, is known as the capillary strength or apparent gas entry pressure and $n$ is the shape factor (pore size distribution index). The porewater saturation $S_w$ is the volume of porewater per volume of pores.

The relative gas/water permeabilities $k_{r,g}$ and $k_{r,w}$ of the Opalinus Clay are described by the approach of Mualem (e.g. Helmig 1997):

$$k_{r,g} = (1 - S_e)^\gamma \left( 1 - S_e^{\frac{n}{n-1}} \right)^{-2(1-1/n)}$$  \hspace{1cm} (Eq. 3-8)

$$k_{r,w} = S_e^{\epsilon} \left[ 1 - \left( 1 - S_e^{\frac{n}{n-1}} \right)^{n+1} \right]^{2}$$  \hspace{1cm} (Eq. 3-9)

with $S_e = \frac{S_w - S_{wr}}{1 - S_{gr} - S_{wr}}$

where $\epsilon$ and $\gamma$ are empirical shape factors, describing the pore connectivity of the medium (present study: $\epsilon = \gamma = 0.5$). According to the Mualem approach, the definition of the effective saturation $S_e$ is slightly modified and includes the residual gas saturation $S_{gr}$. An excellent review of the spectrum relative permeability models in multiphase flow analysis is given in Honarpour et al. (1986).

Enhancement (or reduction) of the gas mobility, as postulated in Croisé et al. (2006) for the interpretation of in-situ gas injection tests at the Mont Terri URL, can be taken into account by introducing a multiplication factor $f_g$ in the relative permeability equation, as follows:

$$k_{r,g} = f_g \cdot (1 - S_e)^\gamma \left( 1 - S_e^{\frac{n}{n-1}} \right)^{-2(1-1/n)}$$  \hspace{1cm} (Eq. 3-10)

In this study a gas enhancement factor $f_g = 1$ was used for all two-phase flow simulations.

A distinct hysteresis is often seen in the capillary pressure relationship, depending on the saturation path, i.e. whether the relationship corresponds to a saturation or desaturation of the porous medium. During the saturation process, the porosity of the medium cannot be saturated completely (residual gas saturation $S_{gr}$), because part of the pore space is poorly connected. On the other hand, assuming an initially fully saturated medium, critical gas saturation has to be exceeded before gas starts to form a continuous phase with a gas permeability $> 0$ (e.g. Dury et al. 1999). In the context of this study, due to the limited experimental data base, no distinction is
made between residual and critical gas saturation. As part of Nagra's RD&D programme, a laboratory programme has been launched to improve the gas-related database by comprehensive water and gas permeability test on Opalinus Clay samples from the Mont Terri URL.

The dependency of capillary pressure on the history of flow is known as the aforementioned capillary pressure hysteresis. The dependence of capillary pressure (and of the relative permeability relationship) on the rate of change of saturation is termed in literature as "dynamic effect" or "non-equilibrium effect". A multitude of references on the dynamic effect are found in the recent literature (Barenblatt et al. 1990, Hassanizadeh et al. 2002, Silin & Patzek 2003, Schembre & Kovscek 2006, Juanes et al. 2006), however, the interpretation of the effect is controversial. Thus, Hassanizadeh et al. (2002) explain the non-equilibrium phenomena as a characteristic feature in the context of their new macroscopic theories of multiphase flow (Hassanizadeh & Gray 1990), whereas Bourgeat & Panfilov (1998) interpret it as consequence of upscaling of two-phase flow parameters. In the present report, the dynamic effect is not considered due to the lack of experimental evidence for ultra-low permeability rock, such as Opalinus Clay. Further insight is expected from Nagra's recent gas-related laboratory programme.

Juanes et al. (2006) investigate hysteresis effects in the relative permeability – saturation relationship as part of a modelling study on CO₂ sequestration. Drawing on experimental evidence, the authors demonstrate by an analysis of pore-scale processes that relative permeabilities are not single functions of fluid saturations ("dynamic effects") and that they display strong hysteresis effects. Permeability hysteresis could be of great importance for the gas release from nuclear waste repositories, because the rock zone around the underground structures is desaturated during the operational phase of the repository. After repository closure, trapped gas in the vicinity of the backfilled tunnels could lower the gas entry pressure of the rock and thus increase its gas transport capacity in the early post-closure period. In the present study, the impact of trapped gas is accounted for by variations of the residual gas saturation in the relative permeability model of the EDZ.

3.2.3 Dilatancy-controlled gas flow

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

Empirical investigations and phenomenological descriptions of dilatancy-controlled gas flow through clay-rich seals were the subject of many geoscientific papers in the field of reservoir engineering (e.g. Clayton & Hay 1994, Ingram et al. 1997, Ingram & Urai 1999, Zweigel et al. 2004). Further evidence for pathway dilation phenomena has been found in other areas such as natural gas storage and CO₂ sequestration. Benson et al. (2002) reviewed the safety results of
underground storage in the United States as part of a comprehensive study considering CO₂ storage in deep geological formations. The authors emphasise the importance of vertical pressure gradients as an indicator for the onset of dilatancy-controlled leakage through the caprocks which cover natural gas storage formations. According to Ibrahim et al. (1970) the critical pressure gradient for dilatancy-controlled gas leakage is bracketed by the hydrostatic gradient (≈ 9.8 kPa/m) and the lithostatic gradient (≈ 22.6 kPa/m assuming a bulk density of the overburden of about 2.3 g/cm³), where the lithostatic pressure gradient represents a lower limit for the initiation of macroscopic fractures (cf. chapter 3.2.4). It is noteworthy that the CSA Standard Z341 (CSA 2006) includes a recommendation that the maximum operating pressure of natural gas storage systems should not exceed 80 % of the fracture pressure of the caprock formation in order to minimise the leakage rates. In the absence of local fracture pressure data, a fracture gradient of 18.1 kPa/m is assumed, which leads to the maximum pressure gradient of 14.5 kPa/m (i.e. 80 % of the fracture gradient). Further references with a collection of case studies on critical pressure gradients in the field of reservoir engineering are found in Evans (2008).

The well-established critical state theory (e.g. Wood 1990, Azizi 2000) forms the foundation for the conceptualisation of rock deformation due to gas transport processes. Coupling of hydraulic and mechanical state parameters (gas / water pressure, rock stress, water saturation) is expressed in terms of an effective stress formulation (e.g. Azizi 2000). Furthermore, empirical relationships are introduced to link rock deformation with porosity and permeability. A consequence of this conceptual framework is that a smooth transition is expected between conventional two-phase flow and dilatancy controlled gas flow (cf. Fig. 3-1), when the geomechanical state of the porous medium changes from poro-elastic towards a plastic deformation. Flow and transport processes in a deformable porous medium are still controlled by visco-capillary forces, which can be expressed by a capillary pressure and relative permeability relationship, respectively. Other parameters, however, such as the "intrinsic" permeability and the gas entry pressure are no more seen as invariants but depend on the state of deformation of the porous medium. Extensive experimental efforts are needed to map the corresponding empirical relationships along the relevant stress and saturation paths.

An important feature of the aforementioned elasto-plastic material behaviour of argillaceous materials is their self-sealing capacity (e.g. Nagra 2002a). Permeability enhancement at elevated gas pressures tends not to be permanent; when the gas pressure is reduced the material consolidates and the hydraulic and mechanical properties of the porous medium approach the values which are characteristic for the undisturbed stress state.

### 3.2.4 Gas flow along macroscopic tensile fractures

As a rule of thumb, a macroscopic tensile fracture (hydrofrac / gasfrac) develops when the gas pressure is larger than the sum of the minimum principal stress and the tensile strength of the rock (e.g. Valko & Economides 1997). The macroscopic fracture is initiated quasi-instantaneously and propagates at about the velocity of a shear wave. Gas flow in such a macroscopic tensile fracture can be seen as a single-phase flow process. The propagation comes to a halt when the gas pressure in the fracture becomes less than the value of the minimum principal stress (shut-in pressure). Large-size hydrofracs are characterised by a fracture transmissivity which increases the bulk permeability of the rock by many orders of magnitude. In a rock with low tensile strength, a macroscopic fracture develops only when the gas pressure build-up is rapid, i.e. when the combined effect of porewater displacement and formation of small-scale fractures (i.e. dilatancy) no longer counterbalances the gas production rate. This is not the case in the post closure period of the L/ILW repository, because the initial gas storage capacity of the backfilled underground structures is sufficiently high to damp the pressure build-up during the
early post closure period when the high gas generation rates are expected. In the late times, the
gas generation rates are slowing down significantly and the gas transport capacity of the host
rock and the engineered gas transport path is sufficient to accommodate the generated gas.
Therefore, hydro- and gas-fracs are not expected under the conditions relevant for the L/ILW
repository.

The conceptual, theoretical and experimental framework for fracture propagation is well docu-
mented in standard hydrocarbon exploration literature (e.g. Valko & Economides 1997).

3.2.5 Scale dependence of parameters
For any of the aforementioned mechanisms, gas transport is controlled by the microscopic
structure of the porous medium. Small-scale heterogeneities may have a distinct impact on the
large-scale transport processes. On the other hand, it is practically impossible to resolve the
heterogeneities in sufficient detail, which is required for a precise numerical simulation of the
transport process on the large-scale. Hence, simplified models of the flow processes are needed,
which still capture the impact of the heterogeneities as far as possible (Dagan 1989, Gelhar
1993).

If the length scale of the flow processes is much larger than the scale of the heterogeneities, the
flow may no longer depend on the details of the small-scale properties. It can then be described
as a flow process in an equivalent homogeneous medium, where the properties of the equivalent
medium capture the impact of the heterogeneities in an averaged sense (e.g. Neuweiler et al.
2003). For miscible fluids, such as gas dissolved in porewater (cf. chapter 3.5.1), the scaling-up
of transport processes in heterogeneous media has been the subject of many theoretical
approaches and experimental verification cases (Dagan 1989, Gelhar 1993). A common concept
is based on the introduction of scale-dependent transport parameters. Thus, the up-scaled disper-
sivity of a heterogeneous medium is proportional to the correlation length and the variability of
its permeability distribution (e.g. Gelhar & Axness 1983).

For displacement processes of one fluid by another immiscible fluid (visco-capillary two-phase
flow and pathway dilation, cf. chapters 3.4.2 and 3.4.3), the flow equations become highly non-
linear and coupled (relative permeability, capillary pressure). With respect to transport, the
mixing is in this case not a mixing of solute concentrations as the two fluids remain immiscible.
However, the spreading of the saturation distribution can be considered as a mixing effect,
which may (or may not!) be described by a dispersive flux term in a homogeneous flow
equation (e.g. Neuweiler et al. 2003). The length scales required for homogenisation of the flow
processes can be far more extended than the typical length scales of miscible flow. Homogeni-
sation approaches for multiphase flow problems have been developed in the fields of contami-
nant transport in groundwater (e.g. Neuweiler & Cirpka 2005) and in reservoir engineering
(Noetinger & Zargar 2004). As part of Nagra's RD&D programme, theoretical studies have been
initiated to review recent developments on multiphase transport in heterogeneous media.

3.3 Gas-related properties of host rock and backfill materials

3.3.1 Materials of concern and gas-related parameters
The quantitative assessment of gas accumulation in the emplacement tunnels and gas transport
from the emplacement caverns along the backfilled underground structures and through the
geosphere requires a comprehensive set of material parameters. Gas storage capacity and gas
transport capacity of the composite gas path are controlled by the transport properties of the
materials which form the different segments of the gas path. Chapter 3.3 provides an overview of the materials of concern, the data sources and discusses the relevant parameters for gas storage and transport.

The composite gas path can be subdivided into the following domains:

- **Opalinus Clay** – gas is released through the microscopic pore throats of the intact host rock and, if existent, along the EDZ around the backfilled underground structures.
- **Backfill of the emplacement caverns**, comprising a mixture of different cementitious materials according to Table 2-2.
- **Seal sections** (cf. chapter 2.6.3), consisting of well-compacted sand/bentonite mixtures (80/20 or 70/30) and the ventilation shaft sealed with pure bentonite.
- **Backfill of branch, operation and access tunnels** (sand/bentonite with low compaction).

For each of the aforementioned elements of the gas path, a variety of representative parameters are required as input for numerical simulations:

- porosity and pore structure as characteristic features, governing both the gas storage and the gas transport capacity;
- intrinsic permeability of the material, characterising the transport capacity of the porous medium independent of the fluid;
- capillary pressure, characterising the coupling between gas and water pressure as a function of saturation;
- relative permeability, characterising the mobility of the different phases as a function of saturation;
- critical pressure for the onset of pathway dilation and lithostatic pressure as indicators for coupled geomechanical processes.

Comprehensive laboratory and field studies have been conducted as part of Nagra's site investigation activities and in the context of the RD&D programme to characterise the gas-related properties of the Opalinus Clay. The investigations provide data bases with well-established test protocols and well-defined quality levels regarding the test analyses. Further dedicated in-house initiatives concern the determination of gas-related properties for sand/bentonite mixtures (the GMT experiment at the Grimsel Test Site under the lead of RWMC; e.g. Shimura et al. 2006) and characterising mortar M1 (Jacobs et al. 1994a and b, Mayer et al. 1998) and mortar M2 (Mayer & Wittmann 1996).

### 3.3.2 Opalinus Clay

**Relevant gas transport paths through the host rock**

As schematically shown in Figure 1-1, the potential gas pathways through the host rock include the microscopic pore space of the intact rock matrix, possible discrete tectonic structures (cracks, fractures, faults) as well as excavation-induced fractures in the vicinity of the backfilled underground structures. From the long-term safety point of view, gas release through the microscopic pore space is of particular significance, because this release path can exist also in the case where tectonic faults and the EDZ can be considered as gas impermeable or when they do not exist at all (e.g. removal of EDZ along seal sections in the SF/HLW concept). In the frame-
work of gas-related studies for the Project "Entsorgungsnachweis" (Nagra 2002a, Nagra 2004) comprehensive databases have been compiled to describe the gas release phenomenologically, conceptually and quantitatively. Further studies on the subject of gas transport through Opalinus Clay were initiated as part of the RD&D programme as well as within the L/ILW programme. Important focal points of the actual investigations are the effect of spatial variability on the gas propagation in the surroundings of a repository (scale dependency of the gas-related parameters) and an improved process understanding of the dependency of the transport capacity of Opalinus Clay on the overburden depth (in-situ stress).

The hydraulic properties of discrete tectonic structures were investigated in the Mont Terri URL (e.g. Marschall et al. 2003). Moreover, the packer test O5 (hydrotest sequence, followed by a gas threshold pressure test) in the Benken borehole was performed at a discrete fault (Nagra 2002a). In both places hydraulic testing did not reveal a significant increase of the rock conductivity. It is thus assumed that geologic faults in Opalinus Clay are generally tight. One cannot exclude however, that a reactivation of such structures may occur if the gas pressure exceeds the magnitude of normal stress acting on the fault plane. For high pressures it is thus possible that preferential gas pathways will form along tectonic structures and a continuous gas transport path through the geosphere will persist until the gas pressure drops below the closure pressure of the tectonic structure. Such structures, however, do not significantly affect long-term radiological safety because gas flow along discrete features is not associated with significant porewater displacement. Furthermore, the discrete structures will close as soon as the gas pressure drops below the magnitude of the normal stress and the flow path will self-seal. The self-sealing capacity of reactivated fractures subsequent to a gas injection sequence was demonstrated in various experiments at the Mont Terri site (e.g. Marschall et al. 2003).

The excavation-disturbed zone (EDZ) around the backfilled underground structures serves a dual function with respect to gas release. As a result of the increased porosity compared to the intact rock the EDZ provides additional storage capacity. In addition, the (self-sealed) fracture network within the EDZ serves as a potential gas pathway through which gas generated in the emplacement caverns can be transported to the backfilled branch, operation and access tunnels. It is expected that following the backfilling and re-saturation of the underground excavations, the EDZ will be reduced either partially or fully, due to the prevailing rock stress ("consolidation"); thus its role as a preferential gas pathway is associated with some uncertainty. Nevertheless, it is obvious that in the case of high gas pressures even a fully reconsolidated EDZ can provide a preferential pathway due to reactivation of the fractures (pathway dilation). Simple process models for pathway dilation within the EDZ are being developed in the framework of the current RD&D programme (see chapter 3.4).

Basic geological characteristics of the Opalinus Clay formation

The Opalinus Clay was identified as the priority sedimentary host rock option for the disposal of spent fuel, vitrified high-level and long-lived intermediate level waste in Switzerland (Nagra 2008c). Site specific investigations were conducted previously for a potential siting area in the Zürcher Weinland (Nagra 2002a). For a L/ILW repository in Northern Switzerland a large portion of the geoscientific basis from the SF/HLW can also be utilised. Site specific differences with respect to the host rock properties (e.g. slightly increased hydraulic conductivity) and the hydromechanical state of the system (e.g. lower magnitude of minimum principal stress) are associated with the lower overburden of a L/ILW repository.

The detailed characterisation of the host rock and the potential siting area in the Zürcher Weinland started in 1994. The key elements of this site investigation programme were 2-D regional seismics, a 3-D seismic campaign in the Zürcher Weinland covering an area of around 50 km².
(Birkhäuser et al. 2001), an exploratory borehole at Benken (Nagra 2001a), experiments as part of the international research programme in the Mont Terri URL (Thury & Bossart 1999), comparative regional studies on Opalinus Clay including analyses of data from deep boreholes in the region (Nagra 2002a), and comparisons with clay formations that are under investigation in other countries in connection with geological disposal (Mazurek et al. 2008). A brief summary of the basic geological characteristics of the formation is given below:

- The Opalinus Clay is part of a thick Mesozoic – Tertiary sedimentary sequence in the Molasse Basin of Northern Switzerland. It was deposited about 180 Ma ago in a shallow marine environment. Geological investigations on the regional and local scale confirmed the remarkable homogeneity of the formation. In the Zürcher Weinland the Mesozoic sediments reveal uniform thickness over a distance of several tens of kilometres, dipping gently to the south-east, and are hardly affected by faulting.

- The Opalinus Clay is a moderately over-consolidated claystone that has been formed by a complex burial and compaction history with two distinct periods of subsidence. In the region of the Zürcher Weinland, the formation reached a burial depth of about 1'000 m during the Cretaceous. A period of uplift of the area in the mid-Tertiary was followed by subsidence in the late Tertiary, when the Opalinus Clay reached its greatest burial depth of about 1'700 m below the surface. From about 10 Ma ago, alpine uplift and erosion brought the Opalinus Clay progressively up to its present burial depth of about 600 – 700 m in the Zürcher Weinland and 300 – 400 m in the Bözberg region. At Mont Terri, the Opalinus Clay reached a maximum depth of about 1'000 m and the present burial depth is about 200 – 300 m.

- On a regional scale, the mineralogical composition of the Opalinus Clay exhibits moderate lateral variability and a slight increase in clay content with depth. Quantitative laboratory analyses of core samples from Benken and Mont Terri provide a total mass fraction of clay minerals of 54 – 66 %, a quartz content of 14 – 20 % and 13 – 16 % calcite. The fraction of swelling clay minerals, with 11 – 14 % illite/smectite mixed layers, is of particular interest for the gas-related studies. Further minerals are siderite, pyrite and feldspar. The mass fraction of organic carbon is < 1 %.

- Field investigations and laboratory experiments suggest a hydraulic conductivity of the Opalinus Clay in the order of $10^{-13}$ to $10^{-14}$ m/s and a moderate anisotropy ratio < 10. Porosity depends on clay content and burial depth; average values of 12 % and 16 % are reported for the Benken site and the Mont Terri URL, respectively. Figure 3-2 depicts a compilation of porosity measurements from various locations in Northern Switzerland as a function of the burial depth; a clear decrease of porosity with depth is observed.
Fig. 3-2: Porosity values of Opalinus Clay in different locations in Northern Switzerland as a function of overburden (after Nagra 2002a).

The porosity values were determined from various methods (Benken and Mont Terri: water-loss porosity; Schafisheim and Weiach: Pycnometer; Herdern-1, Berlingen-1 and Kreuzlingen-1: Porosity from saturation with isopropanol).

Gas-related characteristics of the Opalinus Clay

Gas transport in low-permeability formations is largely controlled by the microstructure of the rock. A balanced assessment of gas transport processes in the Opalinus Clay therefore requires careful consideration of both structure and texture. Figure 3-3 illustrates the mineralogical and structural features of the Opalinus Clay in the Zürcher Weinland on various scales. Petrophysical logs in the Benken borehole indicate moderate variability and a slight increase of clay content with depth, suggesting a division of the Opalinus Clay into 5 lithostratigraphic sub-units (facies). Core inspection reveals a distinct anisotropy, made up of siderite concretions and silt and sandstone lenses, which are embedded in the clay-rich strata. The anisotropy due to bedding is largely a result of microscopic heterogeneity as seen in the thin sections, where diagenetic cementation of the pore space has been observed in the silty and sandy layers. Scanning electron microscope (SEM) images reveal that the size of the mineralogical components (10^{-7} – 10^{-3} m) determines the microstructure of the rock. Quartz minerals may exhibit grain sizes in the range 0.01 – 1 mm, whereas the clay minerals form flake-like packages with typical sizes in the order of 100 nm – 10 μm. The pore space of the rock is formed by a network of micro/meso- and macropores, which is too small (in the order 1 – 100 nm) to be shown by conventional SEM methods. This network of pores actually dominates the flow and transport properties of the rock.
Complementary methods were used to characterise the pore space of the Opalinus Clay, such as the measurement of the adsorption / desorption isotherms and mercury porosimetry (Nagra 2002a). To obtain nitrogen and water isotherms, the powder samples were dried at temperatures of at least 120°C and degassed under vacuum. Nitrogen isotherms were measured at 77 K, water isotherms at 303 K by gravimetry in quasi-equilibrium mode, where water vapour was introduced at a constant, low flow rate. The pore size distributions were obtained by incremental saturation of the sample. Table 3-2 depicts the volume fractions of the different pore classes (definition according to IUPAC 1997), indicating that the majority of pores can be classified as mesopores (1 – 25 nm). The inferred macropore fraction in the order of 20 – 30% represents the pore space which is relevant for gas transport, because these pores are accessible to gases at moderate gas pressures (cf. Young-Laplace's Eq. 3-6).
Tab. 3-2: Volume fractions of the different pore classes, determined by adsorption and desorption isotherms (H$_2$O, N$_2$) after Nagra (2002a).

Complementary experimental evidence suggests that at least 20% of the total porewater can be attributed to the interlayer water.

<table>
<thead>
<tr>
<th>Equivalent radius [nm]</th>
<th>Micropores &lt; 1</th>
<th>Mesopores 1 – 25</th>
<th>Macropores &gt; 25</th>
</tr>
</thead>
<tbody>
<tr>
<td>Assumption: fraction of micropores is 20% (interlayers)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N$_2$-Isotherm</td>
<td>20</td>
<td>46 – 56</td>
<td>24 – 34</td>
</tr>
<tr>
<td>H$_2$O-Isotherm</td>
<td>20</td>
<td>54 – 63</td>
<td>17 – 26</td>
</tr>
</tbody>
</table>

For mercury porosimetry, Hg was injected at increasing pressures into crushed, dried and degassed samples. In the context of the Project "Entsorgungsnachweis" (Nagra 2002a) the maximum injection pressure was 200 MPa, and thus only pores with a radius larger than 3.7 nm could be detected. As part of Nagra's collaboration with the oil & gas industry, new mercury intrusion experiments were conducted in 2004 by the geotechnical laboratories of Chevron (Philip Mariotti, Houston/Texas) using higher injection pressures up to 420 MPa. Two core samples from Benken and Mont Terri were tested – the equivalent pore size distributions are shown in Figure 3-4. The general distributions are consistent with the results of the adsorption/desorption measurements, indicating that majority of pores in the Opalinus Clay can be classified as mesopores. The more detailed comparison of the cores from Benken and Mont Terri reveals that the pore size distributions of the core samples from Benken are shifted towards the lower pore radii. This is a clear indication for the higher degree compaction of the samples from Benken, corresponding to the higher burial depth.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Porosity (%)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>9.9</td>
<td>10.8</td>
<td>8.5</td>
<td>7.6%</td>
</tr>
<tr>
<td>Bulk density (Mg/m$^3$)</td>
<td>2.45</td>
<td>2.43</td>
<td>2.52</td>
<td>2.48</td>
</tr>
<tr>
<td>Grain density (Mg/m$^3$)</td>
<td>2.72</td>
<td>2.73</td>
<td>2.75</td>
<td>2.66</td>
</tr>
</tbody>
</table>

Fig. 3-4: Equivalent pore size distributions of drillcore samples from Benken (sampling depth 614.82 m below ground) and Mont Terri (shaly facies), determined by mercury intrusion methods at Chevron's laboratories in Houston (by courtesy of Philip Mariotti).
Water retention functions describe the capacity of a porous medium to retain water at a given suction head. Thus, the water retention function is in principle identical to the water adsorption isotherm. The main differences are the experimental procedure and the preparation of the samples. Water retention curves of the Opalinus Clay were determined at the geotechnical laboratories of UPC (Universitat Politècnica de Catalunya, Barcelona / Spain), by stepwise desaturation and resaturation of core samples under controlled humidity (Nagra 2002a, Muñoz et al. 2003). More recently, a comprehensive experimental programme was accomplished by GRS (Braunschweig), aimed at comparing the capillary pressure – saturation relationships of different clay formations. Figure 3-5 depicts a compilation of water retention curves of Opalinus Clay samples from Mont Terri, determined in the GRS laboratories (Zhang & Rothfuchs 2007) and by UPC (Muñoz et al. 2003). Characteristic features of the Opalinus Clay are the high capillary pressures in the order of 10 MPa even at high water saturation > 90 % and the marked hysteresis between wetting and drying path.

![Capillary pressure measurements](image)

The experiments were conducted by GRS (Zhang & Rothfuchs 2007) and UPC (Muñoz et al. 2003) as part of the EU-funded VE project.

The mobility of the gas in the intact Opalinus Clay (expressed in terms of a relative permeability relationship) can be determined by water and gas permeameter experiments in the laboratory and by in-situ gas injection tests in boreholes. An experimental data base for the derivation of relative permeabilities of the intact Opalinus Clay was elaborated in the context of the Project "Entsorgungsnachweis". The key references of the corresponding experiments are given in Nagra (2002a) and in Marschall et al. (2005). Further experiments and data analyses have been conducted since then as part of the Mont Terri Project (Croisé et al. 2006) and in the context of the EU-funded integrated project NF-PRO (http://www.nf-pro.org/).


