Technical Report 14-14

Low- and intermediate-level waste repository-induced effects

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This status report presents the result of work in progress and is intended to provide rapid dissemination of current information. The methods used and results obtained will be reassessed in the course of Stage 3 of the Sectoral Plan "Deep Geological Repositories".

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Abstract

This status report aims at describing and assessing the interactions of the radioactive waste emplaced in a low- and intermediate level waste (L/ILW) repository with the engineered materials and the Opalinus Clay host rock. The Opalinus Clay has a thickness of about 100 m in the proposed siting regions. Among other things the results are used to steer the RD&D programme of Nagra. The repository-induced effects considered in this report are of the following broad types:

- **Thermal effects:** i.e. effects arising principally from the heat generated by the waste and the setting of cement
- **Rock-mechanical effects:** i.e. effects arising from the mechanical disturbance to the rock caused by the excavation of the emplacement caverns and other underground structures
- **Hydraulic and gas-related effects:** i.e. the effects of repository resaturation and of gas generation, e.g. due to the corrosion of metals within the repository, on the host rock and engineered barriers
- **Chemical effects:** i.e. chemical interactions between the waste, the engineered materials and the host rock

Deep geological repositories are designed to avoid or mitigate the impact of potentially detrimental repository-induced effects on long-term safety. For the repository under consideration in the present report, an assessment of those repository-induced effects that remain shows that detrimental chemical and mechanical impacts are largely confined to the rock adjacent to the excavations, thermal impacts are minimal and gas effects can be mitigated by appropriate design measures to reduce gas production and provide pathways for gas transport that limit gas pressure build-up (engineered gas transport system, or EGTS). Specific measures that are part of the current reference design are discussed in relation to their significance with respect to repository-induced effects.

The disposal system described in this report provides a system of passive barriers with multiple safety functions. The disposal system has been designed to perform with sufficient safety margin for a range of siting conditions. The barriers include the host rock, its surrounding geological setting, the waste forms, drums and the cementitious backfill. They have a range of attributes that intrinsically favour safety and that avoid or minimise detrimental phenomena and uncertainties or mitigate their effects. Nevertheless, potentially detrimental repository-induced effects remain and in the present report, these are investigated and discussed considering a broad spectrum of parameters, reflecting, among other things, the range of potential siting conditions.

The L/ILW emplacement caverns are designed, constructed, operated and finally backfilled in such a way that formation of excavation damaged zones is limited. Specifically this is achieved by restricting the size of the excavations and the depth of the repository, using a low-deformation, controlled construction and excavation method and by the fact that the excavations will be backfilled relatively soon after construction with grain supported mortar. At expected repository depths, the caverns will need to be supported to ensure stability and worker protection; this will prevent rock falls and further extension of the EDZ. Based on the modelling results, it can be concluded that the extent of the EDZ around the L/ILW emplacement caverns will not exceed a thickness of one cavern diameter and that the hydraulic conductance of the EDZ around the emplacement caverns, access tunnels and shafts will not exceed a value of 10^{-7} m^3/s. Self-sealing of the EDZ and low hydraulic gradients along the tunnels will result in negligible radionuclide transport by the EDZ pathway.

It is shown that gas pressure build-up is controlled by the gas transport capacity of the pathways between the main repository and the access tunnel forming the so-called EGTS. Results obtained with the sensitivity cases for a repository depth of 500 m bgl indicate that the EGTS can be designed in such a way that gas pressures which could damage the repository and/or the host rock will not be reached.

When designing and assessing the performance of a L/ILW repository, the relevant chemical interactions are taken into account. With the current reference design, it is expected that degradation of the cementitious backfill, the concrete tunnel liner and the corrosion of the steel drums and other supporting structures will lead to some alteration of the cementitious nearfield and Opalinus Clay. These detrimental effects are taken into account in dose calculations and have been found not to have a significant impact on the calculated dose rates.

Zusammenfassung

Das Ziel dieses Statusberichts ist es, in einem geologischen Tiefenlager für schwach- und mittelaktive Abfälle (SMA-Lager) die wechselseitige Beeinflussung von eingelagertem Abfall und eingebauten bautechnischen Materialien spezifisch auf das in den vorgeschlagenen Standortgebieten etwa 100 m mächtige Wirtgestein Opalinuston zu untersuchen, um das F&E-Programm der Nagra gezielter ausrichten zu können. Die im vorliegenden Bericht untersuchten lagerbedingten Einflüsse sind dabei:

- **Thermische Effekte:** D.h. Auswirkungen auf das Wirtgestein und die technischen Barrieren, die vor allem durch die vom Abfall bedingte Zerfallswärme und die Hydratation des Zements verursacht werden
- **Felsmechanische Effekte:** D.h. Auswirkungen, die von der mechanischen Beanspruchung des Gesteins durch den Vortrieb der Lagerkavernen und weiterer Untertagbauten hervorgerufen werden
- **Hydraulische und durch Gasdruck bedingte Effekte:** D.h. Auswirkungen durch Wiederaufsättigung des Tiefenlagers und Gasbildung beispielsweise aufgrund von Metallkorrosion im Tiefenlager auf Wirtgestein und die technische Barrieren
- **Chemische Effekte:** D.h. chemische Wechselwirkungen von Abfall, bautechnischen Materialien und Wirtgestein

Geologische Tiefenlager sind so ausgelegt, dass die potenziell nachteiligen Auswirkungen von lagerbedingten Einflüssen möglichst begrenzt werden. Die Beurteilung der lagerbedingten Einflüsse für das in diesem Bericht betrachtete SMA-Lager zeigt, dass sich die chemischen und mechanischen Auswirkungen auf das Gestein in unmittelbarer Umgebung der Untertagbauten beschränken, die thermischen Einflüsse minimal ausfallen und der sich aufbauende Gasdruck über geeignete Auslegungsvarianten ('Engineered Gas Transport System' EGTS, ein System aus Verfüll- und Versiegelungsbauwerken zur kontrollierten Ableitung von Gasen entlang der Zugangsbauwerke) reduziert werden kann. Geeignete Massnahmen werden als Teil des Referenzkonzepts im Hinblick auf ihre Bedeutung für die lagerbedingten Einflüsse diskutiert.

Das Entsorgungskonzept für SMA beschreibt ein System mit multiplen passiven Barrieren und Sicherheitsfunktionen. Dieses Entsorgungskonzept wurde für eine Reihe von Standortbedingungen ausgelegt. Die Barrieren bestehen aus dem Wirtgestein, den einschlusswirksamen Rahmengesteinen, den Abfallgebinden mit den konditionierten Abfällen und der zementhaltigen Verfüllung. Das Barrierensystem weist intrinsische Eigenschaften auf, welche die Sicherheit erhöhen und gleichzeitig die Auswirkung von nachteiligen Phänomenen und Ungewissheiten begrenzen. Nichtsdestotrotz kann es lagerbedingte Einflüsse geben, die sich nachteilig auswirken können; diese werden im vorliegenden Bericht unter Einbezug einer grossen Bandbreite von Parametern, die unter anderem die Bedingungen an möglichen Standorten widerspiegeln, untersucht und diskutiert.

Die SMA-Lagerkavernen wurden so ausgelegt, gebaut, betrieben und schliesslich verfüllt, dass die Bildung einer Auflockerungszone (AUZ)[1] möglichst begrenzt wird. Dies wird erreicht, indem die Grösse der Ausbruchzonen und die Tiefenlage des Lagers begrenzt werden, eine gebirgsschonende, kontrollierte Ausbruch- und Ausbaumethode angewendet wird und dadurch, dass die Lagerkavernen relativ schnell nach ihrem Ausbruch wieder mit einem korngestützten Mörtel verfüllt werden. Auf entsprechender Lagertiefe werden die Lagerkavernen mit Stütz-

[1] *Englisch*: Excavation damaged zone (EDZ).