Reference parameters

The key parameters required for the simulation of gas transport processes in the undisturbed rock zone around a L/ILW repository are:

- porosity of the intact host rock
- intrinsic permeability
- capillary pressure-saturation relationship
- relative permeability-saturation relationship

According to the layout described in chapter 2, the emplacement caverns of the L/ILW repository in the Bözberg siting area are located approx. 300 – 400 m below surface. This depth corresponds approximately to the overburden of the Mont Terri URL (250 – 300 m below surface). It is thus reasonable to consider the geotechnical parameters of the Opalinus Clay determined for the Mont Terri URL to derive the reference parameters. As alternative values, those corresponding to the reference values from the geodataset for the SF/HLW repository in the Zürcher Weinland will be used (Nagra 2002a). Table 3-3 summarises the reference values for a L/ILW repository in the Bözberg region. The parametric models used for the capillary-saturation relationship and the relative permeability of the intact Opalinus Clay are shown in Figure 3-6 (reference values according to Tab. 3-3).

For the quantitative treatment of the gas release in a L/ILW repository, the EDZ plays a subordinate role, because practically all backfilled underground structures (caverns, cavern connections, access tunnel, plugs and seals) have a hydraulic conductivity which is higher than the one expected for the EDZ. The EDZ is modelled in the two-phase flow models as a zone with a thickness of 1 m around the underground structures with the properties documented in Table 3-3. The gas-related properties of the EDZ shown in Table 3-3 have been derived from the hydromechanical considerations in the framework of Project "Entsorgungsnachweis" (Nagra 2002a).
Tab. 3-3: Values for the gas-related parameters of the undisturbed Opalinus Clay for a L/ILW repository in Northern Switzerland and corresponding parameters for the EDZ (RV – reference value; AV – alternative value).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>RV</th>
<th>AV</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Undisturbed host rock</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
| Intrinsic permeability normal to bedding       | $1 \times 10^{-20}$ | $2 \times 10^{-21}$ | RV: corresponds to the reference value for hydraulic conductivity at Mont Terri  
AV: corresponds to the reference value for hydraulic conductivity in the Zürcher Weinland |
| $k_\parallel [m^2]$                           | 5             | -             | RV: according to Nagra (2002a)                                           |
| Capillary pressure – saturation relationship   | Parametric model according to van Genuchten (Eq. 3-7) with coefficient $n = 1.67$ |
| Capillary strength $1/\alpha [MPa]$            | 18            | 5             | RV: derived from capillary pressure measurements (drying path)          |
| Relative permeability – saturation relationship| Parametric model according to van Genuchten/Mualem (Eqs. 3-8 & 3-9) with the following coefficients, $\varepsilon = 0.5$ and $\gamma = 0.5$ |
| Residual water saturation $S_{wr} [-]$         | 0.5           | -             | RV: according to the results of adsorption / desorption measurements, suggesting that 50 % of the total pore space can be classified as micro- and mesopores  
AV: - |
| Residual gas saturation $S_{gr} [-]$           | 0.003         | 0.0           | RV: the residual gas saturation determines the effective gas entry value. Effective gas entry values were determined by gas permeability testing at Mont Terri and Benken (cf. Marschall et al. 2005)  
AV: effective gas entry pressure of the rock is infinitesimal |
| Water loss porosity [%]                        | 12 %          | 16 %          | RV: corresponds to the reference value for the porosity of the Zürcher Weinland. At Mont Terri, the sandy facies exhibits typical porosity values of about 12 %  
AV: Porosity of the shaly facies at Mont Terri: 16 % |
| Lower bound of fracture pressure [MPa]         | 8.125         | -             | RV: lithostatic pressure at repository level $(\rho_{rock} = 2.5 \text{ Mg/m}^3, \text{ overburden } z = 325 \text{ m bg})$  
AV: - |
Tab. 3-3: (continued)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>RV</th>
<th>AV</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Undisturbed host rock</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
| Threshold pressure for pathway dilation [MPa]  | 6.5    | -   | RV: the onset of pathway dilation is assumed at about 80% of the lithostatic pressure  
AV: -                                                        |
| **Excavation Damage Zone (EDZ)**               |        |     |                                                                         |
| Intrinsic permeability $k$ [m$^2$]             | $1 \times 10^{-19}$ |     | RV: corresponds to an increase of hydraulic conductivity by a factor of 10 with regard to $k_{\perp}$ of the undisturbed Opalinus Clay (thickness of EDZ: 1 m)  
AV: no EDZ                                                  |
| Capillary pressure – saturation relationship   |        |     |                                                                         |
| Capillary strength $1/\alpha$ [MPa]           | 2      |     | RV: reduced capillary strength accounts for secondary porosity (EDZ fractures)  
AV: no EDZ                                                  |
| Relative permeability – saturation relationship|        |     |                                                                         |
| Residual water saturation $S_{wr}$ [-]         | 0.25   |     | RV: attributes to the increase of porosity of the EDZ  
AV: no EDZ                                                  |
| Residual gas saturation $S_{gr}$ [-]           | 0.0    |     | RV: accounts for EDZ fractures  
AV: no EDZ                                                  |
| Water loss porosity [%]                        | 14 %   |     | RV: geomechanical models suggest that a full reconsolidation of the EDZ may not be achieved  
AV: no EDZ                                                  |
| Relationship between intrinsic permeability and hydraulic conductivity: |        |     |                                                                         |
| $k \left[ m^2 \right] = \frac{\eta_w}{\rho_w \cdot g} \cdot K \approx 1 \times 10^{-7} \cdot K \left[ m/s \right]$ |        |     |                                                                         |
| $\eta_w$: dynamic viscosity of water, [Pa·s]   |        |     |                                                                         |
| $\rho_w$: density of water, [kg m$^{-3}$]      |        |     |                                                                         |
| $g$: gravitational acceleration, [m s$^{-2}$]   |        |     |                                                                         |
Fig. 3-6: Parametric models of capillary pressure and relative permeability $k_r$ for water (w) and gas (g), representative for the undisturbed Opalinus Clay formation in the Northern Aargau (reference parameter values RV and alternative values AV).
3.3.3 Cementitious backfill of the emplacement caverns

Representation of the backfilled emplacement caverns

The basic design of the emplacement caverns of the L/ILW repository is described in detail in chapter 2.3. For construction and backfilling of the caverns different cementitious materials are used, each of them fulfilling a number of specific functional requirements:

- Construction concrete (lining, technical installations, etc.) and shotcrete are used to provide static stability.
- The waste drums are filled with concrete for fixing and immobilising the raw waste. The waste drums are placed in prefabricated reinforced concrete containers and the void spaces within the containers are backfilled with cementitious mortar M2.
- The mortars (M1 and M2) used to fill the gaps between waste containers and the cavern wall are specially designed to provide high gas storage capacity and high gas permeability, while still withstanding high stresses due to convergence of the caverns after repository closure.

For the purpose of the gas transport simulations on the scale of the repository near-field (chapter 4), a highly resolved representation of all cement-based materials (e.g. waste containers, backfill, liners, etc.) in the emplacement caverns is not necessary. Instead, the modelling efforts can be reduced significantly by an appropriate averaging of the material properties of the backfill. In the subsequent chapters, a traceable approach will be presented to derive homogenised gas transport properties of the backfilled emplacement tunnels.

With respect to their geotechnical properties the materials can be categorised in four different groups (Tab. 3-4). The mortars M1 and M2 correspond to approx. 36% of the total volume to be backfilled. They are characterised by a high gas accessible porosity and a high permeability. Both mortars have been developed and characterised in the framework of earlier RD&D programmes of Nagra (e.g. Jacobs et al. 1994a and b, Mayer et al. 1998; see also Appendix A). The volumetric proportion of shotcrete, construction concrete and special concrete is approx. 28%. Those of the shotcrete essentially determine the transport properties of this material group. Gas accessible porosities and permeabilities of this material group are in general lower than those of the backfill mortar and they vary strongly, corresponding to the construction requirements (Jacobs 1998; Appendix A). For example, shotcrete is normally relatively porous with a moderate permeability in the order of $1 \times 10^{-17} \text{ m}^2$. In contrast, special concretes with enhanced requirements for their geomechanical properties exhibit a low gas accessible porosity (a smaller proportion of connected pores) and a very low permeability (typically: $1 \times 10^{-19} \text{ m}^2$). The third material group consists of the waste package concrete. The porosity and permeability of this concrete are extremely low compared to the special concrete for construction purposes. It should be noted however, that in the waste conditioning process, the drums are normally not completely filled, so that the effective pore volume available for gas storage in this material group is substantially larger (Schwyn et al. 2003). The last material group, with a volumetric proportion of approx. 36% consists of the conditioned waste itself. The complexity of the radioactive waste (see chapter 2.7) cannot be considered explicitly in the calculations performed here; it is rather assumed that the waste exhibits no porosity and is impermeable.

The data base for gas-related properties of cementitious materials has been compiled through a comprehensive literature survey. For the backfill mortars M1 and M2 Nagra's own research work was available with properly documented measurement protocols. Knowledge of the material group of construction concretes is based, however, on literature studies; information
concerning the test set-up, test protocol and measurements are not in many cases directly accessible. For the conditioned waste material it is assumed that the two-phase flow characteristics are similar to high performance cement with low permeabilities and porosities (Schwyn et al. 2003). The major results from the literature study are summarised in Appendix A.

Tab. 3-4: Categories of cementitious materials applied for the backfill of the emplacement caverns and typical parameter values for the gas-related properties.

The references of the data sources are given in Appendix A.

<table>
<thead>
<tr>
<th>Material group</th>
<th>Volume fraction [%]</th>
<th>Porosity [%]</th>
<th>Permeability $^{1)}$ [m$^2$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mortar M1 &amp; M2</td>
<td>36</td>
<td>≈ 30 (M1)</td>
<td>≈ 10$^{-10}$ (M1)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>≈ 35 (M2)</td>
<td>≈ 10$^{-14}$ (M2)</td>
</tr>
<tr>
<td>Shotcrete</td>
<td></td>
<td>≈ 25</td>
<td>≈ 10$^{-17}$</td>
</tr>
<tr>
<td>Normal building concrete</td>
<td>28</td>
<td>≈ 20</td>
<td>≈ 10$^{-18}$</td>
</tr>
<tr>
<td>High performance concrete</td>
<td></td>
<td>15</td>
<td>≈ 10$^{-19}$</td>
</tr>
<tr>
<td>Waste fixation concrete</td>
<td>36</td>
<td>20*</td>
<td>≈ 10$^{-19}$</td>
</tr>
</tbody>
</table>

* Note: the effective pore volume of the backfilled waste drums is significantly higher because the waste drums are not filled up completely
$^{1)}$ Permeability tests performed with water

Reference parameters

For the averaging of the gas-related properties of cavern backfills, a series of simplifying assumptions was made as discussed below.

The maximum possible gas storage volume is simply the sum of all available pore space. Therefore, the effective porosity of the homogenised backfill is determined by weighting the individual porosities of the three material groups (Tab. 3-4) with the corresponding volume fractions $\nu_i$:

$$\Phi_{eff} = \sum_{i=1}^{3} \nu_i \cdot \phi_i = 0.25$$  \hspace{1cm} (Eq. 3-11)

The derivation of the effective intrinsic permeability of the cavern backfill is – due to its tensorial nature – significantly more difficult. Thus, for the estimation of the effective permeability one needs not only the volumetric proportion of the different materials but also their spatial arrangement. In the gas release calculations described in chapter 4, as a simplifying assumption only the axial component of the permeability tensor is considered. Here it is, in particular, the connectivity of the high-permeable backfill mortars determining the axial fluid and gas transport capacity of the cavern backfill. As shown in chapter 2.3, in the cavern ceiling it is foreseen to backfill throughout with mortars M1 and M2 (Fig. 2-6), whereas the lower part of the caverns contains regularly placed (separation of approx. 30 m) concrete walls (Fig. 2-7).
Due to buoyancy effects, the gas will accumulate along the ceiling of the caverns while the transport of dissolved radionuclides in the lower part of the cavern can be affected by these concrete walls. In the numerical modelling these design aspects have not been considered. Instead a homogeneous and isotropic intrinsic permeability of $10^{-15}$ m$^2$ was assigned to the whole cavern backfill. With this relatively low and thus conservative permeability value, one takes into consideration possible long-term permeability changes in the cavern backfills through for example, interactions between waste and cement (cf. chapter 3.4.2).

The estimation of the effective capillary pressure – saturation curve for the cavern backfill can be derived formally through a volume-weighted superposition of the pore size distribution (PSD) of the individual material groups:

$$PSD_{eff}(r) = \sum_{i=1}^{3} \nu_i \cdot PSD_i(r)$$

(Eq. 3-12)

The capillary pressure – saturation relationship is given from the pore size distribution and the relation between the incremental capillary pressure change and the corresponding saturation change with the help of Young-Laplace's formula (Eq. 3-6):

$$\frac{\partial P_c}{\partial S} = \frac{1}{PSD_{eff}(r)} \cdot \frac{2 \cdot \sigma \cdot \cos \alpha}{r^2}$$

(Eq. 3-13)

A simplified approach was chosen for the studies here considering the relatively large uncertainties with respect to the pore size distribution of individual backfill materials (shotcrete, construction concrete, waste). In this approach, the parameter values for the van Genuchten model, as shown in Table 3-5, are determined from the interpretation of documented experiments. An average grain size distribution and the resulting reference parameters of the capillary-saturation relationship was then derived from the calculated pore size distributions of the different materials, according to Young-Lapace's equation (Eq. 3-6), and their volumetric proportion (see Appendix A).

The relative permeability of the cavern backfill has a subordinate role in the numerical calculations, because the intrinsic permeability of the backfill material is orders of magnitude higher than the permeability of the host rock and the cavern plug. For the numerical modelling a parametric model according to van Genuchten/Mualem was used with the reference values as shown in Table 3-5.

Of great significance for the gas pressure build-up is the initial water saturation $S_{wi}$ of cavern backfill, after the cavern is sealed, because this will determine the available gas storage volume in the early phase of gas generation. It can be assumed that the individual backfill materials will not be fully saturated during the emplacement process. For example, the shotcrete and the construction concrete will be dried out during the construction phase as a result of the ventilation of the underground constructions over a long period of time. In addition, during the emplacement of the mortars M1 and M2 only a limited amount of water will be used. Finally, as mentioned above, in the waste packages themselves one should expect the existence of air-filled pore volume. A reference value of 0.5 is assumed for the initial water saturation in the numerical modelling (Tab. 3-5). Because of the great significance of this parameter for the development of the gas build-up an alternative value of 0.7 is also considered.
Tab. 3-5: Reference values RV and alternative values AV for the gas-related parameters of the cementitious backfill material.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>RV</th>
<th>AV</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cavern Backfill</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
| Effective intrinsic permeability k [m²] | $1 \times 10^{-15}$ | $1 \times 10^{-14}$ to $1 \times 10^{-17}$ | RV: effective k value assumed isotropic as explained in the text  
                              AV: - |
| Capillary pressure – saturation relationship | | | Parametric model according to van Genuchten (Eq. 3-6) with coefficient $n = 2.5$ |
| Capillary strength $1/\alpha$ [Pa] | $4 \times 10^3$ | $5 \times 10^2$ | RV: the apparent gas entry pressure is dominated by the high-porosity mortars (see Appendix A)  
                              AV: apparent gas entry pressure of Mortar M1 |
| Relative permeability – saturation relationship | | | Parametric model according to van Genuchten/ Mualem (Eqs. 3-7 & 3.8) with coefficients \( \varepsilon = 0.5 \) und \( \gamma = 0.5 \) |
| Residual water saturation $S_{wr}$ [-] | 0.30 | - | RV: it is assumed, that 30 % of the porosity is not accessible to the gas phase (non-connected pores and micro/mesopores); see Appendix A  
                              AV: - |
| Residual gas saturation $S_{gr}$ [-] | 0.0 | - | RV: The existing references do not indicate any residual gas saturation (see Appendix A)  
                              AV: - |
| Effective porosity [%] | 24 % | - | RV: corresponds to the volume weighted average porosity of the 3 material groups (as explained in the text)  
                              AV: - |
| Initial water saturation $S_{wi}$ [-] | 0.50 | 0.70 | RV: it is assumed, that the concretes are not fully water saturated at the time of repository closure (as explained in the text)  
                              AV: more robust assumption |

Relationship between intrinsic permeability and hydraulic conductivity: cf. Table 3-3
3.3.4 Bentonite-based materials for seals and tunnel backfill

Gas transport processes in bentonite-based buffer materials

Materials containing bentonite are considered for seals due to their favourable retention properties. They are characterised by a very low hydraulic conductivity and they possess excellent sorption properties.

Pure bentonites have a large swelling capacity and an extremely low permeability for water and gas. For certain repository system components, a certain gas permeability is, however, desirable to enable the transport of gas from the emplacement caverns at moderate gas overpressures. In such cases, sand/bentonite mixtures with relatively low bentonite content are suitable, because they have a low hydraulic conductivity and at the same time significant gas permeability. In addition, through the application of appropriate techniques for their emplacement (compaction), their gas transport properties can be modified to correspond to the safety-relevant design requirements (see also chapter 2.5.1). For these reasons comprehensive research studies have been conducted in the past decades to characterise gas transport in sand/bentonite mixtures (e.g. JAEA 1999, Tashiro et al. 1998, Graham et al. 1997; see also Appendix A). In particular, a better understanding has been developed for the microstructure of such mixtures and the importance of this microstructure for gas transport behaviour has been investigated. It has been shown that sand/bentonite mixtures with a moderate bentonite content of 20 – 30 % are characterised by a multi-modal pore size distribution (Olsön 1969, Collins & McGown 1974, Alonso et al. 1987, Gens & Alonso 1992, Hoffmann et al. 2007). The form of the pore size distribution depends on a variety of factors, for example the degree of compaction and the water content of the sand/bentonite mixture (Fig. 3-7). This also explains the ability to design these materials in order to exhibit desired properties, as described in chapter 2.5.1.

As part of the GMT experiment, investigations of sand/bentonite mixtures 80/20 (Kunigel) were performed to derive the dependency of the pore size distribution on the (i) emplacement density and (ii) the degree of saturation (Romero & Castellanos 2004). Figure 3-7a shows that with increasing mixture density the macro-porosity and hence, the pore space available for water flow and solute transport decreases significantly. If the material is saturated with water, the bentonite swells and fills the pore space of the sand matrix, thus resulting in a very pronounced decrease in the macropores as shown in Figure 3-7b and c.

Pure bentonite also exhibits a multi-modal distribution (Hoffmann et al. 2007). This is particularly true if it is present in a granular form and is subsequently compacted. During saturation of compacted bentonites, the macro-porosity and a part of the inter-aggregate porosity is strongly or slightly reduced depending on the saturation history. Important influencing factors are the duration of the saturation and the stress path to which the material is subjected during saturation. A minimisation of the macro and inter-aggregate porosity is expected when the granular bentonite saturates to its maximum swelling capacity (bentonite slurry) through the unlimited supply of water and subsequently is compacted to the desired emplacement density. A bentonite sample treated with the previously described procedure can be considered as a bounding case for a saturation history on a geological scale and leads to minimum gas permeability.

For a L/ILW repository the gas permeability of pure bentonite is not important because gas transport occurs mainly through the sand/bentonite seals of the branch, operation and access tunnels (Fig. 2-13), while the ventilation shaft which is sealed with compacted bentonite is considered as gas tight. Thus, the gas-related properties of compacted bentonite are not been further discussed in the framework of this study.
Fig. 3-7: Evolution of microstructure during wetting at nearly constant volume (after Nagra 2007b).

a) Pore size distribution of sand/bentonite mixtures (80/20) with various densities

b) Pore size distribution of a sand/bentonite mixture (80/20) with different degrees of saturation

c) Environmental Scanning Electron Microscope (ESEM) images of sand/bentonite mixtures with different degrees of saturation.
Reference parameters

The reference concept described in chapter 2.6, which includes the engineered gas transport system (EGTS), foresees sand/bentonite mixtures with relatively low bentonite content (20 – 30 wt%) as backfill and sealing materials of the branch, operation and access tunnels and the seals and plugs (V4 and V5). Special emplacement procedures are adopted to meet the design specifications (chapter 2.5.1).

For the two seals V1 (shaft seal) and V2 (rock laboratory), it is foreseen to use pure compacted bentonite as sealing material. Pure bentonite has a very low gas permeability, and thus, the sealing systems V1 and V2 will not contribute to the engineered gas transport system.

Reference parameters for the gas-related parameters of the bentonite-based backfill materials are presented in Table 3-6. Further geotechnical information is compiled and discussed in Appendix A and B.

Tab. 3-6: Reference values for the gas-related parameters of the bentonite based backfill materials for seals and tunnel backfill.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>RV</th>
<th>AV</th>
<th>Remarks</th>
</tr>
</thead>
</table>
| Intrinsic permeability of repository seal V4 k [m²] | $1 \times 10^{-18}$ to $1 \times 10^{-19}$ | RV: optimised k-value for a L/ILW repository in the Opalinus Clay, ensuring the release of repository gases and, at the same time, efficient radionuclide retention  
AV: alternative values tested to cope with unexpected site conditions (e.g. very low host rock permeability) |
| Intrinsic permeability of cavern plug V5 k [m²] | $1 \times 10^{-17}$ to $1 \times 10^{-19}$ | RV: optimised k-value for a L/ILW repository in the Opalinus Clay; the corresponding permeability could be realised with moderately compacted sand/bentonite mixtures with mixing ratio 80/20  
AV: alternative values tested to cope with unexpected site conditions (e.g. very low host rock permeability) |
| Capillary pressure – saturation relationship of repository seal V4 and cavern seal V5 | | Parametric model according to van Genuchten (Eq. 3-7) with coefficient $n = 2.5$ |
| Capillary strength $1/\alpha$ [Pa] | 4'000       | 100'000     | RV: value based on comprehensive experimental data bases from the GMT experiment at the GTS  
AV: value fitted to results from laboratory experiment on highly compressed sand/bentonite specimen |
Tab. 3-6: (continued)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>RV</th>
<th>AV</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Relative permeability – saturation relationship of repository seal V4 and</td>
<td>0.0</td>
<td>-</td>
<td>RV: value based on comprehensive experimental data bases from the GMT experiment / GTS</td>
</tr>
<tr>
<td>cavern plug V5</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Residual gas saturation $S_{gr}$ [-]</td>
<td>0.0</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Residual water saturation $S_{wr}$ [-]</td>
<td>0.3</td>
<td>-</td>
<td>AV: -</td>
</tr>
<tr>
<td>Water loss porosity [%]</td>
<td>30</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Initial water saturation $S_{wi}$ of cavern plug V5 [-]</td>
<td>0.7</td>
<td>-</td>
<td>RV: optimum compaction of sand/bentonite mixtures 80/20 is achieved for saturations</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>between 0.5 and 0.7</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>AV: -</td>
</tr>
<tr>
<td>Initial water saturation $S_{wi}$ of repository seal V4 [-]</td>
<td>0.95</td>
<td>-</td>
<td>RV: the value accounts for possible resaturation of the repository plug in the early</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>post-closure period</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>AV: -</td>
</tr>
</tbody>
</table>

Relationship between intrinsic permeability and hydraulic conductivity according to Table 3-3
3.4 Impact of coupled phenomena on gas transport

3.4.1 Relevance of coupled processes

The current process and system understanding of gas release suggests that after closure of the L/ILW repository no safety-relevant gas pressures will be developed in the emplacement caverns (see also chapter 4). Deviations from the expected system behaviour could, however, result from the coupled hydromechanical and hydrochemical processes. These include:

- Hydrochemical interactions that can in principle in the long-term reduce the gas permeability of the seals and of the host rock. Such self-sealing processes might lead to an increase of the gas pressures in the emplacement caverns.
Hydromechanical processes along the cavern plugs, which can increase the gas permeability of the rock in the vicinity of the backfilled caverns ("pathway dilation") if the gas pressures exceed a threshold value and hence, these processes ensure that no critical gas pressures will occur.

These processes are described on a phenomenological level in the following chapters and the current state-of-knowledge is presented.

### 3.4.2 Hydrochemical interactions – problem statement

The engineered gas release system presented in chapter 2.6 enables an efficient release of the gas produced in the emplacement caverns along the backfilled underground structures. In order to ensure an effective functioning of this system over the relevant time frame, it has to be ensured that gas release will not be blocked as a result of hydrochemical self-sealing processes. This involves both the gas release through the host rock and the gas release along the repository structures (e.g. engineered gas transport system) which both can in principle be sealed due to interactions of the cement porewater with the Opalinus Clay or the sealing material.

Chemical reactions considered in the cavern near-field

The cavern near-field is the zone which includes the backfilled emplacement caverns and a limited rock zone around the caverns. Most of the relevant hydrochemical processes are restricted to this zone. The following reactions are considered in more detail:

- Reactions of the cement water with the clay minerals of the host rock or of the bentonite in the cavern plugs, tunnel seal and backfill.
- Cement maturation and interaction of the cement with porewater from the host rock ("sulphate attack").
- Interactions between waste and cement (metal corrosion, degradation of organics, sulphate attack).
- Chemical processes in the cavern near-field during the construction and operational phase (calcite precipitation, salt deposition, pyrite oxidation).

Reaction of cement porewater with clay

Porewater from the host rock infiltrating the backfilled caverns, access, branching and operation tunnels during repository resaturation (chapter 4.4) will interact with the cement, which is not stable and will (partially) degrade. Also the cement porewater, which has a high pH value, will diffuse into the sand/bentonite mixture of the cavern plug / tunnel backfill and will lead to a partial conversion of the clay minerals. The mineral transformation will lead to a reduction of the porosity, because typically the secondary minerals have a lower density than the original minerals. In addition, the coupling of the chemical processes with transport will lead to a heterogeneous distribution of the porosity, because the location of the dissolution of the primary minerals is not necessarily identical to the location of the precipitation of the secondary minerals. For this to occur, the pore space has to be at least partially saturated because these chemical processes and the transport are associated with porewater. The affected space around the interfaces is most likely in the cm range and depends on the transport velocity and reaction speed.