mitteln ausgebaut, um deren Stabilität und die Arbeitssicherheit zu gewährleisten. Dadurch wird Nachfall und eine weitere Ausdehnung der AUZ verhindert. Basierend auf Modellrechnungen kann abschliessend festgehalten werden, dass sich die AUZ nicht über einen Tunnelquerschnitt hinaus ausdehnt und dass das hydraulische Leitvermögen der AUZ um Lagerkavernen, Zugangstunnel und Schächte nicht einen Wert von 10^{-7} m^3/s übersteigt. Die Selbstabdichtung der AUZ und die niedrigen hydraulischen Gradienten entlang der Bau- und Betriebstunnel führen zu einem vernachlässigbaren Radionuklidtransport durch die AUZ.

Es wird gezeigt, dass der Gasdruckaufbau durch die Gastransportrate zwischen dem Hauptlager und dem Zugangstunnel bestimmt wird, der seinerseits durch das EGTS bestimmt wird. Die Resultate einer Sensitivitätsanalyse eines Lagers in einer Tiefe von 500 m zeigen, dass das EGTS so ausgelegt werden kann, dass ein Gasdruck, der das Wirtgestein potenziell schädigen könnte, nicht erreicht wird.

Chemische Wechselwirkungen werden sowohl bei der Planung als auch bei der Bewertung der Sicherheit eines SMA-Lagers in Betracht gezogen. Im derzeitigen Referenzkonzept wird erwartet, dass der Abbau des Betons im Tunnelausbau und die Korrosion von Stahlbehältern und anderen stahlhaltigen Stützelementen das zementhaltige Nahfeld und den Opalinuston zu einem gewissen Grad umwandeln. Diese Umwandlungen werden in die Dosisberechnungen mit einbezogen und zeigen keinen signifikanten Einfluss auf die resultierende Dosis.

Résumé

Le présent rapport reflète les connaissances actuelles du traitement des perturbations induites, dans un dépôt profond, par les déchets radioactifs de faible et moyenne activité (DFMA) sur les matériaux des barrières ouvragées et inversement, ainsi que plus spécifiquement sur l'Argile à Opalinus, qui atteint une épaisseur d'environ 100 mètres dans les domaines d'implantation envisagés, pour mieux pouvoir aligner le programme de R&D de la Nagra. Les perturbations provoquées par le dépôt peuvent être réparties en quatre catégories:

- **Effets thermiques :** à savoir les effets sur la roche d'accueil et les barrières ouvragées qui sont dus principalement à la chaleur générée par la décroissance radioactive des déchets et les réactions d'hydratation du ciment.
- **Effets géomécaniques :** à savoir les effets résultant de la perturbation mécanique de la roche causée par l'excavation des cavernes de stockage et d'autres structures souterraines.
- **Effets hydrauliques et effets liés aux émissions de gaz :** à savoir les effets sur la roche d'accueil ou sur les barrières ouvragées qui sont en rapport avec la resaturation du dépôt profond et la production de gaz, notamment consécutive à la corrosion de métaux dans le dépôt.
- **Effets chimiques :** à savoir les interactions de nature chimique entre les déchets, les barrières ouvragées et la roche d'accueil

Les dépôts en couches géologiques profondes sont conçus de manière à éviter ou atténuer tout impact sur la sûreté à long terme. Pour le dépôt considéré ici, l'examen des perturbations provoquées par le dépôt montre que les impacts chimiques et mécaniques se limitent en grande partie au secteur de la roche proche de la zone excavée, que les effets thermiques sont minimes et que les effets des gaz peuvent être atténués par une architecture de dépôt visant, d'une part, à limiter la production de gaz et d'autre part, à empêcher une augmentation de la pression en mettant en œuvre un système technique de transport des gaz, Engineered Gas Transport System (EGTS). Des mesures spécifiques visant à limiter les perturbations provoquées par le dépôt sont envisagées dans le cadre du concept de référence et évaluées quant à leur efficacité.