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7 In Nagra (2008d), the relevant time frame for the L/ILW repository is set at $10^5$ years.
The formation of a "skin" at the interface can constrict the gas flow. The clogging of bottlenecks in the connected porosity may have a distinct effect even if the total pore space is not significantly affected.

With mass balance calculations one can show that in an extreme case, in which the minerals in the cement dissolve, the bentonite completely reacts and all secondary minerals precipitate in the sand/bentonite mixture, the latter looses only one third of the porosity. Because, however, the materials at the interfaces have a high porosity (Mortar M1: 0.25, sand/bentonite: 0.27) with large pores, the blocking of gas flow is rather unlikely even in this extreme case.

Similar to the processes at the cement–sand/bentonite interfaces, the reactions of the cement water with the Opalinus Clay can also lead to sealing effects. The Cement–Opalinus Clay interaction has been addressed in the Project "Entsorgungsnachweis" in connection with the ILW repository (Nagra 2002c). According to those considerations, the reactions are locally restricted and, as at the interface cement–sand/bentonite, zones with reduced porosity will probably occur.

Sealing of the above mentioned interfaces may also occur on the side of the cementitious backfill, for instance by the formation of calcite by the carbonate of the Opalinus Clay (or sand/bentonite) porewater. It is worth mentioning that such cement carbonation may take place also under unsaturated conditions. Due to the high partial pressure gradient for CO₂, the latter will migrate in the gas phase from the adjacent rock to the cement. The reaction will, however, be limited by the availability of CO₂ which is restricted by the buffering capacity and transport of the porewater.

**Curing of concrete and reaction of clay porewater with cement**

The maturation processes in the cement, after its hardening, will continue for years. The process tends to result in a porosity decrease, primarily due to the formation of ettringite and Ca-mono-carboaluminates. According to mass balance calculations, however, this loss of porosity volume in the waste caverns amounts to less than 1 % of the total volume.

Sulphate in the infiltrating host rock porewater will react with the cement minerals to form most probably ettringite and gypsum. Mass balance calculations indicate a porosity loss of up to 17 % from a typical initial porosity of 20 % to about 3 %. However, 200 cavern pore volumes of Opalinus Clay porewater would be necessary to provide the necessary sulphate. Thus, due to the low water exchange in Opalinus Clay, such a porosity loss of the magnitude mentioned above is hardly possible within the time scales considered.

Sulphate can, however, also originate from other sources, for example from the pyrite oxidation during the phase when the caverns are open. In this case, the upper sulphate concentration is limited by the solubility of gypsum.

The production of sulphate from waste components, for example the ion-exchange resins, may also occur.

**Interactions between waste and cement**

The volume increase during metal corrosion may lead to a substantial loss of porosity near the corroding surfaces. This could locally hinder the escape of gas but primarily also the access of water necessary for corrosion. Such a hindrance may be limited, because corrosion layers will most likely be disrupted.
The rate of volume increase and loss of porosity around the corroding surfaces will virtually be proportional to the gas production rate because most of the produced gas originates from metal corrosion. A significant loss of porosity will therefore only occur after a long time period when substantial amounts of gas will already have been released.

Assuming a total conversion of the metals by corrosion the backfilled cavern may lose on average about 20 % of its porosity. Since the metal content of the individual waste types varies substantially, parts of the repository with high metal content would theoretically lose their total porosity. Because, however, the Mortar 1 backfill is hardly compressible, the compressive forces will be transmitted to the relatively plastic Opalinus Clay, contributing progressively to the recompaction of the EDZ. As the mortar is not a hydraulic barrier, porosity reduction and cracking are not expected to influence overall gas transport and water flow in the caverns.

It is assumed that over time, all organic material present in the waste may degrade according to the following simplified chemical equation:

\[2\{CH_2O\} \rightarrow CH_4 + CO_2 \]  
(Eq. 3-14)

Most probably, such degradation would be microbiologically mediated. The resulting methane contributes to the gas generation, whereas the CO₂ reacts with the cement (portlandite) as follows:

\[CO_2 + Ca(OH)_2 \rightarrow CaCO_3 + H_2O \]  
(Eq. 3-15)

The resulting calcite has a volume which is about 2.5 times smaller than the original organic material (assumption of a density of 1 g/cm³) and the Ca(OH)₂. Consequently the porosity will increase.

**Other chemical reactions**

During the period when the repository is open, CO₂ will outgas from the porewater due to the pressure release; as a consequence calcite will precipitate. This process will most probably occur in the EDZ. When the repository is closed, the pressure will build up again and calcite precipitation will cease, before the emplacement caverns and the access tunnels are re-saturated. Due to the very small amount of water that is affected by the pressure decrease, this process can be disregarded.

During the operation phase, CO₂ is introduced into the emplacement caverns through the ventilation. It will react with the cement and carbonate will be formed at the surface of the concrete liner. This carbonation is associated with a reduction of the porosity. Due to the low porosity and the resulting low gas permeability, the carbonation front migrates very slowly into the concrete components (for example the walls of the waste containers) with rates of approx. 1 to 2 cm in 100 years and is thus irrelevant.

**Repository system components affected**

Changes in porosity and pore structures through mineral dissolution and precipitation appear primarily in the interfaces between the various repository components. The interface between the emplacement caverns and the cavern plugs plays the most significant role (Fig. 3-9); but also of importance are the interfaces Opalinus Clay/cavern backfill and the repository seals.
The possibility for formation of impermeable skin zones is considered for the interfaces host rock/cavern backfill and the contact zone between cavern backfill and cavern plug.

3.4.3 Influence coupled hydromechanical processes on gas transport

Dilatancy controlled gas flow is known as a coupled hydromechanical transport mechanism with a high gas transport capacity (chapter 3.2.3). The creation and propagation of dilatant gas pathways around cavern plugs (EDZ) or in the host rock is especially important if the cement/bentonite interactions mentioned in chapter 3.4.2 would lead to a progressive self-sealing of the engineered gas transport system (EGTS) and the gas transport capacity of the sand/bentonite backfill would be significantly reduced. This would cause an increase of the gas pressure in the emplacement caverns and a reduction of the effective stress in the rock. Pathway dilation would be initiated when a critical gas pressure is reached in the caverns (critical pressure for the onset of pathway dilation), giving rise to a gas-pressure dependent permeability increase and thus, to an enhanced gas transport capacity of the host rock around the backfilled repository structures. In this sense, pathway dilation processes along the EDZ is seen as a favourable process which is expected to reduce the gas pressure build-up in the emplacement caverns.

In order to study the creation and propagation of "pathway dilation" in the vicinity of seal and plug systems, new model developments for the propagation of discrete (micro)fractures were initiated within Nagra's RD&D programme. With modelling tools it is possible to simulate discrete fracture patterns, as would be created for example during the excavation of the underground structures as part of the excavation zone around the tunnels (boundary element code FRACOD2D, Shen & Stephansson 1993). Compared to classical geomechanical continuum models, the discrete fracture propagation models have the advantage that they can reflect more realistically the observations (discrete fracture networks in the EDZ). In addition, discrete fracture network models are better suited for the simulation of self-sealing mechanisms in the EDZ after repository closure. The newly developed modelling capabilities for the simulation of fracture propagation processes are expected to improve the understanding of the hydromechanical phenomena, associated with the gas flow along the EDZ. This includes not only the gas pressure-induced fracture propagation process but also the self-sealing which takes place when the gas pressure decreases.
3.5 Evaluation of process understanding

It has been the purpose of chapter 3 to provide an overview of the main gas transport processes, the gas-related parameters and of the coupled processes related to the release of corrosion and degradation gases from the emplacement caverns of a L/ILW repository in the Opalinus Clay. The existing process understanding as developed in the framework of the Project "Entsorgungs-nachweis" (Nagra 2002a, b and c, Nagra 2004) has been confirmed by the gas-related studies of the last few years. An important increase in the state of knowledge has been achieved through the experimental investigations and literature reviews on gas transport in backfill materials (sand/bentonite mixtures, concrete; cf. Lanyon & Rüedi 2008). Aside from this, for the consideration of gas release from a L/ILW repository, the role of the hydrochemical coupled processes must be considered which may under certain circumstances lead to partial self-sealing of the gas transport paths (repository structures, host rock).

The most important conclusions for the process understanding of gas migration from a L/ILW repository can be summarised as follows:

- The Opalinus Clay possesses a significant gas transport capacity, as has been confirmed from numerous recent laboratory and field tests. The gas-related database is supported by gas-related R&D studies performed by Nagra, and also by contributions from other partner organisations as well as by sources derived from Nagra's cooperation with the oil and gas industry.

- Reference values for the gas-related parameters of the various backfill materials were obtained from the literature as well as in-house laboratory and field investigations. The compiled data bases suggest that an efficient engineered gas transport system can be designed. It is foreseen to continue the laboratory programme for the derivation of gas-related parameters of the backfill materials.

- Currently, the experimental database on hydrochemical process interactions is restricted to fully saturated conditions, whereas the understanding of couplings associated with two-phase flow conditions is yet on the level of a phenomenological description. Further laboratory and in-situ experiments are necessary to improve the conceptual understanding with quantitative process models.

- With respect to hydromechanical coupling (dilatancy-controlled gas transport), it is expected that very local stress concentrations around the backfilled underground excavations will appear, that can serve as starting points for pathway dilation if higher gas pressures would occur. The creation of pathway dilation along the backfilled structures would start before the magnitude of the minimum principal stress is reached.

- Dilatancy controlled gas flow is associated with rock deformation, leading to a temporary enhancement of porosity and permeability by micro-fracturing in the time period when gas pressure exceeds the threshold pressure for dilatant flow. Diverse experimental evidence has been gained, that compaction of the dilated claystone will occur at elevated effective stress ("geomechanical self-sealing"), as soon as the gas pressure decreases (Nagra 2002a). Thus, pathway dilation is a process which reduces the risk of extended gas fracs, which could impair the long-term barrier function of the host rock. Nonetheless, the complexity of dilatancy controlled processes, the necessity of obtaining a much larger body of experimental evidence and the need to invoke self-sealing, makes the safety arguments for this transport mechanism more challenging. Therefore, in the context of this generic study it has been the strategy to investigate the possibility of preventing the development of the dilatancy regime in the rock barrier.
Nagra's RD&D programme comprises complementary gas-related research topics, which are expected to provide contributions to the robustness of arguments for the long-term safety of a L/ILW repository. Key issues are hydromechanical and hydrochemical processes, scale dependence of transport properties and the extension of existing data bases on gas-related parameters of Opalinus Clay and backfill and sealing materials. The activities comprise laboratory studies, in-situ experiments in URLs, modeling studies and model developments.
4 Gas transport in the vicinity of the underground structures

After closure of the L/ILW repository, the evolution of the backfilled underground structures will not only be determined by the gas production source term of the waste (chapter 2) and the properties of the backfill materials and of the host rock (chapter 3), but also by numerous other factors related to geology and repository design. The large-scale hydrogeological conditions around the repository will determine the time period for the repository resaturation and the return to the undisturbed porewater pressure regime in the site region (chapter 4.2). The repository layout (tunnel geometry, placement of the seal sections etc.) will have a major impact on the fate of the gas generated within the emplacement caverns (chapter 4.3). An evaluation of the understanding of the porewater circulation in the vicinity of the repository is given in chapter 4.4. This includes a discussion of the pore pressure and saturation conditions in and around the backfilled emplacement caverns after repository closure and an evaluation of the relevance of the resaturation phase in the context of long-term safety assessment.

4.1 Scope of the calculations and approach chosen

The assessment of potential effects of post-closure gas generation on the performance of a L/ILW repository in Northern Switzerland addresses the following aspects:

- Estimation of the repository resaturation time, taking into account the possibility of rapid complete resaturation. The subsequent modeling studies are based on the waste inventory MIRAM 2005, assuming that the gas production is high in the first 10 years after repository closure (Fig. 2-19). In this time period gas pressures could rise quickly, if there is not sufficient gas storage volume available in the emplacement caverns (e.g. hypothetical case of very rapid resaturation of caverns).

- Estimation of the maximum gas pressures in the emplacement caverns. To avoid the risk of extended gas fractures, gas pressure in the backfilled underground structures should not exceed lithostatic stress\(^8\). Furthermore, it is investigated under what conditions it can be ensured that gas transport takes places only in the two-phase flow regime and that the gas pressure does not exceed the critical pressure for the onset of pathway dilation.

- Quantification of porewater flow in the vicinity of the backfilled underground structures induced by gas pressure build-up leading to porewater displacement.

The modelling activities reported in the present synopsis started in 2005 and the majority of calculations were completed by the end of 2007. In this period, the L/ILW disposal concept has undergone various changes with respect to the waste inventory and the repository layout. These changes gave rise to successive model adaptations; the corresponding modifications of the repository geometry and the model input parameters are reflected in the modelling results presented later in this chapter. In this context, it is worth mentioning that modelling was also used as a tool for the refinement and optimisation of the repository layout. Correspondingly, the choice of the modelling parameters was motivated by the specific objectives of the individual modelling tasks and deviations from the reference parameters in chapter 3 were consciously accepted.

Two different models are used for the analyses which differ in the level of detail implemented in the models (geometrical abstraction, process abstraction). The large-scale hydrogeological conditions and the repository resaturation times are investigated with a conventional hydrodynamic

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\(^8\) Due to the generic character of this study, it is assumed that lithostatic stress represents the minimum principle stress and the tensile strength of the host rock is low.
site model. Gas production in the emplacement caverns is not included in the resaturation calculations with this model and thus, the calculations provide a lower limit for the repository resaturation time. In this model, the geological conditions and the underground structures can be represented with a high level of geometric detail. It is also possible with an acceptable computational effort, to simulate complex boundary and initial conditions. Due to the simplified assumptions for the flow conditions however (i.e. Richards' equation for seepage flow), this model does not allow the calculation of gas transport.

The second model, used to calculate the gas transport capacity of the host rock (chapter 4.3.2) and of the underground structures (chapters 4.3.3 and 4.3.4), simulates the combined gas/water transport in and around the backfilled underground structures and in the host rock. The calculations are performed with a two-phase flow simulator, with which complex transport and exchange processes can be represented in detail. However, due to the long computational time, extensive simplifications had to be made with respect to the geometric level of detail (representation of the underground structures) and to the number of parameter variants investigated.

Chapter 4.4 contains an evaluation of the porewater circulation in the vicinity of the repository and includes also the effect of porewater displacement due to gas pressure build-up. In chapter 4.4.1, the consistency between the hydrodynamic site model and the two-phase flow model is checked by comparing the simulation results. This allows the quantitative assessment of the influence of geometric and process model abstractions.

In chapter 4.4.2 the temporal development of the porewater circulation in the vicinity of the backfilled repository under the influence of gas production is evaluated. The influence of possible process coupling is discussed qualitatively. With the help of the simulations performed in chapter 4.3 the relevance of the considered hydrochemical and hydromechanical processes are assessed for the performance of the L/ILW repository.

4.2 Evolution of the groundwater flow systems on the site scale

4.2.1 Motivation and expectations

The groundwater circulation regime at the repository site will be affected significantly through the construction and operation of the L/ILW deep repository. The recovery towards undisturbed hydrogeological conditions (steady-state) will take in the order of $10^4 – 10^5$ years. The temporal evolution of the groundwater flow on the repository site scale is important for the assessment of the long-term radiological safety of the repository. Due to the complex geological situation, but also due to the complex layout of the underground structures, it is necessary to simulate and evaluate a range of boundary conditions and parameter combinations for the groundwater circulation using numerical models. Conceptual and parameter uncertainties, covering geologic and hydrogeological model assumptions, will be systematically analysed through sensitivity studies. In addition, the effect of various construction and operation parameters (e.g. layout variants) on the development of the groundwater flow circulation will be investigated. The expected large-scale flow regime can be derived from the range of the simulation variations.

Poppei & Croisé (2006) have shown in a pre-study (cf. chapter 4.3.1), that sufficient gas storage volume is required to limit the gas pressures in the caverns in the case of high gas generation rates in the early post-closure phase. During this phase, the gas transport through the host rock is not sufficient to compensate for the high initial gas production rate. Such gas transport processes cannot be explicitly simulated with the site-scale hydrodynamic model, but nevertheless, it is possible to improve the understanding of the general repository system behaviour during
the resaturation phase. Of particular interest is the temporal development of the resaturation process up to the complete pressure recovery. The simulations with the single-phase hydrodynamic model provide an estimate of the minimum saturation time, since the gas production that is not considered in the model will prolong the resaturation process. The following model variants are studied with the hydrodynamic site model (without gas development):

- Reference model for a L/ILW repository in the Opalinus Clay formation with parameter variations addressing the geological and hydrogeological situation (variation of the hydraulic parameters, variation of the initial and boundary conditions)
- Variants with repository seals with poorer seal performance (parameter variations for the backfill materials)
- Variants with a steeply inclined fracture zone (variation of the transmissivity of a fracture zone intersecting the repository)

The hydrodynamic site model provides as modelling products, the temporal development of the hydraulic potential and the water fluxes in the repository surroundings. In addition, with the help of particle tracking methods, the flow pathways from the repository caverns to the aquifer systems can be traced. A detailed description of the hydrodynamic site model can be found in Kuhlmann & Marschall (2008).

### 4.2.2 Hydrodynamic model of repository resaturation

The hydrodynamic modelling was performed with the numerical code CASA which was also used in the past for the Wellenberg geosynthesis (Nagra 1997) and the Opalinus Clay geosynthesis (Nagra 2002a). CASA calculates transient groundwater flow conditions with the method of finite elements. Isoparametric elements with quadratic base functions are utilised, which guarantee a more realistic description of curved model boundaries (e.g., tunnels and caverns).

The determination of the hydrogeological units is based on the geologic and hydrogeologic model described in chapter 2 (cf. Fig. 2-1). The following simplifying assumptions for the geologic conditions have been adopted:

- The layering is modelled as horizontal.
- The upper and lower model boundaries are formed by the regional aquifers Hauptrogenstein and Muschelkalk, respectively.
- The Passwang formation is considered as the upper confining rock formation.
- The lithologic units Lias and Keuper are modelled as one hydrogeological unit 'Lias – Keuper' and are considered as the lower confining unit (note: the Gansinger dolomite and the Schilfsandstein can occur locally as aquifers. For the present resaturation studies the significance of local aquifers is low).
- The Opalinus Clay as the host rock forms a separate hydrogeological unit.

All units are modelled as homogeneous, the Opalinus Clay with an anisotropic hydraulic conductivity. For the hydraulic properties of the three hydraulic units, the database of the Opalinus Clay geosynthesis (Nagra 2002a) is used. For the hydraulic head of the aquifers the potential of the local discharge zones is used both for the Hauptrogenstein as well as for the Muschelkalk (Sissle/Bözen: 404 m asl; tributary rivers: 430 m asl). The hydraulic properties of the reference model for the hydrodynamic modelling at the site scale are summarised in Table 4-1.
Tab. 4-1: Hydrogeologic units of the hydrodynamic model for a generic L/ILW repository in Opalinus Clay in the region of northern Aargau and hydraulic parameters for the hydrodynamic model.

<table>
<thead>
<tr>
<th>Hydrogeol. Unit</th>
<th>Thickness [m]</th>
<th>Base [m asl]</th>
<th>K_h [m/s]</th>
<th>Anisotropy factor K_v / K_h [-]</th>
<th>Specific storage [1/s]</th>
<th>Boundary conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hauptrogenstein</td>
<td></td>
<td>282</td>
<td></td>
<td></td>
<td></td>
<td>Top: fixed head:</td>
</tr>
<tr>
<td>Passwang 1)</td>
<td>65</td>
<td>217</td>
<td>$1.0 \times 10^{-10}$</td>
<td>1.00</td>
<td>$3 \times 10^{-6}$</td>
<td>Lateral: no-flow</td>
</tr>
<tr>
<td>Opalinus Clay</td>
<td>100</td>
<td>117</td>
<td>$1.0 \times 10^{-13}$</td>
<td>0.20</td>
<td>$1 \times 10^{-5}$</td>
<td>Lateral: no-flow</td>
</tr>
<tr>
<td>Lias – Keuper</td>
<td>170</td>
<td>-53</td>
<td>$1.0 \times 10^{-13}$</td>
<td>1.00</td>
<td>$3 \times 10^{-6}$</td>
<td>Lateral: no-flow</td>
</tr>
<tr>
<td>Muschelkalk</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Bottom: fixed head:</td>
</tr>
</tbody>
</table>

1) The assumed hydraulic conductivity of the Passwang formation represents an upper limit.

The horizontal extension of the hydrodynamic model is chosen so that a minimum distance of approx. 600 m between the repository and the model boundaries is kept. The resulting surface area of the grid amounts to approx. 2'500 × 1'600 m. The vertical extent includes the hydrogeologic units Passwang and Lias – Keuper, which are adjacent to the host rock and amount to a total thickness of 335 m (cf. Fig. 2-2).

The repository structures are implemented in the model as described in chapter 2.5 with the following simplifying assumptions:

- The model explicitly includes the access tunnel, the central area, the operation tunnel, the test area, the ventilation shaft, the branch tunnels, the emplacement caverns, the pilot facility and the seals/plugs. The unloading and transfer areas are represented as part of the emplacement caverns.

- The cross sections of all underground structures are modelled as circular with the same area as the actual cross section of the respective underground element as shown in Table 2-1. All underground structural elements are centered around the tunnel axis (which implies that the higher lying transfer / unloading area is not represented in detail in the resaturation calculations; cf. Fig. 2-7).

- The inclination of the access and operational tunnel corresponds to the specifications is shown in Figure 2-3. The access tunnel terminates at the lateral boundary of the model, at the boundary with the Passwang unit.

- The various plugs and seals are not modelled in detail; they are rather represented with elements that have the corresponding hydraulic properties.

- The repository caverns are modelled as being horizontal in the axial direction.
Fig. 4-1: Hydrodynamic model for simulating the resaturation of the L/ILW repository.

a) 3-D view comprising the underground structures and the geological units

b) details of the test facility and the ventilation shaft

c) detail of the cavern plug and the junction between branch tunnel and operation tunnel with EDZ
The implementation of the repository structures in the model is shown in Figures 4-1a–c. A 1-m thick excavation disturbed zone in the host rock is modeled with an increased hydraulic conductivity \( K_{EDZ} = 1 \times 10^{-12} \text{ m/s} \), corresponding to the long-term EDZ conductivity according to Nagra 2002a). The lengths and the hydraulic properties of the implemented structures are given in Table 4-2. Further details on the geometrical and hydraulic input data are documented in Kuhlmann & Marschall (2008).

Tab. 4-2: Length and hydraulic parameters of the seals, plugs and tunnel backfill used in the hydrodynamic model.

The locations of the seals and plugs are given in Figure 2-14. S/B: Sand/Bentonite.

<table>
<thead>
<tr>
<th>Seal / Plug / Backfill</th>
<th>Length [m]</th>
<th>K [m/s]</th>
<th>Porosity [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>V2: Test facility plug (S/B: 80/20)</td>
<td>60</td>
<td>(1 \times 10^{-11})</td>
<td>0.3</td>
</tr>
<tr>
<td>V3: Ventilation shaft (bentonite)</td>
<td>65</td>
<td>(1 \times 10^{-13})</td>
<td>0.4</td>
</tr>
<tr>
<td>V4: Repository seal (S/B: 70/30)</td>
<td>82.5 (^1)</td>
<td>(1 \times 10^{-12})</td>
<td>0.3</td>
</tr>
<tr>
<td>V5: Cavern plugs (S/B: 80/20)</td>
<td>52.8</td>
<td>(1 \times 10^{-11})</td>
<td>0.3</td>
</tr>
<tr>
<td>Tunnel backfill (access and operation tunnel, branch tunnel and test facility)</td>
<td>(1 \times 10^{-9})</td>
<td>0.3</td>
<td></td>
</tr>
</tbody>
</table>

\(^1\) Total length including bulkhead (gravel), transitional layer and seal (sand/bentonite)

It is assumed that the activities related to the construction and operation of the test facility and construction of the repository structures will last 20 years, followed by a 15-year long operational period during which the emplacement caverns are successively filled with waste. For the closure of the emplacement caverns and backfilling of the branch tunnels 13 more years are required. The access tunnel will be closed at the end of this stage, whereas the pilot facility and the test area will remain accessible through the shaft for monitoring purposes during the observation phase. After the completion of the observation phase (assumption: 100 years), the remaining open underground structures will also be backfilled and sealed. The implementation of this time sequence in the numerical model represents the various phases of the repository operation and closure concept as described in chapter 2.4.

In the resaturation calculations, the construction and operation phase is simulated by assuming atmospheric pressure conditions in the open underground structures; the host rock is assumed to be fully saturated at all times. The calculated pore pressure distribution in the host rock at the end of the operation phase is used to specify the initial pressure conditions, needed for modelling the subsequent resaturation phase. For modelling the resaturation phase, it is assumed that all repository structures are backfilled. The initial saturation of the backfill is assumed to be 50 % at atmospheric pressure conditions. For the unsaturated backfill a pressure-dependent storage coefficient is derived using a van Genuchten capillary pressure relationship. All initial and boundary conditions are described in greater detail in Kuhlmann & Marschall (2008).

The numerical simulations were run on a workstation with a single CPU (Intel Core 2, CPU 6600 @ 2.4 GHz). Typical run times of the investigated resaturation cases were 30 – 50 hours.
4.2.3 Simulation of repository resaturation: results

The hydrodynamic modelling on the site scale serves as a basis for estimating the time needed for complete resaturation and to investigate the hydrogeological and layout related factors that could lead to an unexpected early saturation of the repository. This includes:

- The accelerated saturation due to a transmissive, steeply inclined fracture, which intersects the operation tunnel.
- The accelerated saturation due to a poor performance of the seal in the access tunnel (V4) and of the cavern plugs (V5).

In the context of this study, all investigated model variants (R_RM01 to R_RM05; see Tab. 4-3) correspond to a hydrogeologic situation with a very low permeability host rock ($K_{OPA,V} = 2 \times 10^{-14}$ m/s, $K_{OPA,H} = 1 \times 10^{-13}$ m/s). The hydraulic parameters used for the host rock are five times lower than the reference values (RV) listed in Table 3-3. The reason for concentrating on cases with a low permeability host rock was motivated by the results of the gas transport simulations (chapter 4.3), which indicate that the likelihood of a rapid pressure build-up during the early post-closure period is most critical for a very tight host rock.