Le système décrit dans le présent rapport comprend une succession de barrières passives remplissant différentes fonctions de sûreté. Le dépôt a été conçu avec une marge de sécurité suffisante en prévision d'une multitude de conditions locales. Les barrières comprennent la roche d'accueil, la zone de confinement géologique, les colis de déchets conditionnés et le comblement en ciment. Le système de barrières présente une série de caractéristiques intrinsèques qui contribuent à la sûreté du dépôt et empêchent ou atténuent les perturbations et les incertitudes, ou du moins en limitent les effets – sans toutefois les éliminer complètement. Le présent rapport s'emploie à étudier les perturbations qui subsistent à la lumière d'une vaste palette de paramètres, en rapport notamment avec différentes conditions qui pourront prévaloir sur les sites d'implantation.

Dès la conception du dépôt, puis au cours des phases de construction, d'exploitation et de comblement, on va faire en sorte de limiter au maximum la formation d'une zone perturbée autour des cavernes pour DFMA. On va ainsi limiter la taille de la zone excavée et la profondeur du dépôt, procéder à l'excavation de manière contrôlée et en ménageant la roche et enfin combler les galeries relativement rapidement après leur construction à l'aide de matériaux gonflants. A la profondeur envisagée pour les dépôts géologiques, il faudra prévoir des soutènements afin de garantir la stabilité des galeries et la sécurité du personnel. Cette mesure évitera que des roches se détachent après l'excavation, ce qui entrainerait une extension de la zone

perturbée. Il est permis d'affirmer, en se fondant sur les modélisations, que la taille de la zone perturbée ne dépassera pas la section d'une galerie et que la conductivité hydraulique de la zone perturbée située autour des galeries et des tunnels et puits d'accès ne dépassera pas 10^{-7} m^3/s. Au vu des propriétés auto-cicatrisantes de la zone perturbée et des faibles gradients hydrauliques le long des tunnels de construction et d'exploitation, le transport de radionucléides dans la zone perturbée sera négligeable.

Les résultats montrent que la montée de la pression des gaz est contrôlée grâce à la capacité de transport des voies reliant le dépôt principal et le tunnel d'accès, lesquelles forment le système technique de transport des gaz (EGTS). Les analyses de sensibilité réalisées pour un dépôt à une profondeur de 500 m indiquent que l'EGTS peut être conçu de manière à empêcher que la pression des gaz n'augmente jusqu'à un niveau susceptible de porter atteinte au dépôt et/ou à la roche d'accueil.

Les interactions chimiques sont prises en compte aussi bien lors de la planification que de l'évaluation du bon fonctionnement d'un dépôt pour DFMA. Pour l'actuel concept de référence, on estime que la dégradation du comblement en ciment et du béton du revêtement, de même que la corrosion des fûts en acier et d'autres éléments porteurs entraîneront certaines altérations du champ proche, à savoir du matériau de comblement (ciment) et de l'Argile à Opalinus. Ces perturbations sont prises en compte dans les calculs de dose; on a constaté qu'ils n'avaient pas d'impact significatif sur les doses calculées.

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1 Introduction

1.1 Background and aims

In Switzerland, the Nuclear Energy Law requires the disposal of all types of radioactive waste in deep geological repositories (KEG 2003). The Swiss Radioactive Waste Management Programme (Nagra 2008a) foresees two types of deep geological repositories: a high-level waste repository (HLW repository) [2] for spent fuel (SF)[3], vitrified high-level waste (HLW) and long-lived intermediate-level waste (ILW), and a repository for low- and intermediate-level waste (L/ILW repository) [4]. The procedure for selecting the sites for the deep geological repositories is specified in the concept part of the Sectoral Plan for Deep Geological Repositories[5] (SGT, BFE 2008) and consists of three stages. The procedure ends with the registration of the selected site for each repository type in the SGT, following which General Licence Applications can be made.