The base case model R_RM01 is characterised by a repository seal and cavern plugs with very low permeability (as-designed). The model comprises eight caverns, including a reserve cavern which accounts for a possible increase of the waste inventory (layout according to the L/ILW reference concept in the year 2006). The results of the simulations with the base case model parameters R_RM01 still reveal unsaturated conditions in the backfilled underground structures after 1'000 years (Fig. 4-2). Even after a period of 10'000 years some of the emplacement caverns are still not fully saturated. The simulations predict the return to hydrostatic conditions after a period of more than 30'000 years.

Further model variants were studied in order to simulate poor performance of the closure systems (Fig. 4-3):

- In the first parameter variation R_RM02, it is assumed that all plugs and seals have a higher conductivity ($K_{seal} = 1 \times 10^{-9}$ m/s) with the exception of the seal in the shaft. Compared to the base case it is shown that after approx. 5'000 years the pilot facility and test area are saturated, whereas all emplacement caverns are still unsaturated (Fig. 4-3b).
- In the second parameter variation R_RM03, only the seal in the access tunnel V4 has an increased permeability (Fig. 4-3c). Access tunnel, operations tunnel and test facility are fully saturated after 5'000 years, whereas the emplacement caverns and the pilot facility are still unsaturated.
- In the parameter variation R_RM04, it is assumed that a vertical regional fracture zone exists, which intersects the operation tunnel between the 4th and 5th cavern. The transmissivity of the fracture zone is assumed to be $1 \times 10^{-9}$ m²/s. In this variant, full saturation is achieved in about 10'000 of years (Fig. 4-3c).
- In the parameter variation R_RM05 (not shown in Fig. 4-3), the repository layout consists of 7 caverns. The simulation allows the results of the hydrodynamic model to be better compared with those from the two-phase flow model which has only 7 caverns (chapter 4.3). A discussion of this comparison is documented in chapter 4.4.

A comprehensive description of the model set-up and the parameter variants, complemented by a discussion of the modeling results can be found in Kuhlmann & Marschall (2008).
Tab. 4-3: Hydrodynamic model of the resaturation of the L/ILW repository: spectrum of model parameters for the sensitivity analyses.

The hydraulic properties of the confining units are given in Table 4-1 and remain unchanged.

<table>
<thead>
<tr>
<th>Model parameters</th>
<th>Parameter values</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Host rock properties</strong></td>
<td></td>
</tr>
<tr>
<td>Hydraulic conductivity</td>
<td>( K_h = 1 \times 10^{-13} \text{ m/s} ) , ( K_v = 2 \times 10^{-14} \text{ m/s} )</td>
</tr>
<tr>
<td>Specific storage</td>
<td>( 1 \times 10^{-5} \text{ m}^{-1} )</td>
</tr>
<tr>
<td>Vertical fault through repository (normal to operations tunnel)</td>
<td>Hydraulically inactive</td>
</tr>
<tr>
<td>Hydraulic conductivity of EDZ</td>
<td>( 1 \times 10^{-12} \text{ m/s} )</td>
</tr>
<tr>
<td><strong>Important state conditions</strong> (reference level: 175 m asl)</td>
<td></td>
</tr>
<tr>
<td>Hydrostatic formation pressure:</td>
<td>2.2 MPa (hydrostatic)</td>
</tr>
<tr>
<td>Initial pressure at repository level:</td>
<td>Atmospheric</td>
</tr>
<tr>
<td><strong>Repository design and backfill properties</strong></td>
<td></td>
</tr>
<tr>
<td>Hydraulic conductivity / porosity of cavern backfill (^2)</td>
<td>( 1 \times 10^{-10} \text{ m/s} ) , 25 %</td>
</tr>
<tr>
<td>Hydraulic conductivity / porosity of cavern plug V5</td>
<td>( 1 \times 10^{-11} \text{ m/s} ) , 30 %</td>
</tr>
<tr>
<td>Hydraulic conductivity / porosity of tunnel backfill</td>
<td>( 1 \times 10^{-9} \text{ m/s} ) , 30 %</td>
</tr>
<tr>
<td>Hydraulic conductivity / porosity of seals V3/V4</td>
<td>( 1 \times 10^{-12} \text{ m/s} ) , 30 %</td>
</tr>
<tr>
<td>Number of caverns modelled:</td>
<td>8</td>
</tr>
<tr>
<td>Length of repository seal V4</td>
<td>82.5 m</td>
</tr>
<tr>
<td>Length of cavern plug V5</td>
<td>52.8 m</td>
</tr>
<tr>
<td>Unsaturated conditions:</td>
<td>Richards' equation / van Genuchten</td>
</tr>
<tr>
<td>Initial saturation (all backfilled underground structures)</td>
<td>0.5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sensitivity Runs</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>R_RM2 (02_P1) (^1)</td>
<td>- hydraulic conductivity of backfill of all underground structures including seals and plugs: ( K = 10^{-9} \text{ m/s} ) (all other parameters corresponding to R_RM01)</td>
</tr>
<tr>
<td>R_RM3 (03_P2) (^1)</td>
<td>- hydraulic conductivity of repository seal V4: ( K = 10^{-9} \text{ m/s} ) (all other parameters corresponding to R_RM01)</td>
</tr>
<tr>
<td>R_RM4 (08_VZ) (^1)</td>
<td>- Vertical fault intersecting the operation tunnel between cavern 4 and 5; transmissivity of the fault ( 10^{-9} \text{ m}^2/\text{s} ) (all other parameters corresponding to R_RM01)</td>
</tr>
<tr>
<td>R_RM5 (09_R7) (^1)</td>
<td>- repository layout with 7 emplacement caverns (all other parameters corresponding to R_RM01)</td>
</tr>
</tbody>
</table>

\(^1\) Run-ID according to Kuhlmann & Marschall (2008)
\(^2\) Average value of the cementitious backfill (mortar, construction and waste fixation concrete)
Fig. 4-2: Resaturation of the L/ILW repository for the base case R_RM01.

a) after 1'000 years

b) after 10'000 years

c) after 20'000 years
Fig. 4-3: Resaturation of the L/ILW repository after 5'000 years.

a) Base case

b) all cavern and repository seals permeable (R_RM02)

c) only the repository seal permeable (R_RM03)

d) vertical fault intersecting the operation tunnel (R_RM04)

Fig. 4-3: Resaturation of the L/ILW repository after 5'000 years.
4.2.4 The impact of the repository on groundwater circulation on the site scale

The simulations of (single phase) groundwater flow on the scale of the repository site illustrate the significance of the general hydrogeological conditions as a determining factor for the resaturation of the repository:

- The time scales of repository resaturation for expected hydraulic conditions (without gas generation) are in the order of several 10'000 of years. Even for unexpected scenarios, such as poor performance of the plugs and seals (repository seal, cavern plugs, test facility plug), the resaturation times of the emplacement caverns are more than 5'000 years. Consequently, during the critical early phase characterised by high gas generation rates (cf. chapter 4.3), the gas storage capacity of the emplacement caverns is still high.

- The resaturation process is controlled by the limited water inflow from the host rock into the backfilled repository combined with the large pore volumes of the repository components to be saturated. The hydrodynamic simulations presented in chapter 4.2 assume an initial water saturation of the backfill materials $S_{wi} = 0.5$. The initial saturation, however, can be adjusted within certain limits.

- The pore pressure decline in the host rock formation, caused by the repository construction and operation, is a phenomenon which is restricted to a zone of few hundreds of meters around the footprint of the repository (cf. Fig. 4-2).

4.3 Combined gas/water transport modelled with the two-phase model

4.3.1 Motivation and modelling approach

For the estimation of the gas pressure build-up in and around the backfilled repository it is important to consider not only the hydrodynamic evolution of the repository as a whole (hydrodynamic model on the site scale; cf. chapter 4.2), but also to assess the combined gas/water flow in and around the individual repository components. Therefore, the gas transport is represented explicitly through the consideration of a mobile gas phase, in contrast to the resaturation model. The gas/water transport simulations are performed with a two-phase flow code (TOUGH2, Pruess et al. 1999). The gas dissipation from the backfilled caverns takes place through the host rock and along the backfilled underground structures (see also Fig. 1-1).

The process of pathway dilation is not included in the two-phase flow calculations presented here. Instead, it is assumed that the rock behaves as an elastic medium, even if the gas pressure in the caverns exceeds the critical threshold pressure for pathway dilation. This modelling approach was chosen for investigating the gas-related optimisation of the engineered gas transport system (EGTS), although it does not describe the actual gas transport processes at high gas pressures in an appropriate manner. In fact, the onset of pathway dilation at high gas pressures increases the gas transport capacity of the host rock significantly and leads to a stabilisation of the maximum gas pressure around the critical threshold pressure for pathway dilation. In the present parametric studies without pathway dilation, the transients of the gas pressure evolution are displayed in graphs, where the indicative levels of fracture pressure (lithostatic pressure as a lower bound) and threshold pressure of pathway dilation (80 % of the fracture pressure) are included.
The gas transport capacity of the various transport pathways was studied with three different model geometries:

- A 2-D vertical model representing a cross section including one emplacement cavern. The simulations here serve to estimate the gas release through the host rock (chapter 4.3.2).
- A 3-D model of the backfilled repository structures under the assumption of an impermeable host rock (chapter 4.3.3). These simulations serve for the estimation of the gas transport along the engineered gas transport system (EGTS), described in chapter 2.6.
- An integrated 3-D model of the complete repository system (gas pathways through the host rock and along the EGTS). These simulations address the interaction of the various gas pathways through the host rock and along the backfilled repository structures (chapter 4.3.4). In addition, the effect of gas transport on the migration of the host rock porewater is investigated.

The first two models mentioned above are suitable for sensitivity studies of the gas pressure build-up in the emplacement caverns. Through a series of parameter variations the most important factors, which control the efficiency of the various gas paths, can be identified (variation of the gas-related parameters of the host rock and the backfill and sealing materials; variation of the initial hydraulic conditions and the boundary conditions).

The integrated 3-D model of the whole repository system is not suitable for comprehensive sensitivity studies due to its large size and complexity. The purpose of this model is to develop an integral understanding of the porewater flow around the repository. This is accomplished through the analysis of a small number of parameter variations which influence the behaviour of the various repository components in different ways during the gas migration and resaturation processes.

The gas generation rates used for the two-phase flow simulations are based on the MIRAM 2005 inventory as described in chapter 2.8. According to MIRAM 2005 the gas production at early time is dominated by hydrogen from the corrosion of metal components with large surfaces and metals with high corrosion rates. These contributions to the total gas production quickly decline and from approximately year 10 to year 1'000 the contribution of methane from the degradation of organic substances increases above the proportion of hydrogen (Appendix C). After 1'000 years the gas production is again dominated by the steel corrosion. This is in contrast to the gas generation rates calculated with the updated inventory MIRAM 2008, where hydrogen from metal corrosion dominates at all times.

For the two-phase flow calculations, the generated gas mixture (hydrogen, methane) is represented by a single gas component with physical and chemical properties corresponding either to those of hydrogen (chapter 4.3.2) or air (chapters 4.3.3 and 4.3.4). The derived mol-equivalent gas generation rate is defined as a ‘realistic gas generation rate’. For the sensitivity studies a so-called ‘conservative gas generation rate’ was additionally defined. It is based on the assumption of a corrosion rate for metals that is 10 times higher (e.g. carbon steel 10 μm/a), whereas the contributions from the degradation of organics are the same as for the realistic gas generation rates. The total cumulative mass of the generated gas is identical in both cases and amounts to about 20 – 30 million m³ (STP). Figure 4-4 shows the temporal evolution of the realistic and conservative rates as well as the cumulative gas mass. The source term for the gas generation rate in the two-phase calculations was defined by uniformly distributing the total gas generation rate along the emplacement caverns.
4.3.2 Gas transport capacity of the host rock

Gas transport capacity of the host rock

The 2-D simulations of the gas pressure build-up in a vertical cross section through a single emplacement cavern serve the purpose of investigating influential factors that are specific to the host rock and hydrogeological setting of the site, as well as the repository design. The sensitivity studies involve simulations with variations of:

- the host rock properties (two-phase flow parameters, intrinsic permeability)
- hydrogeologic boundary and initial conditions (static formation pressure, initial porewater pressure, initial saturation of the emplacement cavern)
- gas generation rates

The 2-D simulations imply a tight cavern plug V5 (Fig. 2-16) with no gas flow along the axis of the emplacement cavern. The flow of gas and water occurs in the plane perpendicular to the axis of the emplacement cavern.

The 2-D simulations were started in late 2005 with the aim of providing a first estimate of the gas overpressures in a L/ILW repository in the Opalinus Clay. Preliminary configuration data were used for modelling the L/ILW disposal system and for representing the geological conditions in the proposed siting region.
The model-set up comprises a finite volume grid with 2'500 cells. The model geometry with the outer model boundaries as well as the cavern contour is shown in Figure 4-5. The cavern contour has a resolution of 10 – 20 cm. The top model boundary is the basis of the Hauptrogenstein (300 m asl, or equivalently 125 above repository level), the bottom boundary is the top of the Muschelkalk (~45 m asl, or equivalently 220 m below repository level). The model includes the Opalinus Clay host rock and part of the confining units below (Lias/Keuper) and above (Passwang formation). The gas-related properties are the same for the host rock and the confining units, respectively. Note that the assumption of low permeability and high entry pressure for the confining units leads to pessimistic estimates of the gas pressure build-up in the emplacement caverns. Thus, the simulations with the 2-D model set-up are intended to explore upper bounding cases for the pressure evolution in the repository.

Fig. 4-5: 2-D simulations of the gas pressure build-up in a vertical cross section through the emplacement caverns: model geometry and boundary conditions.

No-flow boundary conditions are assumed for the vertical model boundaries, representing the symmetry axis through the cavern and at the midpoint between adjacent caverns, respectively. The top and bottom model boundaries are represented by prescribed pressures corresponding to fixed potentials. The hydraulic pressure conditions at the top and bottom boundaries are derived from the local hydrogeological regime (see also chapter 2.2). A reference hydraulic head of
400 m asl is assumed, corresponding to the local discharge areas. This corresponds to a pore-water pressure of 2.2 MPa at the repository level (175 m asl), assuming hydrostatic conditions. Alternative boundary conditions were defined based on a water level of 500 m asl at the surface above the repository. This corresponds to a porewater pressure of 3.2 MPa at the repository horizon assuming hydrostatic conditions.

An operational phase of 10 years was assumed for the simulations. Atmospheric conditions are present in the repository caverns during the operational phase; for modelling purposes the resulting (small) water inflows into the repository caverns from the prescribed atmospheric pressure are withdrawn (i.e. no accumulation of water in the repository caverns during this period). During the operational phase the host rock experiences a progressive depressurisation of porewater pressures around the underground structures. It is assumed that the host rock around the caverns does not desaturate (i.e. no suction pressures are prescribed at the cavern surface).

The resulting flow field in the rock at the end of the operational phase forms the initial conditions for the post-operational phase: the repository caverns now consist of a partially saturated, homogeneous filling of drums, mortar, concrete and shotcrete lining, with defined porosity, compressibility and permeability. The water saturation in the caverns for the base case was assumed to be 30 % at the beginning of the post-operational phase, a value chosen to correspond to the residual saturation of mortar M2. In a sensitivity case a much higher value of 50 % was considered, corresponding to the reference value in Table 3-5.

The start of the post-operational phase represents the onset of resaturation of the repository and gas generation from corrosion and degradation of waste. For these simulations, gas generation rates are introduced as source terms in the backfilled caverns, assuming a total length of the emplacement tunnels\(^9\) of 1'562 m (cf. Fig. 4-1). The properties of the prescribed gas source are taken from its main constituent, hydrogen. A detailed description of all model parameters for the base case and all simulation cases in the framework of the sensitivity analysis can be found in Poppei & Croisé (2006).

**Parameter sensitivity for the evaluation of gas pressure build-up in the emplacement caverns**

An overview of the sensitivity studies with the 2-D model is given in Poppei & Croisé (2006). The model products consist of the transients of the gas pressure in the emplacement cavern, as well as the evolution of saturation and gas/water flows in the host rock. The most important cases are described in Table 4-4 and are discussed in the following. Emphasis is placed on the interpretation of the gas pressure build-up in the emplacement caverns.

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\(^9\) The value for total length of the emplacement tunnels corresponds to the previous L/ILW repository layout in 2006; minor deviations with respect to the reference value in Table 2-1 are accounted.
Tab. 4-4: Simulation for gas dissipation through the host rock: spectrum of the model parameters for the sensitivity analyses with the 2-D vertical-plane model.

<table>
<thead>
<tr>
<th>Model Parameter</th>
<th>Parameter Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Base Case R_HR01</strong> (refers to case R1 in Poppei &amp; Croisé 2006)</td>
<td></td>
</tr>
<tr>
<td><strong>Rock properties (Opalinus Clay &amp; confining units)</strong></td>
<td></td>
</tr>
<tr>
<td>Intrinsic Permeability of host rock</td>
<td>$1 \times 10^{-20}$ m²</td>
</tr>
<tr>
<td>Capillary strength $1/\alpha$</td>
<td>18 MPa</td>
</tr>
<tr>
<td>Porosity</td>
<td>12 %</td>
</tr>
<tr>
<td>Parametric model</td>
<td>van Genuchten ($n = 1.67$)</td>
</tr>
<tr>
<td>Residual water saturation</td>
<td>0.0</td>
</tr>
<tr>
<td>Residual gas saturation</td>
<td>0.003</td>
</tr>
<tr>
<td>Specific storage</td>
<td>$2.6 \times 10^{-6}$ m⁻¹</td>
</tr>
<tr>
<td><strong>Backfill properties</strong></td>
<td></td>
</tr>
<tr>
<td>Intrinsic permeability</td>
<td>$1 \times 10^{-16}$ m²</td>
</tr>
<tr>
<td>Capillary strength $1/\alpha$</td>
<td>500 Pa</td>
</tr>
<tr>
<td>Porosity</td>
<td>25 %</td>
</tr>
<tr>
<td>Parametric model</td>
<td>van Genuchten ($n = 1.29$)</td>
</tr>
<tr>
<td>Residual water saturation</td>
<td>0.25</td>
</tr>
<tr>
<td>Residual gas saturation</td>
<td>0.2</td>
</tr>
<tr>
<td><strong>Important state conditions</strong> (reference Level: 175 m asl)</td>
<td></td>
</tr>
<tr>
<td>Hydrostatic formation pressure</td>
<td>2.2 MPa</td>
</tr>
<tr>
<td>Initial water saturation of backfill</td>
<td>0.3</td>
</tr>
<tr>
<td><strong>Gas Generation</strong></td>
<td></td>
</tr>
<tr>
<td>Gas generation rate</td>
<td>&quot;realistic rates&quot; according to Figure 4-4</td>
</tr>
<tr>
<td>Start of gas pressure build-up</td>
<td>Immediately after repository closure</td>
</tr>
</tbody>
</table>

### Simulation Runs

- **R_HR02 (R0)**<sup>1)</sup> - Hydrostatic formation pressure: 3.2 MPa (the other parameters according to R_HR01)
- **R_HR03 (R8)**<sup>1)</sup> - Intrinsic permeability of the host rock: $1 \times 10^{-19}$ m² (the other parameters according to R_HR01)
- **R_HR04 (R9)**<sup>1)</sup> - Intrinsic permeability of the host rock: $1 \times 10^{-21}$ m² (the other parameters according to R_HR01)
- **R_HR05 (R1a)**<sup>1)</sup> - Initial water saturation of backfill $S_{wi} = 0.5$ (the other parameters according to R_HR01)
- **R_HR06 (R10)**<sup>1)</sup> - Porosity of backfill $\phi_{bf} = 50\%$ (the other parameters according to R_HR01)
- **R_HR07 (R15)**<sup>1)</sup> - Porosity of backfill $\phi_{bf} = 75\%$ (the other parameters according to R_HR01)
- **R_HR08 (R7)**<sup>1)</sup> - Conservative gas generation rate (according to Fig. 4-4) (the other parameters according to R_HR01)

<sup>1)</sup> refers to the identification of cases in Poppei & Croisé (2006)
<sup>2)</sup> host rock assumed to be isotropic
<sup>3)</sup> pore compressibility of $2.4 \times 10^{-10}$ Pa⁻¹ specified in TOUGH2 input
Case R_HR01 is the base case for the sensitivity analyses. Note, that not all the model parameters for the base case are identical to the reference values described in chapter 3 for the gas-relevant parameters of a generic L/ILW repository in the Opalinus Clay of Northern Switzerland. Rather, the model parameters have been selected to capture the most important parameter sensitivities with regard to the maximum gas pressure in the emplacement caverns. Case R_HR02 investigates the influence of the hydraulic boundary conditions and cases R_HR03 and R_HR04 investigate the significance of the host rock permeability. Cases R_HR05 to R_HR07 explore the influence of the available gas storage volume in the repository caverns. Finally, case H_HR08 examines the effect of a conservative gas generation rate (cf. Figure 4-4).

The gas pressure development in the emplacement caverns for the various cases is summarised in Figure 4-6. For most of the cases the maximum gas pressure is below the lithostatic pressure of approx. 8.125 MPa, which is considered an indicator for the development of tensile fractures in the host rock. Only in the cases of very low host rock conductivity ($k = 1 \times 10^{-21} \text{ m}^2$) and for the case of a conservative gas generation rate higher gas pressures of approx. 10 – 12 MPa are obtained. Pressures above the hydrostatic pressure (3.2 MPa in Case R_HR02, 2.2 MPa in all other cases) are reached only after a period of 100 to 1’000 years. The maximum pressure is calculated typically after l’000 to 10’000 years. With a larger gas storage volume in the emplacement caverns the gas pressure build-up can be significantly delayed and, at the same time, the peak gas pressure is reduced (Case R_HR06 and R_HR07).

![Fig. 4-6: 2-D cavern near-field model: spectrum of the temporal development of the gas pressure build-up in the emplacement caverns. Significant gas overpressures are reached typically after between 100 and 1’000 years.](image-url)
The significance of the host rock for gas release

The 2-D simulations of the gas pressure build-up in the emplacement caverns show that the intrinsic permeability of the intact Opalinus Clay is crucial for the gas release through the host rock:

- For the conditions expected for a L/ILW repository in the Opalinus Clay of Northern Switzerland (compare to the gas-related reference parameters RV in Tab. 3-3) the gas transport capacity of the host rock is sufficient to release the waste-generated gas without creation of tensile fractures.

- In the case where the host rock in the site region has a significantly lower permeability (due to higher overburden comparable to the conditions in the Zürcher Weinland), the gas transport capacity of the host rock is not sufficient and, hence, dilatant gas pathways might be created in the host rock when gas pressure build-up approaches the lithostatic pressure.

- Due to the high gas generation rates in the early gas production phase (cf. Fig. 4-4), the amount of the initially available gas storage volume plays a significant role in the development of gas overpressures in the caverns. The gas pressure build-up in the caverns can be reduced strongly, when the initial saturation of the cavern backfill is low and the total pore volume is high. The choice of backfill materials with high porosity, the creation of additional dead volumes through an extension of the emplacement caverns as well as a low initial water saturation of the backfill material are viable options for increasing the initial gas volume at atmospheric pressure (see chapter 2.6).

- Due to the relatively slow gas pressure build-up, over a period of 100 to 1'000 of years, the creation of extended tensile fractures in the undisturbed host rock can be excluded. If gas pressures approach the critical stress, microscopic pathways will form and gas is released in a dilatancy-controlled regime.

The degree of conservatism in the assessment of pressure build-up can be reduced by considering the storage and gas transport capacity of the backfilled and sealed underground structures as described in chapters 4.3.3 and 4.3.4.

4.3.3 Gas transport capacity along the underground structures

Purpose and model set-up

A three-dimensional model of the underground structures with an impermeable host rock is used for estimating the transport capacity of the gas pathway along the backfilled repository structures. The purpose of the model calculations is to:

- obtain an in-depth understanding of the gas pathway along the backfilled underground structures and, in particular, of the functioning of the engineered gas transport system (EGTS), proposed in chapter 2.6, through sensitivity analyses

- optimise the design of the cavern plugs and the repository seal (geometry and hydraulic properties)

For computational reasons, the geometry of the two-phase model is simplified, compared to the hydrodynamic model described in chapter 4.2. The simplifications include square cross sections keeping the same area and orthogonal connections to the access tunnel. The following structures are considered in the model (Fig. 4-5): access tunnel, central area, operation tunnel, test area, shaft, branch tunnels, emplacement caverns, pilot facility as well as the cavern plugs and the
repository seal. The transfer and unloading areas are included as part of the caverns. In the model, the access tunnel ends with the repository seal V4 at the lateral boundary of the model. It is assumed that the host rock is impermeable. On the front surface of the repository seal V4 hydrostatic conditions are assumed.

The parallel version of the two-phase flow simulator TOUGH2_MP (Zhang et al. 2003, Zhang & Wu 2006) is used for simulation of two-phase flow in the present 3-D model. The integrated finite difference grid of the underground structures consists of about 280,000 cells. Further details about grid generation are given in chapter 4.3.4. The different gas components are represented by a single gas phase (air) using the TOUGH2 EOS3 module.

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Fig. 4-7: 3-D variant of the cavern near-field model: model geometry with the various underground structures.

At the start of the post-operational phase, the water saturation in the repository caverns in the base case is assumed to be 70%; it is thus higher than in the vertical cross section model in order to assess a parameter variant, which could lead to a more rapid pressure build-up (see chapter 4.3.2). After closure, the saturation of the repository can only occur through the repository seal V4, because the host rock and the ventilation shaft seal are considered impermeable. For the simulation of the gas pressure build-up, gas generation rates are introduced in the backfilled caverns as source terms. A detailed description of all model parameters of the base case and of all sensitivity runs is given in Senger & Ewing (2009).
Parameter sensitivity of the maximum gas pressure in the repository caverns

The sensitivity calculations performed with the 3-D model are described in Senger & Ewing (2009). The simulations with an impermeable host rock are characterised in Table 4-5 and are discussed here. Focus is on the interpretation of the gas pressure build-up in the repository caverns. The results are described in terms of gas pressure and gas saturation in the repository caverns, and gas and water fluxes along the backfilled underground structures.