For Stage 1 of the process, Nagra proposed six geological siting regions for the repository for low- and intermediate-level waste (L/ILW) and three for the repository for high-level waste (HLW) in November 2008. These siting proposals were prepared on the basis of criteria relating to safety and engineering feasibility, as well as other requirements set out in the Sectoral Plan. It was noted for the three siting regions that were proposed for both the HLW and the L/ILW repositories that the two repository types could be co-located at the same site; the term used for such a facility is a 'combined repository'. The siting regions proposed by Nagra were entered in the Sectoral Plan with a decision by the Federal Council in November 2011.

In Stage 2, proposals for siting the repository surface facility within the so-called planning perimeters of the regions had to be prepared together with the siting regions and the affected Cantons for potential areas. Nagra put forward siting proposals for the surface facility at the beginning of Stage 2 and these then formed the basis for a discussion and cooperation with the regional participation bodies. The proposals were evaluated and reviewed by the regions and the Cantons during the course of Stage 2 and were also, upon their request, modified and supplemented with additional proposals. As a result, Nagra was able to propose at least one siting area for the surface facility in each of the siting regions and to complete the associated planning studies. These planning studies serve as the basis for the socio-economic-ecological impact studies for each region that are prepared under the lead of the Swiss Federal Office of Energy (SFOE) [6] and for the preliminary investigations for the environmental impact assessment to be conducted at a later stage.

Stage 2 also includes a narrowing-down of the potential geological siting regions to at least two for each repository type for further investigation for Stage 3. This is done by conducting a safety-based comparison of the siting regions, with the highest priority being assigned to the long-term safety of the repository. A geological siting region can only be placed in reserve in Stage 2 if it shows clear disadvantages in terms of safety compared with the other regions. Aspects of spatial planning, ecology, economy and society are of secondary importance as selection criteria and the socio-economic studies have no impact on the selection of the geological siting regions. Requirements for these safety analyses are set out in BFE (2008) and in ENSI 33/075 (ENSI 2010).

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[2] *In German*: HAA-Lager.

[3] According to the current legislation, spent fuel is classified as radioactive waste.

[4] *In German*: SMA-Lager.

[5] *In German*: Sachplan geologische Tiefenlager (SGT).

[6] *In German*: Bundesamt für Energie (BFE).

The present report addresses the specific requirement that the long-term behaviour of the repository barrier system should be demonstrated. In particular, ENSI requires that Nagra analyses the safety-related impact on the barriers of repository-induced effects, such as desaturation effects, thermal effects, the effects of any high-pH plume and the effects of gas generation and gas pressure build-up (ENSI 2011, Request #38). ENSI requires that these analyses address all potential host rocks in a site-specific manner. The repository-induced effects are described in greater detail in Appendix 1 of the "Sachplan Geologische Tiefenlager – Konzeptteil" (BFE 2008).

The present report focuses on a L/ILW repository constructed in Opalinus Clay, which is the host rock proposed in SGT Stage 2 for this repository type. The aim of this report is to assess the effects of the waste emplaced in the repository and of the repository engineered materials on each other and on the Opalinus Clay host rock in order to better align the RD&D efforts of Nagra. A separate report deals with repository-induced effects for the HLW waste repository (Leupin et al. 2016).

The repository-induced effects by a co-disposal of HLW and L/ILW are discussed in Appendix A of the companion report on the repository-induced effects of a high-level waste repository (Leupin et al. 2016).

The effects considered are of the following broad types:

- **Thermal effects:** i.e. effects arising principally from the heat generated by the waste and setting of cement
- **Rock mechanical effects:** i.e. effects arising from the mechanical disturbance to the rock caused by the excavation of the emplacement caverns and other underground structures
- **Hydraulic and gas-related effects**[7]**:** i.e. the effects of repository resaturation and of gas generated, e.g. by the corrosion of metals within the repository, on the host rock and engineered barriers
- **Chemical effects:** i.e. chemical interactions between the waste, the engineered materials and the host rock

For the barrier system to be acceptable, it needs to be shown that such effects will not adversely affect repository performance and safety.