Run R_EBS01 is the base case for the sensitivity analyses. Not all of the model parameters of the base case are identical to the reference values for a generic L/ILW repository the Opalinus Clay of Northern Switzerland (RV column in Tab. 3-4). The model parameters were rather chosen to best capture the most significant parameter sensitivity of the maximum gas pressure in the repository caverns. In particular, the permeabilities of the backfill, plugs and seals were set to very low values. Runs R_EBS02, R_EBS03 und R_EBS05 investigate the effect of the permeability of the repository seal V4 and the cavern plugs V5. Run R_EBS04 evaluates the effect of the repository seal length.

Figure 4-8 shows the temporal evolution of the gas pressure build-up for all the runs described in Table 4-5 (Reference: emplacement cavern no. 1). The base case R_EBS01 clearly shows that for an impermeable host rock and very low permeability seals \((k_{V4} = k_{V5} = 1 \times 10^{-19} \text{ m}^2)\), the engineered gas transport system (EGTS) cannot transport the gas generated in the emplacement caverns without the gas pressure rising significantly higher than the lithostatic pressure. Thus, dilatancy-controlled gas transport through the host rock (especially in the EDZ along the seals) is expected. In the simulation, the maximum gas pressure is reached after approx. 30'000 years, which coincides with gas breakthrough across the repository seal V4 in the access tunnel.

The pressure build-up in the emplacement caverns can be markedly reduced by increasing the permeability of the repository seal V4 (R_EBS02) and of the cavern plugs V5 (R_EBS03) one order of magnitude. In addition, a reduction of the length of the repository seal from 37.5 m to 25 m (R_EBS04) results in a significantly earlier gas breakthrough. Nevertheless, the gas pressures still exceed the lithostatic pressure and pathway dilation in the host rock (especially in the EDZ along the seals) cannot be excluded. Critical gas pressures above lithostatic pressures result after approx. 500 to 1'000 years. In run R_EBS05, the permeability of the repository seal V4 and of the cavern plugs V5 is set at the value of \(1 \times 10^{-16} \text{ m}^2\) which results in peak pressures below lithostatic pressure and even below the threshold pressure for pathway dilation. Thus, even in the case of an impermeable host rock it is possible to transport all the gas generated in the emplacement caverns through the engineered gas transport system without reaching critical gas pressures.
Tab. 4-5: Simulation for gas transport through the engineered gas transport system (EGTS): spectrum of model parameters for the three-dimensional model.

<table>
<thead>
<tr>
<th>Model Parameter</th>
<th>Parameter Value</th>
</tr>
</thead>
</table>
| **Base Case R_EBS01**  
(case EBS7n_QGR8c in Senger & Ewing 2009) | |
| Repository seal and cavern plug | |
| Length of repository seal V4 | 37.5 m |
| Intrinsic permeability of repository seal V4 | $1 \times 10^{-19}$ m$^2$ |
| Intrinsic permeability of cavern plug V5 | $1 \times 10^{-19}$ m$^2$ |
| Backfill properties / caverns | |
| Intrinsic permeability of backfill | $1 \times 10^{-15}$ m$^2$ |
| Capillary strength $1/\alpha$ | 500 Pa |
| Porosity | 25 % |
| Parametric model (relative permeability) | van Genuchten/Mualem ($n = 1.29$) |
| Residual water saturation | 0.25 |
| Residual gas saturation | 0.2 |
| Important state conditions, (reference level: 175 m asl) | |
| Hydrostatic formation pressure / lithostatic pressure: | 2.2 MPa / 8.125 MPa |
| Initial water saturation of backfill: | 0.7 |
| Gas Generation | |
| Gas generation rate: | "realistic rates" according to Figure 4-4 |
| Start of gas pressure build-up: | Immediately after repository closure |

<table>
<thead>
<tr>
<th>Simulation Runs</th>
<th></th>
</tr>
</thead>
</table>
| R_EBS02  
(EBS8n_QGR8c) | - intrinsic permeability of seal V4 and plugs V5: $k_{V4} = 1 \times 10^{-18}$ m$^2$  
(the other parameters according to R_EBS01) |
| R_EBS03  
(EBS2c_QGR4) | - intrinsic permeability of plug V5: $k_{V5} = 1 \times 10^{-16}$ m$^2$  
(the other parameters according to R_EBS02) |
| R_EBS04  
(EBS6n_QGR4c) | - length of repository seal $L_{V4} = 25$ m  
(the other parameters according to R_EBS02) |
| R_HR05  
(EBS9n_QGR8c) | - intrinsic permeability of seal V4: $k_{V4} = 1 \times 10^{-16}$ m$^2$  
(the other parameters according to R_EBS03) |
Evaluation of the efficiency of the engineered gas transport system EGTS

The efficiency of the engineered gas transport system (EGTS) has been studied with a 3-D model. Particular attention was given to the contribution of the individual components of this gas pathway to the gas storage and gas release. The simulations of the gas build-up in the emplacement caverns show that the gas generated in them can be effectively transported by the EGTS system with appropriate selection of seal/backfill properties. The following issues are of importance:

- After the closure of the L/ILW repository, a sufficiently large gas storage volume should be available to accommodate the generated gas with moderate gas pressures over a period of approx. 100 years. An increase of this volume reduces the pressure build-up and delays the time of the gas pressure breakthrough.

- Once the gas pressure in the repository exceeds the hydrostatic pressure (reference value 2.2 MPa according to chapter 2.2), gas will be released along the engineered gas transport system. Note in this context, that the gas entry pressure of sand/bentonite mixtures with low bentonite content is typically < 1 MPa. Through the gas pressure, a small fraction of the porewater in the repository seal V4 will be displaced followed by the formation of a continuous gas pathway. The transport capacity of this pathway is sufficient to release the gas generated in the emplacement caverns through the access tunnel.

- The maximum gas pressure in the emplacement caverns is reached just before the breakthrough of the gas phase in the backfilled access tunnel ("gas breakthrough"). The maximum gas pressure depends primarily on the design of the repository seal V4 and secondarily, on the total available gas storage volume. Through an appropriate design of the repository seal V4 the maximum gas pressure can be kept below the lithostatic pressure.

Fig. 4-8: 3-D model of the engineered gas release system with impermeable host rock: spectrum of the temporal development of the gas pressure build-up in the emplacement caverns.

Impact of the seal and plug design on the pressure build-up in cavern no. 1.
The most important design parameters of the repository seal are the permeability of the sealing material and the length of the sealed section. For the design of the repository seal, site specific parameters, in particular the formation pressure of the local aquifer system and the local formation stresses, must be considered. For the assumed geological setting and the layout of the generic repository (cf. chapter 2) the transport capacity of the EGTS is sufficient, when the length of the repository seal $V_4$ is less than 37.5 m (e.g. 25 m) and the intrinsic permeability of the sand/bentonite mixture is higher than $1 \times 10^{-18}$ m$^2$ (e.g. $1 \times 10^{-16}$ m$^2$).

A gas permeable shaft seal $V_3$ (e.g., sand/bentonite backfill 80/20, similar with the V5 cavern seal) is a possible design variant of the EGTS, which can increase the gas transport capacity. Furthermore, in the test area additional gas storage volume can also be made available.

### 4.3.4 Combined gas release through the host rock and along the repository structures

**Purpose and model set-up**

The interaction of the various gas paths (i.e. host rock and EGTS), which contribute to gas storage and gas release, is simulated with an integrated 3-D model. The purpose of the simulations is to assess the evolution of the repository system focusing on the following aspects:

- Estimation of the temporal evolution of the gas pressure build-up in the emplacement caverns. The spectrum of the defined runs addresses both conceptual as well as parametric uncertainties with respect to the gas release.
- Quantitative description of the porewater circulation in the vicinity of the repository (the porewater displacement due to gas generation).
- Quantitative description of the saturation distribution in the emplacement caverns and in the surrounding host rock (also relevant for self-sealing processes through hydrochemical interactions).

The geometry of the integrated 3-D model is the same as the one used for the 3-D model described in chapter 4.3.3. In addition gas pathways through the host rock are now explicitly included, as described in chapter 4.2 (Tab. 4-1). The development of the 3-D model geometry was automated using the visualization software 'mView' (Calder & Avis 2006). The horizontal geometry is represented by a nested grid with refinements near the tunnels and caverns, resulting in 8'329 elements per layer (Fig. 4-9a). The vertical discretization is represented by 36 horizontal layers, comprising the low-permeability host rock (Opalinus Clay) and the higher permeability Passwang Formation at the top and Lias-Keuper Formation at the bottom (Fig. 4-9b). The entire model is comprised of 299'844 elements. In comparison, the 3-D model as described in chapter 4.3.2 (including the disturbed zone around the cavern and tunnels) consists of only 27'822 elements. Detailed views of various repository components are shown Figures 4-9c and d.
Fig. 4-9: 3-D model with repository structures and geosphere (note vertical exaggeration).

a) Plane view of the model grid on the repository level
b) Vertical cross section along cavern no. 4
c) Vertical cross section along the access and operation tunnel
d) Vertical cross section along the axis of an emplacement cavern.
The numerical simulations were run on a Linux cluster with 24 CPUs (Intel Xeon CPU 5150 @ 2.66 GHz). The base case in Table 4-6 required 14'924 time steps with a total run time of 66.3 hours.

**Gas pressure development in the emplacement caverns**

A series of simulation runs were defined and performed with the 3-D model; these are described in Senger & Ewing (2009). From these simulations the following modelling results were extracted: the temporal evolution of the water pressure, the gas saturation, as well as the gas and water fluxes in and around the underground structures. The most important cases are documented in Table 4-6 and are discussed below. The hydraulic properties of the confining units are given in Table 4-1.

Run R_CM01 is the base case for the sensitivity analyses. The model parameters for the base case are not identical to the reference values given in chapter 3 (RV column in Tab. 3-3). In fact, the base case parameters were specified for investigating a repository configuration which is associated with the development of high gas pressures. In particular, the host rock permeability in the R_CM01 was set five times lower than the reference value for the L/ILW repository, which corresponds to the reference value of a SF/HLW repository in the Zürcher Weinland. In addition, the intrinsic permeability of the cavern plugs was decreased by an order of magnitude compared to the value of the reference design.

Run R_CM02 studied the influence of an increased permeability of the repository seal ($k_v = 1 \times 10^{-18}$ m$^2$), whereas in R_CM03 the host rock permeability corresponds to the reference value according to Table 3-3.

Runs R_CM04 to R_CM06 were defined as sensitivity runs for evaluating the influence of the two-phase flow parameters of the host rock and of the engineered barriers (variation of capillary strength and residual water saturation of the host rock, length of the repository seal). In run R_CM07 a conservative gas generation rate, as shown in Figure 4-4, was chosen. Run R_CM08 was conducted without gas generation to compare the modeling results of resaturation with the hydrodynamic site model (cf. chapter 4.4.1).

The simulations with the integrated 3-D model are complemented with runs R_CM09 and R_CM10. These two runs are aimed at assessing the impact of an enlarged waste inventory as discussed in chapter 2.7 ("bounding inventory" with a L/ILW volume of 200'000 m$^3$ according to Nagra 2008e). For this purpose, the realistic gas generation rate according to the waste inventory MIRAM 2005 is multiplied by a factor of 2.5. The repository geometry, however, remained unchanged, i.e. the enhanced gas transport capacity of the host rock due to an extended disposal area is not considered here. Thus, runs R_CM09 and CM10 represent conservative bounding cases for the bounding inventory for L/ILW. Run R_CM09 is based on the configuration parameters according to run R_CM04, whereas in run R_CM10 the repository seal $V_4$ and the cavern plugs $V_5$ exhibit a permeability $k_{V_4} = k_{V_5} = 1 \times 10^{-17}$ m$^2$ which is enhanced by a factor of 10.
Tab. 4-6: Simulation for the combined gas transport through the host rock and the repository structures: spectrum of the model parameters for the sensitivity analyses with the 3-D model (properties of the confining units given in Tab. 4-1).

<table>
<thead>
<tr>
<th>Model Parameters</th>
<th>Parameter Values</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Base case R_CM01</strong> (refers to case SMA4_QGR1 in Senger &amp; Ewing 2009)</td>
<td></td>
</tr>
<tr>
<td><strong>Host rock properties</strong></td>
<td></td>
</tr>
<tr>
<td>Intrinsic permeability of host rock:</td>
<td>$k_h = 1 \times 10^{-20} \text{ m}^2$, $k_v = 2 \times 10^{-21} \text{ m}^2$</td>
</tr>
<tr>
<td>Capillary strength</td>
<td>18 MPa</td>
</tr>
<tr>
<td>Porosity</td>
<td>12 %</td>
</tr>
<tr>
<td>Parametric model (two-phase flow)</td>
<td>van Genuchten ($n = 1.67$)</td>
</tr>
<tr>
<td>Residual water saturation $S_{wr}$</td>
<td>0.3</td>
</tr>
<tr>
<td>residual gas saturation $S_{gr}$</td>
<td>0.0</td>
</tr>
<tr>
<td>Specific storage</td>
<td>$1.7 \times 10^{-6} \text{ m}^{-1}$</td>
</tr>
<tr>
<td>Intrinsic permeability of EDZ</td>
<td>$1 \times 10^{-19} \text{ m}^2$</td>
</tr>
<tr>
<td><strong>Properties of cementitious backfill (cavern)</strong></td>
<td></td>
</tr>
<tr>
<td>Intrinsic permeability</td>
<td>$1 \times 10^{-15} \text{ m}^2$</td>
</tr>
<tr>
<td>Capillary strength</td>
<td>4 kPa</td>
</tr>
<tr>
<td>Porosity</td>
<td>25 %</td>
</tr>
<tr>
<td>Parametric model</td>
<td>van Genuchten ($n = 2.5$)</td>
</tr>
<tr>
<td>Residual water saturation $S_{wr}$</td>
<td>0.3</td>
</tr>
<tr>
<td>Residual gas saturation $S_{gr}$</td>
<td>0.0</td>
</tr>
<tr>
<td><strong>Properties of sand/bentonite (access tunnels /seals)</strong></td>
<td></td>
</tr>
<tr>
<td>Intrinsic permeability of tunnel backfill</td>
<td>$1 \times 10^{-16} \text{ m}^2$</td>
</tr>
<tr>
<td>Intrinsic permeability of repository seal V4</td>
<td>$1 \times 10^{-19} \text{ m}^2$</td>
</tr>
<tr>
<td>Intrinsic permeability of cavern plug V5 and test area seal V3</td>
<td>$1 \times 10^{-18} \text{ m}^2$</td>
</tr>
<tr>
<td>Capillary strength</td>
<td>4 kPa</td>
</tr>
<tr>
<td>Porosity</td>
<td>30 %</td>
</tr>
<tr>
<td>Parametric model</td>
<td>van Genuchten ($n = 2.5$)</td>
</tr>
<tr>
<td>Residual water saturation $S_{wr}$</td>
<td>0.3</td>
</tr>
<tr>
<td>Residual gas saturation $S_{gr}$</td>
<td>0.0</td>
</tr>
<tr>
<td><strong>Important state conditions</strong> (reference Level: 175 m asl)</td>
<td></td>
</tr>
<tr>
<td>Hydrostatic formation pressure / assumed lithostatic pressure:</td>
<td>2.2 MPa / 8.125 MPa</td>
</tr>
<tr>
<td>Initial water saturation of cavern backfill:</td>
<td>0.7</td>
</tr>
<tr>
<td><strong>Gas Generation</strong></td>
<td></td>
</tr>
<tr>
<td>Gas generation rate</td>
<td>&quot;realistic rates&quot; according to Fig. 4-4</td>
</tr>
<tr>
<td>Start of gas generation</td>
<td>Immediately after repository closure</td>
</tr>
</tbody>
</table>
Tab. 4-6: (continued)

<table>
<thead>
<tr>
<th>Model Parameters</th>
<th>Parameter Values</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Base case R_CM01</strong></td>
<td></td>
</tr>
<tr>
<td>(refers to case SMA4_QGR1 in Senger &amp; Ewing 2009)</td>
<td></td>
</tr>
<tr>
<td><strong>Simulation Runs</strong></td>
<td></td>
</tr>
<tr>
<td>R_CM2 (QGR2)</td>
<td>- permeability of repository seal V4: ( k = 1 \times 10^{-18} \text{ m}^2 ) (all other parameters according to R_CM1)</td>
</tr>
<tr>
<td>R_CM3 (QGR4)</td>
<td>- permeability of host rock: ( k_h = 5 \times 10^{-20} \text{ m}^2 ), ( k_v = 1 \times 10^{-20} \text{ m}^2 ) (all other parameters according to R_CM2)</td>
</tr>
<tr>
<td>R_CM4 (QGR9)</td>
<td>- inverse of capillary strength of host rock ( 1/\alpha = 5 \text{ MPa} ) (all other parameters according to R_CM5)</td>
</tr>
<tr>
<td>R_CM5 (QGR8)</td>
<td>- residual water saturation of host rock and EDZ: ( S_{wr} = 0.5 ) (all other parameters according to R_CM3)</td>
</tr>
<tr>
<td>R_CM6 (LBNL2)</td>
<td>- permeability of cementitious backfill: ( k = 1 \times 10^{-17} \text{ m}^2 ), seal length V4: 82.5 m; V5: 52.8 m as specified in Table 4-3 (all other parameters according to R_CM1)</td>
</tr>
<tr>
<td>R_CM7 (QGR8)</td>
<td>- conservative gas generation rate (all other parameters according to R_CM5)</td>
</tr>
<tr>
<td>(R_CM8) (SAT1)</td>
<td>- resaturation without gas generation (all other parameters according to R_CM1)</td>
</tr>
<tr>
<td>R_CM9 (QGR11)</td>
<td>- gas generation rate, accounting for an enlarged waste inventory: gas generation rates of MIRAM 2005 multiplied by factor 2.5 (all other parameters according to R_CM4)</td>
</tr>
<tr>
<td>R_CM10 (QGR12)</td>
<td>- permeability of repository seal V4 and cavern plug V5: ( k = 1 \times 10^{-17} \text{ m}^2 ) (all other parameters according to R_CM9)</td>
</tr>
</tbody>
</table>

Figure 4-10 presents the evolution of the gas pressure (note, in the fully saturated model domains gas pressure is equal to porewater pressure; cf. Eq. 3-7) in the vicinity of the repository for the base case (R_CM01) at different times after repository closure and onset of gas generation. Figure 4-10a shows the pressure distribution in a three-dimensional representation after 1'000 years. A series of contour plots of the gas pressure in the 2D horizontal plane of the repository level is displayed in Figure 4-10b – d. According to Figure 4-10b the gas pressure increases to about 5.7 MPa in the emplacement caverns and to about 4.2 MPa in the surrounding near-field after 1'000 years. Gas pressure in the caverns exceeds the hydrostatic formation pressure, while the surrounding rock zone of the test area is still affected by the sub-hydrostatic conditions from the construction and operational phase. The gas pressure in the operations tunnel is about 5 MPa and decreases across the test area plug to about 2.9 MPa. In the access tunnel the gas pressure decreases from about 5 MPa to about 4.6 MPa near the repository seal, resulting in a steep gradient across the repository seal V4, which is represented by hydrostatic pressure boundary conditions on the outer model boundary.

After 1'000 years (Fig. 4-10c) the gas pressures in the rock around the caverns have not changed significantly from those after 1'000 years. However, the pressures increase to about 7.4 MPa in the caverns and to about 7.3 MPa in the operation tunnel. In the access tunnel the pressure decreases to about 7.1 MPa towards the repository seal V4 and to about 7.2 MPa across the test area plug.
Fig. 4-10: Evolution of gas pressure in the vicinity of the repository for base case R_CM01.
Fig. 4-11: 3-D model with gas release through the host rock and along the repository structures: spectrum of the temporal evolution of the gas pressure in the emplacement caverns.

Impact of the repository seal design and host rock properties on the pressure build-up in cavern no. 1.

After 100,000 years (Fig. 4-10d) the gas pressure increases to about 7.9 MPa in the caverns and to about 7.8 MPa in the operations tunnel with only a small decrease to 7.6 MPa toward the repository seal V4. However, the pressure in the rock zone around the cavern decreases to near hydrostatic pressure of about 2.5 MPa. The cavern pressure of 7.9 MPa after 100,000 years is lower than the peak pressure which occurs after about 50,000 years as shown in the pressure development in cavern no. 1 for the base case R_CM01 in Figure 4-11.

Figure 4-11 shows the gas pressure evolution in cavern no. 1 for the cases R_CM01 to R_CM04. Only for the base case the critical gas pressure increases to over 8 MPa; in this case the host rock permeability is very low and at the same time very low permeability repository seal V4 and cavern plugs V5 are assumed ($k_{V4} = 1 \times 10^{-19} \text{ m}^2$, $k_{V5} = 1 \times 10^{-18} \text{ m}^2$). The maximum pressure is reached, in this case, after about 50,000 years. In case R_CM02, the permeability of the repository seal V4 is increased by one order of magnitude. For the first 1,000 years the pressure development is practically identical to that of the base case, because the gas pressure in the underground structures is below the effective gas threshold pressure of the sand/bentonite mixture of the repository seal and the repository represents a largely closed gas storage system. The gas breakthrough in the access ramp occurs after 1,000 years, displacing some porewater and developing a distinct gas pathway through the repository seal V4. After the gas breakthrough, a quasi-stationary gas flow occurs along the access tunnel, represented by a gradual decrease in gas flow corresponding to the decline in the gas generation rate and a concomitant decrease in gas pressure in the repository. The difference in the pressure build-up between the base case R_CM01 and R_CM02 is solely caused by the difference in the permeability of the repository seal V4, representing the largest effect in terms of the overall pressure build-up compared to the other cases in Figure 4-11.
Cases R_CM03 and R_CM04 were defined to investigate the role of the host rock. The important host rock parameters are the intrinsic permeability and the capillary strength. In case R_CM03, the host rock permeability was increased by half an order of magnitude compared to the base case, corresponding thus to the reference values defined in Table 3-3. In case R_CM04, the capillary strength was reduced from 18 MPa to 5 MPa and the residual water saturation (for relative permeability) was increased from 0 to 0.5. Case R_CM05 was modified from Case R_CM03 considering only the effect of the increased residual water saturation of the host rock and of the EDZ. All three cases used the higher permeability of the repository seal (V4) according to Case R_CM02. Both cases show differences in the gas pressure development compared to the base case R_CM01 and Case R_CM02 after a few decades. The increase in host rock permeability by half an order of magnitude results in a delay and in a decrease of the peak pressure in the repository from 6'160 kPa after about 3'000 years for Case R_CM02 to 5'570 kPa after about 8'000 years for Case R_CM03. The reduction in capillary strength of the host rock (Case R_CM04) results in a decrease in the peak pressure to 5'120 kPa without shift in the peak compared to Case R_CM02.

Further cases were evaluated to study parameter sensitivities with respect to the backfill materials and different gas generation rates (Fig. 4-12). The results of Case R_CM05 considering only the effect of increased residual water saturation yielded a slightly higher peak pressure of 5'670 kPa after 7'750 years, compared to Case R_CM03. For Case R_CM06 it was assumed that the cementitious backfill of the caverns has lower intrinsic permeability, namely $1 \times 10^{-17}$ m², and the lengths of the seals V4 and V5 correspond to those used in the hydrodynamic model (82.5 m and 52.5 m according to Tab. 4-3). Case R_CM06 yielded a peak pressure of 7'800 kPa after 7'700 years, which is a significantly higher pressure build-up than Case R_CM03.
Case R_CM07 considered the same model parameters as in R_CM05, but assumed a conservative gas generation rate as shown in Figure 4-4. The peak pressure for Case R_CM07 increased to 10'100 kPa after 5'500 years (Fig. 4-12).

Except for case R_CM07, no gas pressures that lie above the lithostatic pressure were obtained. It is apparent that the decrease of the capillary strength decreases the gas pressure build-up only marginally, whereas the reduction of the gas permeability of the cavern backfill results in a significant increase in the pressure in the caverns; the gas generated in the caverns can only migrate slowly along the engineered gas release system. Case R_CM07 demonstrates clearly that for conservative gas generation rates the gas transport capacity of the EGTS needs to be increased. This could be achieved, for example, by increasing the intrinsic permeability of the repository seal V4.

The simulation cases R_CM09 and R_CM10 are dedicated to the impact of an enlarged waste inventory for L/ILW. For this purpose, the realistic gas generation rate according to the waste inventory MIRAM 2005 is multiplied by a factor of 2.5 (Figure 4-13). The repository geometry and in particular the size of the emplacement caverns remains unchanged. Thus, runs R_CM09 and CM10 represent conservative bounding cases for the bounding inventory for L/ILW, because (i) the initial gas storage capacity of the repository structures and (ii) the overall gas transport capacity of the host rock are underestimated significantly. Run R_CM09 is based on the input...
parameters according to run R_CM04, which represents a realistic configuration for a repository in the Bözberg area. The evolution of gas pressure in cavern no. 1 is displayed in Figure 4-13. A rapid pressure build-up develops within the first 10 years after repository closure, which can be attributed to the fact that the model does not account for the additional initial gas storage capacity of a repository for an enlarged L/ILW inventory. The maximum pressure is approximately 8.5 MPa, exceeding slightly the critical gas pressure, which corresponds to the level of lithostatic stress (8.125 MPa). A significant reduction of the maximum pressure is obtained by increasing the transport capacity of the engineered gas transport system. Enhancement of the permeability of the repository seal and the cavern plugs by the factor 10 ($k_{V4} = k_{V5} = 1 \times 10^{-17} \text{ m}^2$) leads to a maximum pressure of 7.6 MPa as shown in run R_CM10. Further issues for design optimization were not assessed in this study. The presented simulations demonstrate clearly the potential for further optimisation of the repository design, to ensure that gas over-pressure build-up remains in the desired range even for an enlarged L/ILW inventory.

Saturation distribution in the vicinity of the backfilled underground structures

The development of the saturation conditions in the backfill of the underground structures and in the surrounding near-field is particularly important for the assessment of hydrochemical interactions, which according to the discussion in chapter 3.4 can lead to self-sealing processes in the host rock and the backfill. Such self-sealing processes could also affect the function of the engineered gas release path.

The saturation conditions in the repository near-field are discussed using the base case R_CM01 as example. This case represents a combination of a low permeability host rock and an engineered gas release path with reduced gas transport capacity. Such a design variant for the repository seal would not be chosen for a L/ILW repository in a very low permeable host rock and in this sense case R_CM01 can be considered as a conservative parameter variant. Nevertheless, for the development of a fundamental understanding of gas transport in the repository near-field, the base case is well suited because the desaturation around the emplacement caverns and in the backfill due to the increased gas pressure is more prominent than it would be for the realistic model variant (i.e., case R_CM03).