Effects such as those associated with biological organisms trapped in the repository or with the radiation field around the wastes are either considered to be minor, or are subsumed within the broad categories given above.

The processes giving rise to repository-induced effects are described in detailed process reports that either exist already or are under development. The descriptions given in the present report are thus limited to synopses and the reader is referred to the detailed process reports for further information. Furthermore, the main emphasis of the report is on repository-induced effects on the host rock, which are covered with more detail in the following chapters than effects on the engineered barrier system (EBS).

The datasets and indicator criteria used to assess the repository-induced effects were cleared in 2015 (or before) and thus might to some extent vary from the more site specific data and indicator criteria that will be cleared for Stage 3. This affects especially effects related to gas pressure build-up, rock mechanics and thermal effects. The method developed in this status report will be reassessed in the course of stage 3 of the sectoral plan.

[7] Hydraulic and gas-related effects are also referred to as "two-phase flow" phenomena in the text.

1.2 Methodology

The methodology adopted in this report comprises the following broad steps and key questions (Fig. 1.2-1):

1. describe the reference repository (configuration / design)
2. identify and describe processes with potentially adverse effects on safety functions[8]
3. make a first qualitative assessment of these effects based on pre-existing data
4. if significant adverse consequences cannot be excluded on qualitative grounds, make a quantitative assessment of these consequences, including, if necessary, radionuclide release and transport calculations
5. based on the insights from Steps 1 – 4, provide input to the design of the repository with the aim of avoiding or mitigating effects that may have a significant and detrimental impact on repository safety

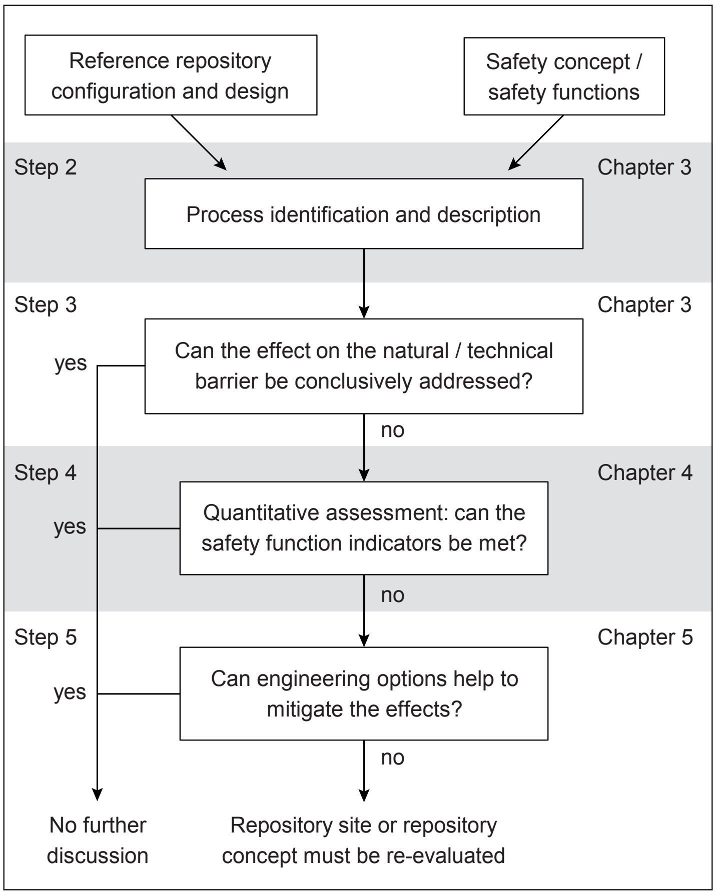

Fig. 1.2-1: Methodological steps and the chapters of this report where each step is applied.

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[8] The overall criterion for evaluating repository safety is the risk criterion issued by national regulators which is usually expressed as a maximum dose, or risk, to a representative individual in the group in the biosphere exposed to the greatest risk. To evaluate the dose or risk from a repository a detailed and quantitative understanding of all processes that affect the repository together with the associated uncertainties is needed. Dose and risk are therefore not very practical entities to use for the study of individual repository components. To resolve this, the concept of "safety functions" has been introduced. A safety function is a description of how an individual barrier contributes to the confinement and retardation of radionuclides. Safety functions can be defined based on the understanding of the properties of the components and the long-term evolution of the system.

1.2.1 Qualitative assessment of adverse consequences

The third step is a qualitative assessment, based on pre-existing data, of the specific effects that the identified thermal, rock-mechanical, hydraulic- and gas-related, and chemical processes could have on the repository safety functions.

When assessing the potentially adverse consequences for the safety functions, current understanding of these effects and all associated uncertainties are taken into account. Specific aspects that are assessed include:

- **the reversibility of any impact:** if the impact of a process is reversible, then its adverse consequences are likely to be more limited than if it is irreversible
- **the relevant period:** some effects only occur for a limited period, e.g. fast aerobic corrosion can only happen while oxygen is present and, if radionuclides are fully contained during this period, there may be a few if any consequences for repository safety
- **the spatial extent of any impact:** some processes will affect, e.g. the repository near field only, whereas others may propagate further into the repository host rock
- **the relevance to siting:** given that an objective of SGT Stage 2 is to select at least two geological siting regions for a L/ILW repository for further geological investigations, any relevance of site-specific conditions to the adverse consequences of repository-induced effects is clearly of interest

It is important not only to consider direct (i.e. thermal, rock-mechanical, gas-related and chemical) consequences of repository-induced effects, but also the couplings between these, as illustrated schematically in Tab. 1.2-1.

Tab. 1.2-1: Schematic illustration of couplings between thermal, rock-mechanical, gas-related and chemical effects for a L/ILW repository.

[T] Temperature-related processes; [RM] rock mechanics-related processes; [G] gas-hydraulic-related processes; and [C] for chemical processes. Colors are used for better readability.

Temperature		T → RM	T → G	T → C
Rock mechanics	RM → T		RM → G	RM → C
Gas-hydraulic	G → T	G → RM		G → C
Chemistry	C → T	C → RM	C → G	
	Temperature	Rock mechanics	Gas-hydraulic	Chemistry

In some cases, it is possible to argue convincingly, on qualitative grounds, that the detrimental impacts of the processes on the repository safety functions will be negligible. In other cases, a more quantitative evaluation of consequences is necessary in Step 4, below.

1.2.2 Quantitative assessment of remaining effects on repository barriers and safety functions

Where significant detrimental impacts on the repository safety functions cannot be excluded on qualitative grounds, a quantitative assessment of impacts is carried out. A set of criteria is established to support this assessment. Following the terminology of SKB (the Swedish Nuclear Fuel and Waste Management Company), these criteria are termed safety function indicator criteria. The criteria concern indicators that can be evaluated in calculations of repository evolution (or specific aspects thereof), such as e.g. peak temperature within and around the repository, or the radial extent of any excavation damaged zone (EDZ). The criteria give limits for how high (or low) the indicators need to be before certain adverse consequences could potentially arise. If the limits can be shown not to be reached for any plausible path of evolution, then the corresponding adverse consequences can be excluded.

If safety function indicator criteria cannot be formulated, or if the criteria cannot unequivocally be shown to be met, then additional radionuclide release and transport calculations are carried out (or existing radionuclide transport calculations are re-examined) to evaluate the nature and extent of any detrimental effects and assess the implications in terms of safety indicators, principally the annual individual dose.