Figure 4-14 shows the development of the gas saturation ($S_g = 1 - S_w$) and the specific gas flux in the near-field of the repository cavern no. 1 at 1'000, 10'000 and 100'000 years. The specific gas flux is depicted in the figure in a vector form. The length of the flux vector represents the magnitude of the gas flux on logarithmic units and is scaled according to the following relationship:

$$\text{Log-Velocity} = \text{Vector_Length}/2 + \text{Log (min. Velocity)}$$

where the minimum velocity (i.e., cutoff value) was set $1 \times 10^{-15} \text{ m/s}$; that is a vector length of 10 m corresponds to a specific flux of $1 \times 10^{-10} \text{ m/s STP}$, and a vector length of 2 m corresponds to a specific flux of $1 \times 10^{-14} \text{ m/s}$).
Fig. 4-14: Evolution of gas saturation and specific gas flux in the vicinity of the repository for base case R_CM01.
The contour representation of the gas saturation distribution is also given in a logarithmic scale ranging between a minimum of $1 \times 10^{-4}$ and a maximum of 1. The saturation distribution in Figure 4-14 clearly shows that for the entire simulation period the desaturation of the host rock is limited to a few meters in the immediate near-field of the caverns. The gas saturation in this zone is a few percent (or equivalently the water saturation $S_w$ is typically > 0.9). The gas flux in the repository system indicates two flow regimes: (1) one part is flowing axially along the underground structures (engineered gas transport system), and (2) another part is flowing radially into the host rock. The radial gas flux into the host rock is confined to the immediate vicinity of the caverns. This is in contrast to the 2-D calculation shown in chapter 4.3.2, where the gas flow extends relatively far into the host rock. The results of the 3-D model show that the gas release to the adjacent rock is limited and the dominant gas flow is through the EGTS. Nevertheless, as the comparison with the 3-D model in chapter 4.3.3 shows, the host rock is important for the gas release, because considering the host rock leads to a significant reduction in the pressure build-up in the early gas production phase. The contribution of the host rock increases due to an increasing effective radial surface area of the underground structures, allowing for advective and diffusive outflow of dissolved gas.

Porewater circulation in the vicinity of the backfilled underground structures

The analysis of porewater circulation in the vicinity of the repository is important for the transport of dissolved radionuclides. As a result of high gas pressures in the caverns, contaminated porewater could be displaced into the geosphere over long time periods. The investigation of the two-phase flow conditions in the near-field helps to better understand the significance of gas pressure as an additional driving force for mass transport. The porewater circulation in the vicinity of the repository caverns will be discussed in the following, also in the context of the base case R_CM01.

The gas pressure$^{10}$ and the specific water flux in the repository cavern no. 1 near-field are shown in Figure 4-15 for different vertical sections for 1'000, 10'000 and 100'000 years. Similarly to Figure 4-14, the specific water flux is introduced in vector form, where the length of the flux vector represents the magnitude of the specific water flux in logarithmic units (vector length of 10 m corresponds to a specific water flux of $1 \times 10^{-10}$ m/s). The porewater circulation around the cavern shows a complex spatial and temporal evolution. At early times (1'000 years) the resaturation of the access tunnel and gas pressure build-up in the emplacement caverns result in a flow pattern, where porewater from the caverns is displaced into the host rock, whereas porewater inflow is observed towards the access tunnel. The specific fluxes from the caverns into the host rock are typically between $1 \times 10^{-12}$ and $5 \times 10^{-12}$ m/s.

After 10'000 a, significant overpressures are observed in all underground structures. The water fluxes are equally distributed both in upward and downward directions with specific fluxes in the range $1 \times 10^{-12}$ to $1 \times 10^{-13}$ m/s. The host rock zone around the repository which is affected by the displacement of porewater exceeds the cross-sectional area of the repository by about 100 – 150 m.

After 100'000 a, when the peak overpressure in the repository has been exceeded and the gas generation in the caverns ceases, the specific fluxes in the vicinity of the repository drop to values below $5 \times 10^{-14}$ m/s. This means that in this time period there is effectively no displacement of contaminated porewater into the host rock and the flow direction ultimately reverses until the caverns are fully water saturated.

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$^{10}$ Note: In the fully saturated rock, gas pressure is equal to water pressure according to Eq. 3-7.
Specific fluxes from the caverns into the host rock were also calculated for R_CM04, which is more representative for the expected site conditions in the Bözberg area. The corresponding fluxes are slightly higher due to the higher permeability of the rock, but still in a range, where radionuclide transport is a diffusion-dominated process. After 1'000 a the specific fluxes from the emplacement caverns into the host rock range between \(3 \times 10^{-12}\) and \(3 \times 10^{-11}\) m/s, after 10'000 a between \(2 \times 10^{-13}\) and \(1.4 \times 10^{-12}\) m/s and after 100'000 a the flow reversed into the cavern and fluxes decreased to less than \(1 \times 10^{-13}\) m/s.

Assessment of the combined gas release through host rock and along the engineered gas transport system

The integrated 3-D model simulates the interaction of the different gas pathways, i.e. through the host rock and along an engineered gas transport system (EGTS). Compared to the separate consideration of the gas pathway in the host rock (chapter 4.3.2) and in the EGTS (chapter 4.3.3), it is shown that the repository system in many ways acts in a much more robust way with respect to the gas overpressures in the repository caverns. In combination, the two gas pathways allow an effective transport of the gas generated in the emplacement caverns, during which the porewater circulation in the repository near-field and its long-term evolution is hardly affected. The most important conclusions from the model of the gas migration in the repository near-field are:

- During the early phase of gas pressure build-up, when one expects high gas generation rates (Fig. 4-4), the available gas storage volume increases due to the gas-permeable cavern plugs. Through this effect the gas pressure build-up in the first 1'000 years is slowed down markedly, even for the cases with very low host rock permeability. The maximum gas pressure in the caverns for the reference case of the sealing system (length 37.5 m; \(k = 1 \times 10^{-18}\) m²) is approximately 5 – 6 MPa, which is 3 – 4 MPa above the hydrostatic pressure conditions. This pressure is significantly lower than the expected lithostatic pressure, so that dilatancy-controlled gas transport processes can be excluded outright.

- Even in the case of relatively low host rock permeability, the EGTS ensures an efficient transport capacity for gases from the emplacement caverns. Through the optimisation of the EGTS (for example, gas permeable seal V2, shorter cavern seal etc.) appropriate design variations can be developed that would allow the transport of gas without extreme overpressures, even for the case of extreme site conditions (very low host rock permeability, high formation water pressure).

- In the early post closure phase (\(\leq 1'000\) a) the specific flux from the emplacement caverns into the host rock is in the order of \(1 \times 10^{-12}\) and \(3 \times 10^{-11}\) m/s (corresponding to the simulation runs R_CM01 and R_CM04, respectively). No significant displacement of contaminated porewater will occur as a result of gas release after the maximum overpressure is past: after 100'000 years, the value of the specific water flux through the host rock formation is in the order of magnitude of \(1 \times 10^{-13}\) m/s, so that one can expect diffusion-dominated radionuclide transport in this time period.

- The interfaces between the cavern backfill and the host rock, as well as the sand/bentonite backfill of the cavern plug remain partially saturated during the entire period of gas generation. This also ensures that a complete self-sealing of these interfaces due to hydrochemical interactions is very unlikely.
Fig. 4-15: Evolution of pressure and specific water flux in the vicinity of the repository for base case R_CM01: cross sections in the X-Z plane (a – c) and Y-Z plane (d – f).

- a) Vertical cross-section X-Z after 1'000 a
- b) Vertical cross-section X-Z after 10'000 a
- c) Vertical cross-section X-Z after 100'000 a

Specific pore water flux: $10^{-10}$ m/s, $10^{-11}$ m/s, $10^{-12}$ m/s
f) Vertical cross-section Y-Z after 10'000 a

c) Vertical cross-section Y-Z after 10'000 a

d) Vertical cross-section Y-Z after 1'000 a

Specific pore water flux: $10^{-10}$ m/s, $10^{-11}$ m/s, $10^{-12}$ m/s

Fig. 4.15: (continued)
4.4 Evaluation of system understanding

4.4.1 Evolution of the repository system after closure

The evolution of the system after repository closure was analysed with two complementary system models, which differ with respect to the degree of detail of the model implementation (geometrical abstraction, process abstraction, abstraction of the development scenarios). The conventional hydrodynamic site model (chapter 4.2) was mainly used to assess the evolutionary uncertainties associated with the hydrogeological site conditions (e.g. hydraulic boundary conditions, characteristics of the hydraulic units, impact of regional faults). In this model, the geological conditions and the underground structures were represented with a high degree of geometric detail. Due to the simplified assumptions for the representation of the flow processes in the hydrodynamic model (Richards’ equation for unsaturated groundwater flow), it is not appropriate for the simulation of gas transport processes. However, when gas production in the emplacement caverns is not considered, the pressure recovery in the host rock and the resaturation process in the backfilled repository structures can be represented, with certain limitations, with simplified flow laws. Such calculations are important for estimating the resaturation times of the caverns as a determining factor for the gas storage capacity of the cavern backfill in the early post-closure time.

The combined effect of the repository resaturation and the transport of waste-generated gas along the underground structures and through the geosphere can be simulated appropriately with the two-phase flow model described in chapter 4.3.4. However, due to the more extensive computational effort required for two-phase flow simulations, extensive simplifications had to be made in terms of the geometric detail (representation of the underground structures) and the number of alternative calculational cases had to be limited. To evaluate the consistency of the two complementary models with respect to the evolution of the repository saturation, several comparison cases were conducted. The bases for the comparison were simulation runs R_RM5 (Tab. 4-3) for the hydrodynamic site model and R_CM8 (Tab. 4-6) for the two-phase 3-D model. Because the laws for flow in an unsaturated/saturated medium are formulated differently in the two cases, two different variants of the initial conditions were examined:

- **Variant 1**: During the construction and operation phase of the repository, the pressure in the underground structures is equal to the atmospheric pressure. After repository closure, it is assumed that the initial saturation of the backfilled underground structures is $S_{wi} = 1$; this implies that the underground structures become fully saturated instantaneously. This model variant can help to assess the influence that the geometrical differences (e.g. orthogonal cross sections, layout of the underground structures) in the model implementation have in the development of the pressure recovery in the saturated host rock.

- **Variant 2**: During the construction and operation phase of the repository, the pressure in the underground structures is equal to the atmospheric pressure. After repository closure, it is assumed that the initial saturation in the backfilled underground structures is $S_{wi} = 0.7$. According to case R_CM8 (Table 4-6). This model variant examines the influence of the simplified formulation of the unsaturated-saturated flow on the simulation of the saturation of the repository using the hydrodynamic model.

For both variants which differ in the implemented initial conditions, the evolution of the hydraulic potential was examined in different locations in the models, which include (i) the centre of caverns 1 and 4, (ii) the intersection of the access tunnel with the pilot facility, and (iii) the test area. The various observation locations are indicated in the 3-D view of the two-phase flow model shown in Figure 4-16a (note that due to the different model geometries, the node location of the observation points in the two-phase flow model do not exactly correspond to those in the
hydrodynamic model). Figure 4-16b shows the results for Variant 1 for the hydrodynamic model (HDM) and the two-phase flow model (TPF). The evolution of the pressure build-up is very similar for both models. Because of the assumption of initial full saturation in all the underground structures, the pressure rises already after a few years in the backfilled access tunnels and caverns and after about 120 years in the test area. Approximate steady-state hydrostatic conditions are reached after several thousand years. The exceptionally good agreement of the models indicates that the differences in the geometric detail in the modelling of the repository behaviour have only a very small effect on the simulated resaturation times.

The simulations of Variant 2 indicate more complex behavior. The HDM uses the Richards' equation for simulating unsaturated flow associated with the saturation of the engineered structures. For this, a saturation-dependent storage coefficient is calculated with the help of the assumed capillary pressure relationship according to van Genuchten. This implementation requires that the initial and residual water saturation in the chosen formulation of the van Genuchten relationship are equal; thus, the model parameters of the cavern backfill used in TPF run R_CM8 ($S_{wr} = 0.3$, $S_{wi} = 0.7$) could not be exactly reproduced in the HDM. Therefore, in order to guarantee that the initial water saturation of the cavern backfill is essentially the same in both models, the residual water saturation $S_{wr}$ in HDM has to be shifted towards the value of the initial water saturation $S_{wi}$ in the TPF model. A residual saturation of $S_{wr} = 0.68$ in the HDM is appropriate to represent the initial saturation of the underground structures as shown in Kuhlmann & Marschall (2008). A further simplification in the HDM is the representation of the unsaturated storage coefficient $S_s(S_w)$ of the tunnel backfill material. In the present study, only a single relationship $S_s(S_w)$ was applied, which does not describe adequately the differences between unsaturated storage coefficients of the cementitious backfill and the sand/bentonite, respectively.

Figure 4-16c displays the simulated pressure evolution of Variant 2 for both models. The same observation points as in Variant 1 are used. The simulated pressure recovery in the two caverns compare fairly well between the HDM and TPF model, respectively. The simulations indicate the onset of the pressure recovery in cavern 1 after about 5'000 years. The pressure recovery of the caverns in the center of the repository starts later and requires significantly longer than 10'000 years to approach hydrostatic pressure. A closer look at the pressure transients reveals the differences between the two modeling approaches. The HDM simulations exhibit a distinct kink in the pressure build-up, when the caverns are "quasi-saturated", whereas the TPF simulations show a smoother pressure increase, which is attributed to the capillarity of the buffer material. Nevertheless, the overall resaturation times of the caverns are reasonably well captured, except that significant deviations are seen in the resaturation of the access tunnel and the test area. As mentioned above, this discrepancy is probably due to the use of a single representation of the unsaturated storage coefficient $S_s(S_w)$ of the different backfill materials. More refined formulations of the unsaturated material properties are expected to reduce the discrepancy of the HDM in future simulations.

The comparison runs show that for the investigation of the temporal evolution of pressure recovery in the host rock formation and for the repository saturation without gas generation, the HDM model and the TPF model can be applied as complementary modelling tools. The strengths of the HDM are found in its flexibility to represent complex geological and engineering geometries in great detail and its ability to execute the simulations with reasonable computational effort. For a detailed analysis of the resaturation process in the underground structures however, the TPF model is more suitable, because it can better represent the two-phase behaviour of the flow of the gas and the fluid and the associated phase interference effects. For example, as shown in Senger & Ewing (2009), during the resaturation of the repository tunnels and seals opposing fluxes of gas and water occur; which cannot be reproduced with the HDM because in this model no mobile gas phase is accounted for.
Fig. 4-16: Comparison of resaturation results for 2 variants of initial conditions.

a) Various observation points in a 3-D view of the two-phase flow model
b) Variant 1 with fully saturated underground structures
c) Variant 2, starting with partial saturation of the repository system.
4.4.2 Impact of coupled phenomena on the evolution of the repository system

The model calculations for the development of the gas pressure in a L/ILW repository (chapter 4.3) show clearly that an engineered gas transport system (EGTS) can release the gas that is produced in the emplacement caverns very efficiently through the underground structures to the backfilled access tunnel and into the adjacent formation. Consequently, at no point in time are excessive gas pressures to be expected. Deviations from the expected system behaviour however, could result from the conceptual uncertainty associated with possible process couplings, such as hydrochemical interactions and hydromechanical processes in the immediate vicinity of the backfilled underground structures. Phenomenological evidence and the conceptual basis for the treatment of these coupled processes were discussed in detail in chapter 3.4. It was shown that primarily hydrochemical interactions can impair the long-term performance of the repository by reducing the gas transport capacity of the EGTS and the host rock. Such self-sealing processes can increase the possibility of developing critical gas pressures in the emplacement caverns.

The gas transport mechanisms and relevant hydromechanical and hydrochemical couplings were analysed and evaluated in chapter 3.4. This detailed process understanding is used below to provide a qualitative description of the long-term evolution of the emplacement caverns under the influence of gas generation. In particular, it is examined if hydrochemical interactions could lead to a sealing of the EGTS and of the gas paths through the host rock, respectively. For this purpose, the development of the repository is divided into the following phases (Fig. 4-17):

- operational phase of the deep repository, during which the open underground structures are continuously ventilated
- initial post-closure phase with a low degree of saturation of the backfill in the caverns
- initiation of the resaturation of the emplacement caverns after exceeding the maximum gas pressure in the emplacement caverns
- end of the gas production phase associated with a return to fully saturated conditions

The fluxes of gas and water in the vicinity of the caverns change significantly between each repository evolution phase defined above. For self-sealing processes to occur, the porewater flow regime (flow into, respectively, out of the cavern) and the degree of saturation of the cavern near-field are of main importance. Hydrochemical interactions can occur, for all practical purposes, only in the fully saturated portion of the pore space, whereas potential self-sealing processes in the gas-filled pore space are considered unimportant. In the following, the relevant transport processes in the different phases are discussed.
Fig. 4-17: Schematic sketch showing the evolution of cavern near-field during the operation phase and after closure.

- **a)** Development of an unsaturated zone during the operation phase
- **b) – d)** Mass transfer processes in the early time, mid time and late time after closure
- **e)** Mass transfer processes around the cavern plug after closure.
Operational phase of the deep repository (Figure 4-17a)

During the operation of the repository the underground structures will be continuously ventilated. The relative humidity of the inflowing air will be significantly below 100 % at an average temperature of around 20 – 30°C at repository level (depending on the depth of the repository). The reduced relative humidity in the cavern will impose a significant capillary suction pressure at the tunnel/cavern walls, resulting in a steep gradient for water flow from the surrounding rock into the tunnel/caverns. Due to the low permeability of the host rock, an unsaturated zone will develop in the host rock surrounding the underground structures, as the water from the host rock adjacent to the cavern surface is drained more readily into the cavern than it can be supplied from the surrounding rock. This results in an unsaturated zone in the vicinity of the cavern, characterised by significant suction pressures (i.e., negative water pressure). This unsaturated zone can have a thickness of several meters, whereby the zone with significant desaturation ($S_w < 0.9$) is restricted to a thickness of typically less than 1 m. Through the evaporation of the porewater in the repository atmosphere, precipitation of originally dissolved solids (e.g. Cl, $\text{SO}_4^{2-}$) will occur on the cavern surface.

In the framework of the EU co-funded project NFPRO (http://www.nf-pro.org/) at the Mont Terri URL, comprehensive scientific studies have been carried out on the development of the unsaturated zone around a ventilated tunnel (Mayor et al. 2007). In an in-situ experiment lasting more than 5 years, they observed the development of a capillary fringe within the unsaturated zone of a ventilated tunnel section and simulated a sequence of saturation and desaturation phases with numerical models. In addition, geo-chemical concentration profiles were determined in radial boreholes indicating salt enrichment in the unsaturated zone (e.g. Fernandez et al. 2007). The evolution of the cavern near-field during the operational phase can thus be described relatively well, both qualitatively and quantitatively, on the basis of the available experimental data. It is not expected that the build-up of mineral deposits during the operational phase will be of any importance for gas transport in the host rock during the post-operational phase.

Early post-operational phase until maximum gas pressure is reached (Figure 4-17b)

At the time of closure of the emplacement caverns, the backfill materials and the EDZ are not fully water saturated (chapter 3.3.3). After a short phase of aerobic corrosion (a few years only) which is of low significance for the following considerations, the onset of anaerobic corrosion processes will change the saturation conditions in the backfill and the surrounding host rock. The water saturation in the backfill may be reduced in the case of very low rock permeability ($K_{OPA} \leq 10^{-21} \text{ m/s}$), because the water consumption$^{11}$ by the corrosion process cannot be fully compensated from the influx of porewater through the host rock (cf. Eq. 2-4 / magnetite reaction: 1.33 mol of hydrogen per mol of corroded iron are formed; see also the scoping calculations in Appendix C). Furthermore, gas pressures will build up in and around the caverns that will limit the influx of porewater from the host rock for a very long time period. Therefore, it is expected that the unsaturated zone in the host rock will increase and the degree of saturation in the cavern backfill will stabilise for a long time close to the level of the residual saturation, $S_{wr} = 0.3$.

A closer observation of the two-phase flow processes in the unsaturated zone clearly shows that with an increasing gas pressure the gasfilled pore space in the host rock remains unchanged (macropores > 25 nm), whereas the influx of porewater is restricted to pores with smaller pore radii (micro- and mesopores; Tab. 3-2). Possible hydrochemical interactions are consequently

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$^{11}$ Water consumption by corrosion is neglected in the calculations presented in this report. An evaluation of the effect of water consumption on gas pressure build up is found in Poppei & Croisé (2006).
restricted predominantly to diffusion processes in the continuously water filled meso- and micropore space of the host rock; these interactions could lead at most to a partial self-sealing (green dashed line in Fig. 4-17b).

The model runs of the two-phase flow conditions in the cavern near-field clearly show that the emplacement caverns as well as the EDZ in the host rock exhibit relatively high gas saturations over time periods of 100'000 of years (Fig. 4-14). Because gas pressures in the emplacement caverns exceed the hydrostatic pressures already occur after a few decades, permanent pore-water flow out of the emplacement caverns into the host rock develops (Fig. 4-15). The water needed for maintaining anaerobic corrosion is provided predominantly through vapour diffusion from the host rock. The gas transport takes place predominantly along the EGTS, and to a lesser extent through the host rock (Fig. 4-14).

The model calculations support the conclusion that after the closure of the emplacement caverns, self-sealing processes due to hydrochemical interactions are of low significance even over very long time periods. As a result of gas overpressures in the emplacement caverns the gas migration pathway through the host rock and the engineered gas release system will be kept open over a period of more than 10'000 years. Thus, the unsaturated zone in the rock zone around the emplacement caverns will also provide an important contribution to gas migration, because possible hydrochemical sealing processes will be restricted principally to the water-saturated pore space within the micro- and mesopores, whereas the effective gas transport capacity of the unsaturated zone will be determined by the gas-filled macropores.

Begin of the saturation of the emplacement caverns (Figure 4-17c)

The emplacement caverns will begin to saturate only after the gas pressure decreases and approaches the hydrostatic pressure. The water influx to the caverns takes place through the host rock and also through the cavern plugs (Fig. 4-17e). Due to buoyancy effects it can be assumed that water saturation will increase preferentially in the lower part of the caverns, whereas the remaining gas will move upwards. It should be noted however, that the saturation distribution in the cavern backfill will basically be determined by the capillarity of the different backfill materials. This means that the construction concrete in the cavern base, which has small pores, will be saturated rather than the Mortar M1 in the cavern roof and the cavern sides, which has large pores. In the fully saturated areas of the cavern, self-sealing processes could occur on the boundary surface of the rock due to hydrochemical interactions. The self-sealing processes will be controlled by advective transport (porewater flow from the host rock into the caverns) and diffusive transport (mass flux along a chemical gradient), so that self-sealing can occur both in the saturated cement matrix and in the host rock, as shown by the red and green skin zones in Fig. 4-17c. The generated corrosion gas could still circulate freely in the unsaturated areas of the caverns, for example in the roof or in the highly porous mortar M1 in the cavern side walls, so that transport through the host rock and along the EGTS is still possible.

On the basis of the model calculations (chapter 4.3.4), it is expected that saturation of the emplacement caverns will eventually occur after more than 100'000 years, in the late gas generation phase (Fig. 4-4). At that point in time, an unsaturated zone of several meters will have formed in the host rock around the caverns, in which the mobility of gas is significantly increased. This is valid also for the cavern plugs and the backfilled access and operation tunnels (Fig. 4-17e). In this gas-filled pore space, occurrence of self-sealing processes due to hydrochemical interactions can be practically excluded, so that the gas transport capacity of EGTS and the host rock will not be in essence, reduced. Considering the reduced gas generation rate during this late phase, a renewed gas pressure build-up through hydrochemical self-sealing processes can be excluded.
End of the gas generation phase (Figure 4-17d)

At the end of the gas generation phase, the unsaturated zone in the host rock and the cavern backfill will decrease and the gas pressure in the caverns will equilibrate with the hydrostatic pressure. Some isolated zones with free gas phase will remain (trapped gas, most likely at the top of the cavern), which will disappear eventually through dissolution processes. Hydrochemical interactions as a result of advective and diffusive mass fluxes could lead to a self-sealing process at the host rock/concrete matrix contact in the saturated space and thus can reduce the porewater flux. With respect to the gas release however, this evolutionary phase of the cavern near-field is of no relevance and will not be further discussed in here.

4.4.3 Importance for long-term safety assessment

The numerical simulations presented in chapter 4 were aimed at developing a comprehensive understanding of the long-term evolution of the backfilled and sealed repository system concerning the impact of continuous gas production in the emplacement caverns. For this purpose a range of calculations were made to assess the behaviour of a generic L/ILW repository in the Opalinus Clay of Northern Switzerland due to gas generation. The key conclusions are:

- The time scale of repository resaturation is in the order of tens of thousands to over a hundred thousand years. Even for poor performance of the seals, the resaturation times are at least several thousands of years. For a very low permeability host rock, water consumption due to corrosion also contributes to a slowing of resaturation. Consequently, during the critical early phase of gas generation, the gas storage capacity of the emplacement caverns is still high. The creation of extended gasfracs which could impair the hydraulic barrier performance of the host rock can be excluded, because this fracture mechanism requires high pressure build-up rates.

- Through optimisation of the engineered gas transport system (EGTS), appropriate design variants can be developed that allow the release of gas without extreme overpressures, even for the case of very low permeability host rocks. Both the release of gas along the EGTS and through the host rock will contribute to keep the gas pressures at moderate levels.

- For a low permeability host rock gas flow is largely restricted to the EGTS and to a narrow host rock zone around the backfilled repository. Consequently, the breakthrough of the gas into the upper confining units is expected to occur locally around the backfilled access tunnel. The bulk of the host rock remains fully saturated at all time.

- Displacement of porewater into the host rock formation and along the EGTS due to the gas overpressures is of significance only during the early gas pressure build-up phase before the maximum gas pressure is reached.

- The radiological significance of porewater displacements from the emplacement caverns discussed in chapter 4.3 can be assessed by comparing the calculated transient flow rates with calculated doses for various steady-state water flowrates through L/ILW caverns that have been evaluated in Nagra (2008e). For a steady-state specific water flux of $10^{-11}$ m/s the calculated dose would be a factor of ten below the regulatory dose limit of 0.1 mSv/a (see Fig. A5.2-1 in Nagra 2008e). Consequently, an even lower dose rate would be expected for the case of a transient flow field with a maximum flux of $5 \times 10^{-12}$ m/s (corresponding to the maximum flux in simulation case R_CM01). This is confirmed by specific calculations in the framework of the on-going safety studies.
5 Summary and conclusions

Evaluation of the relevance of gas generation, accumulation and transport for a L/ILW repository in Opalinus Clay

In a Swiss repository for L/ILW it is expected that a total of 20 – 30 millions of cubic meters (STP) of gas will be generated by metal corrosion and degradation of organic substances. The potential impact of gas generation, accumulation and migration on the performance of both the engineered barriers and the natural geological barrier system is regarded as an important issue in the assessment of long-term radiological safety of a L/ILW repository, in particular when situated in a very low permeability host rock formation such as the Opalinus Clay of Northern Switzerland. Gas production in the disposal area may give rise to significant gas overpressures in the backfilled and sealed underground structures. Thus, the barrier function of both the host rock itself and of the engineered barrier system could be affected. An important factor to be assessed for the radiological long-term safety is the possibility for displacement of contaminated porewater from the emplacement caverns into the geosphere as a result of gas pressure build-up.

The present study provides an assessment of the gas issue for a generic geological repository for L/ILW in the Opalinus Clay of Northern Switzerland. The report draws on the L/ILW repository design and on the waste inventories, which were elaborated for the so-called Sectoral Plan for Geological Repositories, representing the framework for site selection within the Swiss nuclear waste disposal programme. For this report a potential siting region was selected to host the generic repository study in order to provide realistic geological conditions for sensitivity studies of the gas transport processes in the repository system. A gas-related design option was studied to evaluate the feasibility of an engineered gas transport system (EGTS), allowing for a controlled gas storage and gas transfer at moderate gas overpressures along the backfilled underground structures. Finally, simulation and assessment tools were elaborated to optimise the layout of a L/ILW repository with respect to the effects of post-disposal gas generation. The results show that gas pressure in a repository in Opalinus Clay is expected to remain below a level that could lead to a degradation in performance of the repository. The main findings with respect to gas generation rates, gas pressure build-up, design measures to mitigate overpressures and porewater displacement are discussed in the following sections.

Waste inventory and gas source term

The estimates of the gas generation rates for the L/ILW repository are based on Nagra's waste inventories MIRAM 2005 and MIRAM 2008. The waste inventory MIRAM 2008 includes a total mass of approximately 40'000 tons of steel, around 400 tons of aluminium and zinc and about 100 tons of Zircaloy. Organic matter is considered as a further gas-producing material, with a total mass of about 2'200 tons.

The gas generation rates calculated include hydrogen gas produced by anaerobic corrosion of the different metals and methane and carbon dioxide produced by degradation of organic components of the waste and consider degradation and corrosion rates specific for the different materials in the waste. Due to a very low $\alpha$-activity in L/ILW the gas generation from the radiolysis of water is not considered in the calculations. Revisions in the gas source term were made in the last years, caused by improvements in the waste inventories. The present report refers to the L/ILW waste inventories MIRAM 2005 (basis for all calculations) and MIRAM 2008.

The total amount of gas produced until the gas-producing material is degraded is approximately 20 – 30 million cubic meters (STP) in terms of mol-equivalent units. The highest gas generation
rates are expected in the early post-closure period. This early phase will last up to several hundreds of years, followed by a steady decline of the gas source term. The expected total duration of the gas generation phase is in the order of 200'000 years.

Repository layout and engineered gas transport system

The total gas storage volume in the backfilled repository is in the order of 58'000 m³, comprising the emplacement caverns (37'000 m³) and all other structures in the Opalinus Clay formation (21'000 m³). The comparison of the available pore volume with the total amount of gas produced reveals that the corrosion and degradation gases cannot be contained in the backfilled and sealed underground structures over the lifetime of the repository without reaching unacceptable pressure build-up. Consequently, the release of gas through the host rock and/or along the backfilled underground structures will occur.

Various engineering measures were assessed to reduce the possibility of excessive gas overpressures in the emplacement caverns. The options that are primarily considered are associated with an increase in the gas storage volume and an increase in the gas transport capacity of the backfilled underground structures. The concept of an engineered gas transport system (EGTS) was elaborated, aimed at a controlled release of the generated gases along the backfilled repository structures. Advantage is taken of specially designed backfill materials. Thus, high porosity mortars are selected as backfill materials for the emplacement caverns in order to increase the gas storage capacity. Sand/bentonite mixtures with a bentonite content of 20 – 30 % are chosen as backfill materials for the access tunnels and for the seals. The sand/bentonite mixtures with low bentonite content exhibit the favourable feature of low permeability to water, whereas the gas permeability is enhanced. With the EGTS concept the gas transport capacity of the backfilled underground structures can be increased significantly without significant negative impact on their radionuclide retention function.

This study is generic with respect to the geological and hydrogeological site conditions. Simplifying assumptions were made for a potential siting area in the Northern Aargau, such as hydrostatic head in the aquifer systems and horizontal layering of the hydrogeological units. Reference parameters for the hydraulic rock properties were derived from site investigations in the Zürcher Weinland and the Mont Terri URL. The uncertainties associated with the local hydrogeological conditions at a real L/ILW repository site were investigated and may have an impact on the detailed design of the EGTS. Sensitivity studies reveal, among other optimisation aspects, that the length and the permeability of the seals are key design parameters which can be adapted within a wide range to the site specific conditions, allowing for the release of the repository gases at moderate overpressures.

Possibility of high gas overpressures in the backfilled and sealed emplacement caverns

When gas overpressures in the emplacement caverns of a backfilled repository exceed a critical threshold value, dilatancy-controlled gas transport will occur ("pathway dilation"). This critical pressure level that characterises the onset of pathway dilation is determined by both the strength of the host rock and by the local stress conditions around the emplacement caverns. Although pathway dilation is not considered to be very critical for host rock barrier performance due to the excellent self-sealing properties of the Opalinus Clay, as a precautionary principle it is nevertheless investigated if and how much the gas pressure can be kept below this critical threshold value. Due to the generic character of this study, without detailed knowledge of the site specific rock stress, the critical gas overpressures may be inferred from experience in other disciplines such as natural gas storage and CO₂ sequestration. The Canadian Standards Associa-
tion recommends e.g., in order to minimise gas leakage from storage facilities, that the maximum operating pressure of natural gas storage systems shall not exceed 80 % of the fracture pressure of the cap-rock formation. In rocks with low tensile strength such as the Opalinus Clay formation, the lithostatic pressure is often used as an indicator for the fracture pressure. Hence, in the context of this generic study the assumed lithostatic pressure at repository level is 8.125 MPa and the corresponding threshold pressure for the onset of pathway dilation is assumed to be 6.5 MPa (reference repository level: 175 m asl).

The development of gas overpressures in the backfilled emplacement caverns is unavoidable, because the produced corrosion and degradation gases can neither be dissolved completely in the porewater of the cavern near-field nor stored in the gas-accessible pore spaces. For the expected gas generation rate, cavern volume and design, and typical gas permeability of the host rock, the gas pressure is expected to stay below the critical threshold pressure of 6.5 MPa. For such conditions, no additional design measures are needed to mitigate gas impacts. For the case of conservative gas generation rates, or the case of a very low gas permeability of the rock of \( \leq 10^{-21} \text{ m}^2 \), the gas pressure could rise above the critical threshold pressure. As a result, the placement of gas-permeable plugs at the exit of each cavern would be a prudent design measure. Calculations indicate that such an approach could keep pressures in the range of 3 – 4 MPa above hydrostatic pressure even in the case of very low permeability rock. A range of cases are discussed in the subsequent paragraphs to evaluate possible effects of the gas pressure on the evolution of the repository system.

In the early gas production phase immediately after repository closure (< 100 years) the pressure build-up is controlled by the initial gas storage volume, represented by the gas-filled pore space of the cementitious cavern backfill. Without gas release along the repository structures (e.g. engineered gas transport system), pressure will build up and displace the water in the backfill until the capillary threshold pressure of the host rock is reached (capillary threshold pressure = gas entry pressure + liquid pressure in the host rock around the cavern). When the gas pressure exceeds the capillary threshold pressure, gas starts to displace the porewater in the connected porosity of the host rock. The gas pressure increases further, until equilibrium is reached between the gas generation rate and gas release rates (peak pressure in the emplacement cavern). For intrinsic host rock permeabilities of \( 10^{-20} \) to \( 10^{-21} \text{ m}^2 \) the expected time to approach the peak pressure is in the order of several thousands to several tens of thousands of years.

Special conditions arise when the capillary threshold pressure is higher than the threshold pressure for pathway dilation. In this case, microfractures will develop in the rock as soon as the gas pressure reaches the critical pathway dilation pressure. The gas transport capacity of the rock around the emplacement caverns increases as a result of the onset of microfracturing processes, leading to a quick stabilisation of the gas pressure when the gas permeability of the dilatant gas paths is sufficient to carry the generated gas. Hence, in the case of pathway dilation, it can be expected that the peak pressure in the emplacement caverns will not exceed significantly the threshold pressure for pathway dilation. Furthermore, the development of microfracturing is largely restricted to the rock mass in the immediate vicinity of the backfilled underground structures, where distinct pressure gradients are expected. In this context, it is worth mentioning that the two-phase flow simulations presented in chapter 4 did not account for possible pathway dilation processes, resulting in gas pressures which are significantly above the lithostatic pressure.

The likelihood of very high gas pressures is strongly associated with the case in which the intact host rock represents the only viable release path for the produced gas. For such conditions, the assessment of the gas-related effects concentrates on two key aspects, namely the availability of sufficient gas storage volume in the early post-closure period and the gas transport capacity of
the rock at pressures below the critical threshold pressure. As indicated in chapter 2, the cementitious cavern backfill is not fully water-saturated during the waste emplacement period. The initial gas storage capacity of the air-filled void space in the backfill is sufficient to take up the gas for a period of several hundred years, without approaching excessive gas pressures in the cavern. Even extreme resaturation scenarios, such as poor performance of the repository seal or groundwater inflow into the access tunnel through high-permeability fault zones would not change significantly the gas storage capacity of the emplacement caverns in the early time (cf. chapter 4.2). Furthermore, there is a potential for further design optimisation with regard to the initial gas storage capacity of the cavern backfill materials.

As stated above, the gas transport capacity of the rock is the other critical aspect to be evaluated, when the intact host rock formation is the only viable gas path. The gas transport capacity is controlled by the intrinsic permeability and the corresponding gas entry pressure of the rock. The existing data base on hydraulic properties of clay-rich formations indicates that the permeability decreases and the gas entry pressure increases with burial depth. Thus, very high gas entry pressures and ultra-low permeabilities in the range \( k \leq 10^{-21} \text{ m}^2 \) were measured in the Opalinus Clay of the Zürcher Weinland. For such rock characteristics it cannot be guaranteed a priori that the actual gas pressure in the emplacement caverns will remain below the critical gas threshold pressure. In this context it is worth mentioning that the proposed siting regions for the L/ILW repository represent shallower host rock formations, suggesting higher intrinsic permeability and lower gas entry pressure than observed at Benken, more comparable to the situation in the rock laboratory at Mont Terri.

The concept of the EGTS as an additional (engineered) gas transport path makes the management of the gas issue much more efficient and reliable. It is possible, for a wide range of situations and configuration parameters to design an engineered gas transport system for a L/ILW repository, which restricts the gas overpressures in the emplacement caverns to values below the critical threshold pressure. The numerical simulations presented in chapter 4.3 indicate moderate overpressures in the order of 3 – 4 MPa (above hydrostatic) even for the cases with very low host rock permeabilities.

The assessment of the possibility of gas overpressures includes an evaluation of possible deviations from the expected behaviour of the repository system after closure. The focus was on self-sealing processes in the host rock and along the engineered gas path due to hydrochemical interactions between the sand/bentonite of the cavern plug and cementitious backfill material. Such a long-term reduction of the gas permeability of the cavern plugs increases the likelihood of excessive gas overpressures in the emplacement caverns. Self-sealing processes can occur for all practical purposes only in the fully saturated part of the pore space, whereas potential hydrochemical interactions in the gas-filled voids are regarded as unimportant in the context of potential disruption of gas flow. Recalling the numerical simulations presented in chapter 4.3, it is considered very unlikely that the cavern plugs could fully resaturate in the period during which significant gas production rates are expected (<10'000 years). Consequently, the likelihood of poor performance of the engineered gas transport system due to hydrochemical interactions is negligible. Nevertheless, the current understanding of hydrochemical processes in the unsaturated near-field of the emplacement caverns is restricted to a phenomenological description of the contributing chemical interactions and further laboratory and in-situ experiments are foreseen to improve the conceptual understanding and the corresponding quantitative process models.
Displacement of contaminated porewater by gas overpressures in the emplacement caverns

The combined flow of porewater and gas in the repository near-field is of importance for the assessment of radionuclide transport. As a result of the elevated gas pressures in the caverns, porewater containing dissolved radionuclides will be displaced into the geosphere. Furthermore, the gas pressure build-up as an additional driving force for mass transport also tends to increase the path length for radionuclide transport in the host rock, an effect which is further enhanced by the anisotropy of the intrinsic rock permeability. The displaced water is widely spread over the footprint area of the repository towards the adjacent rock formations above and below the host rock.

The numerical simulations (chapter 4.3.4) indicate specific water fluxes in the host rock of up to $10^{-11}$ m/s in the very early gas generation phase (< 1'000 years after repository closure). The fluxes reduce steadily with time until the regime of diffusion-dominated transport is reached in the late times of the gas production phase (specific water flux typically < $10^{-13}$ m/s after several 10'000s of years). In Nagra (2008e), dose calculations were performed for a L/ILW repository in the Opalinus Clay formations for a wide range of steady state fluxes through the repository area. Calculations with the conservative assumption of a steady-state specific water flux of $10^{-11}$ m/s indicate that the dose would be a factor of ten below the dose limit of 0.1 mSv/a (see Figure A5.2-1, Safety Report, Nagra 2008e). Consequently, an even lower dose rate would be expected for the case of a transient flow field. It can thus be concluded that gas effects on the movement of contaminants from a L/ILW repository in Opalinus Clay will not compromise safety.

Applicability of the gas-related conclusions to future site specific assessments

The presented repository concept is generic in the sense that the corresponding repository configuration data can be easily adapted to future projects. Thus the EGTS can be optimised with respect to the site specific conditions such as the actual host rock permeability, the pore pressure conditions and the local stress conditions, respectively. This also includes consideration of the enlarged waste inventory as it has been used for preparing the proposal for siting regions (Nagra 2008c). For this enlarged inventory the overall conclusions regarding gas pressure build-up in the emplacement caverns and the displacement of porewater from the emplacement caverns would not change significantly.
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Appendix A: Gas-related properties of cementitious backfill materials

In the first section of this Appendix, the results of a literature survey on cementitious materials are summarised to show the existing information on different cementitious materials. The second section contains the methodology applied to obtain bulk parameters for the entire tunnel backfill.

Normal concretes and mortars

Normal concretes and mortars will be used for engineering purposes as well as for waste packaging. The major requirement of these materials is their static behaviour and their ability to retain water inflow into the tunnel during construction and emplacement.

Concrete consists of cement (often Ordinary Portland Cement – OPC), aggregate (e.g. sand or gravel), water, chemical additives (retarders, plasticisers, super-plasticisers, corrosion inhibitors) and mineral additives (e.g. fly ash, silica flume). In some applications it is commonly reinforced with fibres or networks of reinforcing materials (steel, glass or synthetics). The properties of the concrete are affected by the water-cement (w/c) mixing ratio and the "curing process" (hydration) and time.

Key references

The available data derive largely from the work done within the Nagra RD&D (Jacobs et al. 1994a and b) and associated Swiss workers at ETH and more recent French studies. Table A-1 lists the different data sources considered.

Tab. A-1: Key data sources for two-phase flow properties of concrete.

<table>
<thead>
<tr>
<th>Source</th>
<th>Concrete</th>
<th>Measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jacobs et al. 1994b</td>
<td>OPC w/c = 0.4 – 0.7</td>
<td>Water permeability, gas permeability and Klinkenberg coefficient as a function of saturation and other properties (porosity, thermal &amp; mechanical)</td>
</tr>
<tr>
<td>Abbas et al. (1999)</td>
<td>OPC w/c = 0.66 ϕ = 12.6 %</td>
<td>Gas permeability and Klinkenberg coefficient as a function of saturation</td>
</tr>
<tr>
<td>Jacobs (1998)</td>
<td>OPC w/c = 0.45, 0.6, 0.8 ϕ = 10.1, 12.7, 15.7 %</td>
<td>Gas permeability as a function of saturation and curing</td>
</tr>
<tr>
<td>Mayer et al. (1992)</td>
<td>&quot;Normal&quot; concrete w/c 0.4 – 0.8</td>
<td>Gas and water (very limited) permeability as a function of saturation</td>
</tr>
<tr>
<td>Monlouis-Bonnaire (2003)</td>
<td>OPC w/c = 0.48 ϕ = 13.2 %</td>
<td>Capillary pressure and relative permeability to gas as a function of saturation</td>
</tr>
<tr>
<td>Baroghel-Bouny et al. (1999)</td>
<td>Cement pastes and concretes using OPC BO w/c = 0.48</td>
<td>Capillary pressure as a function of saturation for cement pastes and concretes</td>
</tr>
</tbody>
</table>
Porosity
The major factor influencing the porosity is the w/c ratio. For normal concretes porosities are around 15 % for w/c ratios of 0.4 (mass ratio), increasing almost proportionally to about 20 % for w/c ratios of 0.7. A similar increase is observed for mortars although the admixture of aggregate increases the initial porosity to about 20 % (Jacobs et al. 1994b). Note that a considerable proportion of the water is chemically bound and, therefore, is usually not accounted for in the documented total porosity. Subsequently, the measured total porosity depends, to some extent, on the analytical method applied.

Long-term studies with cement have shown that porosities are reduced by up to 20 – 30 % over the 28 years of the test duration with a corresponding reduction of gas permeability of up to one order of magnitude.

There are no references for shotcrete porosities but the usually high w/c ratios of around 1 applied for shotcreting implies porosities of 25 – 35 %.

Permeability
There are significant differences in measured permeability to water and gas (or other fluids such as ethanol). Water is present in concrete both within the pore system and the concrete matrix as calcium silicate hydrate (CSH). Thus water flow may be accompanied by processes such as hydration, dissolution etc. These processes depend on the chemical equilibrium of the fluid with the concrete porewater. Within this section measured water permeability is reported, where available, which should be adequate for the modelling task, but chemical processes associated with fluid flow may be significant in the long-term (cf. chapter 3.4). Similar uncertainties apply to relative permeability measurements.

Gas permeability and its dependence on saturation is important for understanding the durability of concrete and is more easily measured than water permeability (see Abbas et al. 1999).

As expected from the porosity evolution, gas permeability increases with increasing w/c ratio. Doubling the w/c ratio will increase the gas permeability by at least 0.5 orders of magnitude (Jacobs 1998, Lanyon et al. 2001, Jacobs et al. 1994b). Laboratory experiments with different concrete materials have shown that for intrinsic permeabilities below about $10^{-14}$ m² consistent differences can be observed between water and gas permeability reaching up to 3 orders of magnitude for gas permeabilities of $10^{-16}$ m² (Jacobs et al. 1994b). The typical range of intrinsic gas permeabilities is presented in Table A-2 and is about $10^{-16}$ to $10^{-18}$ m² which is 1 to 4 orders of magnitude higher than for water permeabilities ($10^{-17}$ to $10^{-21}$ m²).

Tab. A-2: Typical ranges and suggested average of concrete porosity and intrinsic permeability to water and gas.

<table>
<thead>
<tr>
<th>Material</th>
<th>Porosity [%]</th>
<th>Intrinsic water permeability [m²]</th>
<th>Intrinsic gas permeability [m²]</th>
</tr>
</thead>
<tbody>
<tr>
<td>High performance concrete and waste packages</td>
<td>15 %</td>
<td>$10^{-19}$</td>
<td>$10^{-17}$</td>
</tr>
<tr>
<td>Normal building concrete</td>
<td>20 %</td>
<td>$10^{-18}$</td>
<td>$10^{-16}$</td>
</tr>
<tr>
<td>Shotcrete</td>
<td>25 – 35 %</td>
<td>$10^{-17}$</td>
<td>$10^{-16}$</td>
</tr>
<tr>
<td>Average</td>
<td>25 %</td>
<td>$10^{-18}$</td>
<td>$10^{-16}$</td>
</tr>
</tbody>
</table>
Relative permeability

For concretes, relative gas permeability decreases exponentially with increasing water content (Jacobs 1998, Abbas et al. 1999, Monlouis-Bonnaire et al. 2003, Lanyon et al. 2001, Lanyon & Rüedi 2008). Many results indicate that this decrease is continuous from 0 to 100 % saturation but some results indicate that gas breakthrough occurs instantly for saturations below about 90 % and a maximum is reached at about 10 – 20 % saturation. For the relative water permeabilities flow starts above a saturation of about 40 – 50 % and exponentially approaches the maximum for 100 % saturation, where half of the maximum is reached for a saturation of about 95 %.

Capillary pressure

The increase of capillary pressure with decreasing saturation is quite similar for different cements with ambient pressures of $5 \times 10^6$ Pa and a van Genuchten $n$ of about 1.5 to 2.5 (Monlouis-Bonnaire et al. 2003, Baroghel-Bouny et al. 1999). To show the applicability of the van Genuchten model an indicative function is depicted in Figure A-1. The observed differences between the data sources in the higher saturation range most likely originate in the experimental procedure (i.e. determination of total porosity or time for equilibration).

![Capillary pressure as a function of water saturation for different experiments with concretes.](image)

The black line indicates the van Genuchten model curve with a residual water saturation of 5 %, a van Genuchten $n$ of 2 and an apparent air entry pressure $1/\alpha$ of 25 MPa.
A survey of modelling studies was conducted to evaluate the parameter spectrum for the two-phase flow parameters of cementitious materials. An overview of recent investigations and parameter values is given in Table A-3.

**Tab. A-3: Compilation of recent modelling studies on concrete materials.**

<table>
<thead>
<tr>
<th>Source</th>
<th>Material</th>
<th>Properties</th>
<th>Purpose</th>
<th>Code</th>
</tr>
</thead>
<tbody>
<tr>
<td>Talandier et al. 2006</td>
<td>High Performance Cement Overpack</td>
<td>(\phi = 0.15), (k = 10^{-19} \text{ m}^2), (vG_n = 1.54), (vG_1/\alpha = 2 \times 10^6 \text{ Pa})</td>
<td>Simulation of hydrogen generation and migration</td>
<td>TOUGH2 EOS5</td>
</tr>
<tr>
<td></td>
<td>Concrete</td>
<td>(\phi = 0.15), (k = 10^{-18} \text{ m}^2), (vG_n = 1.54), (vG_1/\alpha = 2 \times 10^6 \text{ Pa})</td>
<td></td>
<td>TOUGH2 EOS5</td>
</tr>
<tr>
<td>Poppei &amp; Croisé 2006</td>
<td>Low permeability concrete barriers (includes effective properties salt filled zones)</td>
<td>(\phi = 0.13), (k = 10^{-15} \text{ m}^2), (vG_n = 1.5), (vG_1/\alpha = ) Davies correlation (S_{gr} = 0.16), (S_{sw} = 0.1)</td>
<td>Simulation of gas generation and migration in salt caverns.</td>
<td>TOUGH2 EOS7</td>
</tr>
<tr>
<td>Senger et al. 2006</td>
<td>Ordinary concrete silo</td>
<td>(\phi = 0.2), (k = 10^{-18} \text{ m}^2), (vG_n = 2), (vG_1/\alpha = 10^6 \text{ Pa}) (S_{gr} = 0.01), (S_{sw} = 0.25)</td>
<td>Gas migration through bentonite/ sand from a vented concrete silo</td>
<td>TOUGH2 EOS3</td>
</tr>
<tr>
<td>Mayer et al. 1992</td>
<td>Normal concrete w/c 0.4 – 0.7</td>
<td>(\phi = 0.13), (k_{\text{gas}} = 10^{-16} \text{ m}^2), (k_{\text{water}} = 1.2 \times 10^{-15} \text{ m}^2), (vG_1/\alpha = 10^5 \text{ Pa}) (Pc Narasimhan form (\nu = 1.3)) (S_{gr} = 0.18), (S_{sw} = 0.3)</td>
<td>Validation of gas flow into partially saturated concrete lab test</td>
<td>TOUGH</td>
</tr>
<tr>
<td>Ando et al. 2006</td>
<td>Lining/invert</td>
<td>(\phi = 0.19), (k_{\text{gas}} = 3 \times 10^{-15} \text{ m}^2) (k_{\text{water}} = 4.1 \times 10^{-18} \text{ m}^2), (vG_1/\alpha = 5 \times 10^6 \text{ Pa}) (Pc Narasimhan form (\nu = 1.05))</td>
<td>Gas migration from TRU repository</td>
<td>TOUGH2 &amp; TMVOC</td>
</tr>
<tr>
<td>COUPLEX Gas/ Benchmark by Andra</td>
<td>Waste package concrete</td>
<td>(\phi = 0.15), (k = 10^{-19} \text{ m}^2), (vG_n = 1.54), (vG_1/\alpha = 2 \times 10^6 \text{ Pa}) (S_{gr} = 0.0), (S_{sw} = 0.01)</td>
<td>Resaturation of a ILW disposal cell.</td>
<td>Various codes</td>
</tr>
</tbody>
</table>

1) Internal reference in Lanyon & Rüedi (2008)

**High porosity mortars**

High porosity mortars were especially designed to provide high porosity for gas storage and transport while still withstanding high axial stresses (Jacobs et al. 1994b). The mono-grain mortar (M1) and the flowing mortar (M2) were tested both on laboratory and larger scale engineering experiments for different levels of compaction. Additionally, M2 type mortar with lower \(w/c\) ratio as used for waste fixation at Beznau power plant was tested.
Porosity and permeability

The porosities of the different types of mortars are displayed in Table A-4 below. For experiments with M1 mortars the results of small-scale and larger size tests were quite similar. The emplacement experiment of M1 mortar showed that, realistically, a density of up to about 1800 kg/m³ can be reached. For M2 mortar the emplacement experiment only reached densities of up to 1900 kg/m³, with corresponding permeabilities of $10^{-13}$ to $10^{-12}$ m².

Tab. A-4: Summary of results from small and large-scale experiments with mortars M1 and M2.

<table>
<thead>
<tr>
<th>Material</th>
<th>Density [kg/m³]</th>
<th>Strength [N/mm²]</th>
<th>Porosity [%]</th>
<th>Intrinsic water permeability [m²]</th>
<th>Intrinsic gas permeability [m²]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mortar M1 (non-compacted)</td>
<td>1650 ± 50</td>
<td>5.4</td>
<td>35 ± 3</td>
<td>$3.1 ± 0.4 \times 10^{-10}$</td>
<td></td>
</tr>
<tr>
<td>Mortar M1 (compacted)</td>
<td>1800 ± 50</td>
<td>10 ± 5</td>
<td>22 ± 3</td>
<td>$2.7 ± 0.4 \times 10^{-10}$</td>
<td>$2.25 ± 0.3 \times 10^{-10}$</td>
</tr>
<tr>
<td>Mortar M1 (highly compacted)</td>
<td>2200 ± 50</td>
<td>34.6</td>
<td>13 ± 1</td>
<td>$2.7 ± 0.4 \times 10^{-10}$</td>
<td>$2.25 ± 0.3 \times 10^{-10}$</td>
</tr>
<tr>
<td>Mortar M2 (non-compacted)</td>
<td>2200 ± 100</td>
<td>38 ± 2</td>
<td>32 ± 3</td>
<td>$3.1 ± 0.6 \times 10^{-14}$</td>
<td>$5 ± 4 \times 10^{-13}$</td>
</tr>
<tr>
<td>Mortar M2 (Beznau)</td>
<td>2250</td>
<td>24 ± 2</td>
<td>2.5 ± 6</td>
<td>$2.5 ± 6 \times 10^{-15}$</td>
<td></td>
</tr>
<tr>
<td>Backfill</td>
<td>1800</td>
<td>35</td>
<td>3 × 10^{-10}</td>
<td>2.5 × 10^{-10}</td>
<td></td>
</tr>
</tbody>
</table>

* Large-scale experiment (Mayer & Wittmann 1995; internal ref. in Lanyon & Rüedi 2008)
** Small-scale experiment (Jacobs et al. 1994b)
*** Emplacement experiment (Mayer & Wittmann 1995; internal ref. in Lanyon & Rüedi 2008)

For mortars, experimental evidence only originates from Jacobs et al. (1994b), where gas flow starts below a saturation of about 80 % and reaches a maximum for about 30 %. For water permeabilities, flow starts above a saturation of about 40 – 55 % but then almost linearly approaches the maximum permeability at 100 % saturation.
Capillary pressure

The only evidence of capillary pressure increase with decreasing saturation is documented in Jacobs et al. (1994b). The results indicate that residual water contents are about 30%. However, the results are not fully conclusive because capillary pressure curves were only measured to pressures of up to 3000 Pa. The parameters resulting from modelling as listed in Table A-5 lead to ambient pressures of 500 Pa and a van Genuchten \( n \) of 2 (Mayer et al. 1998).


<table>
<thead>
<tr>
<th>Parameter</th>
<th>Reference Value</th>
<th>Range</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k ) Intrinsic permeability to water</td>
<td>( 4 \times 10^{-10} )</td>
<td>( 10^{-10} ) to ( 10^{-14} )</td>
<td>m²</td>
</tr>
<tr>
<td>( \phi ) Porosity</td>
<td>0.25</td>
<td>0.25 – 0.4</td>
<td>-</td>
</tr>
<tr>
<td>( E_s ) E-Modul</td>
<td>( 1 \times 10^{-10} )</td>
<td>( 9 \times 10^{-9} ) to ( 2 \times 10^{-10} )</td>
<td>Pa</td>
</tr>
<tr>
<td>( \nu ) Poisson's ratio</td>
<td>0.25</td>
<td>0.1 – 0.35</td>
<td>Pa</td>
</tr>
</tbody>
</table>

Capillary pressure curve

Relative permeability to water

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Reference Value</th>
<th>Range</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( S_{wr} ) Residual Water Saturation</td>
<td>0.3</td>
<td></td>
<td>-</td>
</tr>
<tr>
<td>( S_{gr} ) Residual Gas Saturation</td>
<td>0.3</td>
<td>0.2 – 0.3</td>
<td>-</td>
</tr>
</tbody>
</table>

Relative permeability to gas

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Reference Value</th>
<th>Range</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( S_{wr} ) Residual Water Saturation</td>
<td>0.3</td>
<td>0.2 – 0.3</td>
<td>-</td>
</tr>
<tr>
<td>( S_{gr} ) Residual Gas Saturation</td>
<td>0.3</td>
<td></td>
<td>-</td>
</tr>
<tr>
<td>( f_{\text{gas}} ) Gas permeability multiplier</td>
<td>1</td>
<td></td>
<td>-</td>
</tr>
</tbody>
</table>

Approach to obtain capillary pressure curves

As explained in chapter 3.3, the homogenisation of all cementitious materials in the backfill tunnel requires a traceable and well founded approach. This section will show the sources of information for the different types of cements and mortars and how the averaging process was performed and what average gas transport parameters resulted from it.

Porosity

As the total porosity defines the maximum pore volume, the porosities were simply averaged considering the volumetric proportions of the different cementitious materials (Eq. A-1). The porosities for the different cementitious materials considered cover a relatively large range of...
possible values and thus the final average values is linked with high uncertainties (Tab. 3-4). It is suggested to test an alternative value of 0.2 as a lower extreme.

\[ \phi_{\text{eff}} = \sum_{i=1}^{n} \phi_i = 0.25 \]  \hspace{1cm} (Eq. A-1)

**Permeability**

The arguments for the derivation of the effective intrinsic permeability of the cavern backfill are given in chapter 3.3; the reference values for the different cementitious materials are listed in Table 3-4.

The relative gas permeabilities usually follow an exponential decrease by 1.5 to 2 orders of magnitude with increasing water saturation (Fig. A-2). Please note that both absolute and relative gas permeability depends strongly on the material used and, in particular, its cement-water ratio and the grain size and distribution of the mortar matrix (sand or gravel).

**Capillary pressure**

There is consistent information available on building concretes (Fig. A-1). On the other hand, the data for the mortars M1 and M2 are not consistent and/or they are not fully understood.

The capillary pressure vs. saturation functions of the different materials cannot be just averaged because they are a product of the pore structure of the different materials. Therefore, an approach is used here to obtain average parameters for modelling the emplacement tunnel that is based on the approach of van Genuchten who developed a method to directly link pore size distribution and capillary pressure. He expresses the relation between porosity and capillary pressure with:

\[ \theta(p_c) = \theta_{res} + \frac{\theta_{sat} - \theta_{res}}{[1 + \alpha \cdot p_c]^m} \]  \hspace{1cm} (Eq. A-2)

\[ \theta(p_c) = \theta_{sat} \]  \hspace{1cm} (Eq. A-3)

With \( m = 1 - 1/n \)

The capillary pressure can be related to a certain pore radius using Young-Laplace's equation:

\[ p_c (r) = \frac{2 \cdot \gamma \cdot \cos(\varepsilon)}{r} \]  \hspace{1cm} (Eq. A-4)

With the surface tension \( \gamma = 0.0728 \text{ J/m}^2 \) (at 20°C) and the wetting angle \( \varepsilon = 0.35 \text{ rad} \) (at 20°C).

These two equations directly lead to a relation between porosity and pore radius or the cumulative pore size distribution.
Fig. A-2: Effective permeability to gas as a function of water saturation.

a) Cements with gravel and sand (w/c = 0.67) (from Abbas et al. 1999)

b) Specimen with different w/c ratio (6 samples with w/c = 0.45 and \( \theta = 0.10 \); 5 samples with w/c = 0.6 and \( \theta = 0.13 \); 8 samples with w/c = 0.8 and \( \theta = 0.16 \)). Each symbol represents one sample, on each sample up to four measurements of gas permeability are made: after 2 years of storage (from Jacobs 1998).
\[ \theta_{\text{cum}}(r) = (\theta_{\text{sat}} - \theta_{\text{res}}) \cdot \frac{1}{[1 + \alpha \cdot 2 \cdot 0.0728 \cdot \cos(0.35)]^n} \]  
(Eq. A-5)

With the above equation the capillary pressure-saturation relations provided in literature (e.g. Fig. A-1) can be transferred to the cumulative pore size distribution function. If available (e.g. Fig. A-3), the latter one can be used directly.

Fig. A-3: Pore size distribution of different single corn mortars analysed after 90 days using MIP (from Jacobs et al. 1994b).

The sum of the three pore size distributions is displayed in Figure A-4 using model parameters and material volumes as listed in Tables A-4 and A-5. It can be seen that the curve cannot be reproduced with a van Genuchten type function without defining the goal of the subsequent calculations. In this case the major goal is to model the distribution of the gas in the emplacement tunnel. Therefore, the main parameters to be reproduced are the air entry behaviour (large pores) and the maximum gas storage volume (i.e. porosity accessible for gas transport). The latter one is limited to pores accessible to gas pressures up to about 10 MPa, corresponding to a pore radius of about \(10^{-8}\) Pa, respectively. The fitting parameters are:

\[ \theta_{\text{sat}}: \quad 0.25 \text{ (Tab. 3-4)} \]

\[ \theta_{\text{res}}: \quad 0.007 \text{ (or 28%)} \]

\[ \alpha: \quad 0.002 \]

\[ n: \quad 1.25 \]
It can be seen that the apparent air entry pressure is dominated by the high-porosity mortar and the total available gas storage volume is about 70% of the total pore space. However, as mentioned above, this value depends largely on the actual materials used and can be adapted to some degree by the final choice of the cements.

Fig. A-4: Cumulative pore size distribution (PSD) for the three major cement materials (red curve) and modelled distribution using parameter values as listed above (yellow curve).
Appendix B: Gas-related properties of sand/bentonite materials

Key references

The data used for sand/bentonite mixtures derive mainly from RWMC's Kodoka Project, the GMT experiment at GTS (incl. laboratory experiments), JAEA's H12 related studies and SKB and AECL's programmes on various sand/bentonite mixtures. The key documents are listed in Table B-1. Further references are found in Lanyon & Rüedi (2008).

Tab. B-1: Key references for sand/bentonite mixtures.

<table>
<thead>
<tr>
<th>Document</th>
<th>Mixture and bentonite</th>
<th>Relevant Contents</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lanyon et al. (2001)</td>
<td>20/80 Kunigel V1</td>
<td>Summary of laboratory data testing performed for GMT together with summary of results from RWMC Kodoka Project for sand/bentonite, mortar and concrete</td>
</tr>
<tr>
<td>Romero et al. (2003)</td>
<td>20/80 Kunigel V1</td>
<td>UPC material characterisation and hydromechanical tests on 80/20 sand/bentonite</td>
</tr>
<tr>
<td>Romero &amp; Castellanos (2004)</td>
<td>20/80 Kunigel V1</td>
<td>UPC air permeability tests on 80/20 sand/bentonite</td>
</tr>
<tr>
<td>JAEA Buffer material database</td>
<td>Varying bentonite fraction Kunigel V1</td>
<td>Compilation of results of tests performed on pure bentonite and sand/bentonite mixtures for varying density, bentonite fraction and water chemistry</td>
</tr>
<tr>
<td>JAEA H12 report</td>
<td>Varying bentonite fraction Kunigel V1</td>
<td>Supporting material for compacted bentonite and sand/bentonite.</td>
</tr>
<tr>
<td>Mata (2002)</td>
<td>30/70 MX-80</td>
<td>Laboratory testing performed at UPC on 30/70 bentonite crushed rock material in support of Äspö Plug and Backfill test</td>
</tr>
<tr>
<td>Engelhardt et al. (2003)</td>
<td>30/70 SPV Volclay/Calcigel</td>
<td>Laboratory testing and modelling (TOUGH2/ITHOUGH2) performed at University Tübingen, PC on 30/70 bentonite crushed rock material in support of experiments at Äspö</td>
</tr>
<tr>
<td>Dixon et al. (2002)</td>
<td>50/50 Avonlea</td>
<td>Description of two large-scale sealing experiments using 50/50 bentonite sand at URL</td>
</tr>
</tbody>
</table>

1) Internal reference in Lanyon & Rüedi (2008)
Appendix C: Back-of-the-envelope calculations of gas transport from a L/ILW repository in Opalinus Clay

Introduction

The release of the gases produced in the backfilled emplacement caverns of a L/ILW repository can be accomplished by a variety of transport mechanisms. Phenomenological considerations suggest the following subdivision of the basic gas transport mechanisms as presented in chapter 3.2 (Fig. 3-1): (i) advective-diffusive transport of gas dissolved in the porewater, (ii) visco-capillary two-phase flow, (iii) dilatancy-controlled gas flow and (iv) gas transport in macroscopic tensile fractures. Potential transport routes are (i) the excavation-damaged zone around the underground structures, (ii) the engineered barrier systems and (iii) the host rock formation (Fig. 1-1).

This Appendix is aimed at assessing the gas transport capacity of the gas path through the host rock with advection and diffusion of dissolved gas as the prevailing transport mechanisms. The gas transport capacity of these transport mechanisms is calculated for simplified repository configurations. The results of the calculations are compared with the total gas production rates of the waste inventory MIRAM 2005 (Fig. 4-4).

Simplified repository configuration - key assumptions

Simplified assumptions are made for describing the L/ILW repository configuration (Tab. C-1).

Tab. C-1: Configuration data of the L/ILW repository used for the scoping calculations.

<table>
<thead>
<tr>
<th>Configuration Data</th>
<th>Parameter Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Repository configuration</td>
<td></td>
</tr>
<tr>
<td>Repository level</td>
<td>160 m asl, in the centre of the host rock</td>
</tr>
<tr>
<td>Thickness of Opalinus Clay</td>
<td>100 m</td>
</tr>
<tr>
<td>Number of emplacement caverns</td>
<td>7</td>
</tr>
<tr>
<td>Length of emplacement caverns</td>
<td>200</td>
</tr>
<tr>
<td>Equivalent diameter of emplacement caverns</td>
<td>12.6 m</td>
</tr>
<tr>
<td>Footprint area (emplacement caverns only)</td>
<td>200 m × 600 m = 0.12 km²</td>
</tr>
<tr>
<td>Footprint area (caverns, pilot &amp; test facility, access tunnel)</td>
<td>400 m × 1'000 m = 0.4 km²</td>
</tr>
<tr>
<td>Average cavern porosity</td>
<td>25 %</td>
</tr>
<tr>
<td>Total gas storage volume in Opalinus Clay (Tab. 2-3)</td>
<td>57'924 m³</td>
</tr>
<tr>
<td>Total excavated volume (caverns, pilot facility; Tab. 2-2)</td>
<td>170'568 m³</td>
</tr>
<tr>
<td>Rock properties (Opalinus Clay)</td>
<td></td>
</tr>
<tr>
<td>Intrinsic Permeability of host rock</td>
<td>$1 \times 10^{-20} \text{ m}^2$</td>
</tr>
<tr>
<td>Porosity</td>
<td>12 %</td>
</tr>
<tr>
<td>Hydromechanical site conditions</td>
<td></td>
</tr>
<tr>
<td>Vertical hydraulic gradient</td>
<td>0.01 – 1</td>
</tr>
<tr>
<td>Hydrostatic pressure at repository level</td>
<td>2.2 MPa</td>
</tr>
<tr>
<td>Lithostatic pressure at repository level</td>
<td>8.125 MPa</td>
</tr>
</tbody>
</table>
Gas production and water consumption

The following scoping calculations are based on the waste inventory MIRAM 2005 (cf. chapter 2.8). The corresponding gas generation rate and the cumulated volume of gas at atmospheric pressure are given in Figure 4-4. The total volume of gas produced after 100 years is in the order of 1 million m$^3$ (STP) and 30 millions m$^3$ (STP) at the end of the gas production phase.

It is of further interest to evaluate the contributions of corrosion and organics to the overall source term separately. Figure C-1 exhibits for the waste inventories MIRAM 2005 and 2008 the contributions from metal corrosion and organics to the total gas generation rate. The cumulated volume of the gas produced by corrosion (MIRAM 2005: 25 millions m$^3$ STP; MIRAM 2008: 22 millions m$^3$ STP) exceeds the gas production by organics (MIRAM 2005: 1.3 millions m$^3$ STP; MIRAM 2008: 0.92 millions m$^3$ STP) by more than a factor 10. It is worth mentioning, that the organics contribute significantly to the overall gas production in the period between 10 and 1'000 years.
Fig. C-1: Realistic gas generation rates and cumulated volumes of gas for the waste inventories: (a) MIRAM 2005 and (b) MIRAM 2008.

The contributions from corrosion of metals and degradation of organic matter are displayed separately.

Anaerobic metal corrosion consumes water. In order to estimate the water consumption due to metal corrosion, simple scoping calculations are performed, assuming that iron corrosion is the prevailing chemical reaction as presented in chapter 2.8.3. Accordingly, 1 mol water is needed
to produce 1 mol of hydrogen. The molar volume of the hydrogen gas is 0.0224 m$^3$/mol and the molar weight of water is 18 g/mol. Figure C-2 shows the water consumption rate and the cumulated volume of water consumed by the corrosion processes in the closed repository. The consumed water per cavern meter (Cm) can be calculated by dividing the total rate by the total length of the caverns (caverns 1 – 7 plus pilot facility: 1'380 m; Tab. 2-1). Approximately 1 m$^3$/Cm of water is consumed in the first 1'000 years. At the end of the gas generation phase, the amount of consumed water is 16 m$^3$/Cm, corresponding to about 65 % of the total gas storage volume per cavern meter (cf. Tabs. 2-1 and 2-3). Thus, water consumption is relevant for the case of a host rock with very low permeability ($k \leq 1 \times 10^{-21}$ m$^2$), when water consumption in the early time is in the same order of magnitude as the water inflow from the host rock.

![Fig. C-2: Water consumption by metal corrosion according to MIRAM 2005.](image)

It is assumed that iron corrosion is the prevailing chemical reaction.

**Gas storage capacity of the backfilled underground structures**

For the estimation of the gas storage capacity, it is assumed that the backfilled and sealed repository is a closed system, i.e. host rock and repository seal V5 are impermeable. The maximum acceptable gas pressure in the closed repository $p_{\text{max}}$ corresponds to the lithostatic pressure $\sigma_v$ at repository level ($\sigma_v = 8.125$ MPa; cf. Tab. 3-3). The total gas storage volume of all backfilled structures in the Opalinus Clay $V_{\text{total}}$ is represented by the total volume of gas-filled voids before repository closure ($V_{\text{total}} = 57'924$ m$^3$; Tab. 2-3).

The maximum gas volume $V_{\text{max}}(\text{STP})$ that can be stored as a free gas phase in the closed repository at a gas pressure $p_{\text{max}} = \sigma_v$ is calculated according to the gas law of Boyle-Mariotte:

$$V_{\text{max}}(\text{STP}) = V_{\text{total}} \cdot \frac{p_{\text{max}}}{p_{\text{atm}}} = 4.7 \times 10^6 \text{ m}^3 \text{ (STP)}$$
Where \( p_{\text{atm}} \) is pressure at atmospheric conditions (\( p_{\text{atm}} = 100 \text{ kPa} \)). For the waste inventory MIRAM 2005, the maximum gas volume of \( 4.7 \times 10^6 \text{ m}^3 \) (STP) is reached after less than 3'000 years. Thus, it is concluded that the gas cannot be contained in the backfilled underground structures of the closed repository without exceeding the critical gas overpressure. Possible routes of gas release through the host rock and along the backfilled repository structures need to be assessed.

**Transport of gas dissolved in porewater**

The possibility of gas dissolving in the porewater, and being transported from the repository by diffusion and advection is considered in this section.

The solubility of a gas in water can as a good approximation be represented by Henry's Law (chapter 3.2.1). Solubilities of hydrogen, carbon dioxide and methane are given in Table 3-1. Henry's law is used to calculate the total volume of gas \( V_{\kappa \text{ max}}(p) \), that can be dissolved in the porewater of the emplacement caverns at a given gas pressure \( p \):

\[
V_{\kappa \text{ max}} = K_\kappa \cdot S_w \cdot \phi \cdot V_{\text{caverns}} \cdot p
\]

Where \( K_\kappa \) is the Henry constant of the species \( \kappa \), \( S_w \) and \( \phi \) are the water saturation and porosity of the emplacement caverns and \( V_{\text{caverns}} \) is the total excavated cavern volume (Tab. 2-1). Assuming full saturation of the caverns, an average cavern porosity of 25 %, a total excavated cavern volume of about 170'000 \text{ m}^3 and a gas pressure of 8.125 MPa (corresponding to the lithostatic stress level), the total amount of dissolved hydrogen is \( 5.5 \times 10^3 \text{ kg} \). Given a molar weight of 2 g/mol and a molar volume of 0.0224 m\(^3\)/mol, the mass of hydrogen can be converted in \( 6.1 \times 10^4 \text{ m}^3 \) (STP). This is significantly less than the cumulated gas volume after 1 year of gas production (cf. Fig. 4-4). It is concluded, that dissolution of gas in the porewater of the caverns is not relevant for the assessment of gas pressure build-up after repository closure.

Transport of the dissolved gas is described by the advection-diffusion equation:

\[
\phi \cdot \frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c - c \cdot u)
\]

where \( \phi \) is porosity, \( c \) is the gas concentration in the porewater, \( D \) is the diffusion coefficient and \( u \) is the transport velocity. The transport velocity can be expressed in terms of Darcy velocity \( v_f \) divided by the porosity. It should be noted that dispersion can be neglected due to the low transport velocity.

In the case of pure advection the total flux \( q \) of dissolved gas out of the repository by natural groundwater flow can be estimated by:

\[
q = c_o \cdot A \cdot v_f \cdot F
\]

where \( q \) is the gas flux, \( c_o \) is the concentration of dissolved gas at a given pressure, \( A \) is the cross-sectional area normal to the flow, \( v_f \) is the Darcy velocity and \( F \) is the flow enhancement factor, which accounts for the enhanced permeability of the backfill materials in the emplacement caverns.
The concentration \(c_o\) of the dissolved gas depends linearly on the gas pressure (Henry's law). For hydrogen the solubility was given as 1.58 mg/l at 100 kPa. Correspondingly, a total of about 35 mg hydrogen per liter of porewater (corresponding to 0.39 m\(^3\) H\(_2\) STP / m\(^3\) of porewater) can be dissolved at a gas pressure of 2.2 MPa, which is the hydrostatic pressure at repository level.

Assuming vertical porewater flow through the repository, driven by the hydraulic gradient between the regional aquifers above and below the repository level, the footprint area of the emplacement area is about 0.12 km\(^2\) (Tab. C-1). The footprint area of the entire repository is about 0.4 km\(^2\).

The Darcy velocity depends on the hydraulic gradient and on the hydraulic conductivity of the host rock. A range between \(1 \times 10^{-12}\) and \(1 \times 10^{-14}\) m/s is assumed here.

The flow enhancement factor for vertical flow can be derived analytically. For the geometry of slablike caverns the enhancement factor in z-direction is \(F_z = 1.2\).

Table C-2 summarises the total advective hydrogen fluxes calculated for a variety of Darcy velocities and two different footprint areas. The calculated fluxes are in the order of a few cubic meters per year or less. The comparison with the gas generation rates (Fig. 4-4: gas generation rates between \(10^5\) and \(10^3\) m\(^3\) H\(_2\) / a (STP) in the first thousand year) shows clearly that advection of dissolved gas is of very limited relevance for the assessment of gas pressure build-up in the emplacement caverns.

<table>
<thead>
<tr>
<th>Darcy velocity</th>
<th>Footprint area</th>
<th>(v_f = 1 \times 10^{-12}) [m/s]</th>
<th>(v_f = 1 \times 10^{-13}) [m/s]</th>
<th>(v_f = 1 \times 10^{-14}) [m/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(A = 0.12) km(^2)</td>
<td>1.8 m(^3) H(_2) / a (STP)</td>
<td>0.18 m(^3) H(_2) / a (STP)</td>
<td>0.018 m(^3) H(_2) / a (STP)</td>
</tr>
<tr>
<td></td>
<td>(A = 0.4) km(^2)</td>
<td>5.8 m(^3) H(_2) / a (STP)</td>
<td>0.58 m(^3) H(_2) / a (STP)</td>
<td>0.058 m(^3) H(_2) / a (STP)</td>
</tr>
</tbody>
</table>

In the case of pure diffusion, the flux of dissolved gas from an infinite circular cylinder, maintained at constant concentration \(c_o\), into rock, with initial concentration zero is (Carslaw & Jaeger 1959):

\[
q(t) = \frac{8 \phi \cdot l}{\pi} \int_0^\infty \frac{1}{u \left( J_0^2(Ru) - Y_0^2(Ru) \right)} e^{-2\nu t} du
\]

Where \(\phi\) is the porosity of the host rock, \(l\) is the length of the caverns, \(D\) is the diffusion coefficient, \(c_o\) is the concentration of dissolved gas at hydrostatic pressure, \(J_0\) and \(Y_0\) are Bessel functions of order zero and \(R\) is the radius of the caverns. The integral can be calculated numerically. At small times the flux can be approximated:

\[
q(t) \approx 2 \phi \cdot l \cdot D \cdot c_o \cdot \sqrt{\frac{\pi \cdot R^2}{D \cdot t}} \left[ 1 + O \left( \sqrt{\frac{D \cdot t}{R^2}} \right) \right]
\]
Figure C-3 shows the transients of the diffusive flux of hydrogen from the caverns into the host rock according to the aforementioned short-time solution for two different effective diffusion coefficients. The fluxes are significant only in the very early time after the onset of gas production. After 1 year, total hydrogen fluxes in the range 1 – 10 m³/a are expected, which are decreasing rapidly. The comparison with the gas generation rates (Fig. 4-4) shows clearly that diffusion of dissolved gas is of very limited relevance for the assessment of gas pressure build-up in the emplacement caverns.

Fig. C-3: Diffusion of dissolved hydrogen from the caverns into the host rock according to the short-term solution given by Carslaw & Jaeger (1959).