The site-specific characteristics of the rock are, where relevant, taken into account:

- when formulating the safety function indicator criteria, and
- when performing calculations to test whether the criteria are met

Thus, the model assumptions and parameter values that are used are intended to cover the full range of expected conditions in the potential siting areas for a L/ILW repository in Opalinus Clay. The model assumptions and parameter values are therefore based, where possible, on site-specific field observations and measurements, complemented by laboratory experiments, supporting calculations and, where necessary, expert judgement. Expert judgement is required because not all characteristics of the potential siting areas are well known at the present stage of the programme. Some assumptions may also be challenged by stakeholders. Thus, especially for less well known and potentially sensitive characteristics, some more extreme model assumptions and parameter values are considered that are outside the ranges expected at the potential siting areas but are still physically plausible, in addition to realistic assumptions and parameter values. The more extreme calculation cases can illustrate the robustness of the repository concept by showing that, even under highly pessimistic, hypothetical assumptions, the nature and extent of any detrimental effects are still insufficient to compromise safety. An example of this type of calculation is that of porewater flow and radionuclide transport along the EDZs of the repository tunnel system, assuming a hypothetically very high EDZ hydraulic conductivity, even though the expected evolution is that the EDZ, once formed, will reseal to some extent. The calculation is discussed further in Section 4.6.2, with details given in Poller et al. (2014).

Nagra's internal data clearance procedure was used to ensure the consistent use of parameter values in all model calculations. This data clearance procedure is an integral part of Nagra's Quality Management System and requires that the data user (client) sets out the data to be used and the purpose to which the data will be put. By signing off the data, the data producer confirms that the data are suitable for their intended use. A data clearance committee oversees the application of this procedure.

1.2.3 Input to the design of the repository

If, based on the insights from Steps 2 – 4, repository-induced effects and associated processes are identified that could conceivably give rise to unacceptable impacts on the repository and its safety functions, then future iterations of the repository design should aim to avoid or mitigate these effects. Thus, the present study provides input to the repository design process.

1.3 Report structure and relation to other reports

The remaining chapters of this report are structured as follows:

- Chapter 2 describes the reference configuration for a L/ILW repository in Opalinus Clay assumed in this report. This description includes the repository engineered and natural barriers, the safety functions that they perform, and the safety function indicators that are evaluated in the later chapters to assess the impact of repository-induced effects on the safety functions.
- Chapter 3 identifies, and provides a qualitative description of thermal, rock-mechanical, gas-related and chemical repository-induced effects, including the couplings between them and, based on this description, provides a summary of the evolution of the repository, taking into account those effects that are judged to be potentially significant. This chapter thus covers Step 3 of the methodology described above.
- Chapter 4 provides a quantitative assessment of those effects that are judged to be potentially significant, including the safety function indicator criteria used to judge actual significance, dose calculations of specific effects that cannot be excluded based on these criteria and a synthesis of system behaviour under site conditions. This chapter thus covers Step 4 of the methodology.
- Chapter 5 summarises the input that the present study provides to the repository-design process and thus covers Step 5 of the methodology.

The present report and the companion report on repository-induced effects in the context of a HLW repository (Leupin et al. 2016) refer to the findings documented in SGT Stage 2:

- the main technical report for SGT Stage 2 (Nagra 2014a) provides the formal safety-related comparison of the repository siting regions currently under consideration
- a geological synthesis (Nagra 2014b)
- a safety report (Nagra 2014c)
- a report on the operational risks (Nagra 2014e)

These reports, together with more detailed and specific process reports, provide the technical foundation for the present report.

2 Description of the reference repository configuration and design

2.1 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 2008b and c) 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 2002a) for the ILW repository. Although the repository concept used is generic, the corresponding repository configuration data can easily be adapted to future project requirements, e.g. by making site-specific modifications to the repository layout and updating waste inventories.

2.1.1 Components of the repository system

Fig. 2.1-1 presents a schematic view of a generic layout of the L/ILW repository, displaying the main elements of the underground structures, namely access ramp and shafts, operations and access tunnels, pilot repository, facility for underground geological investigations, seal sections and the emplacement caverns. The generic layout was adapted to geological conditions in the candidate siting regions, in particular taking into account the burial depth and thickness of the host rock formations, their geotechnical properties (rock strength and hydraulic conductivity) and the environmental conditions with regard to relevant state variables (stress state, head distribution).

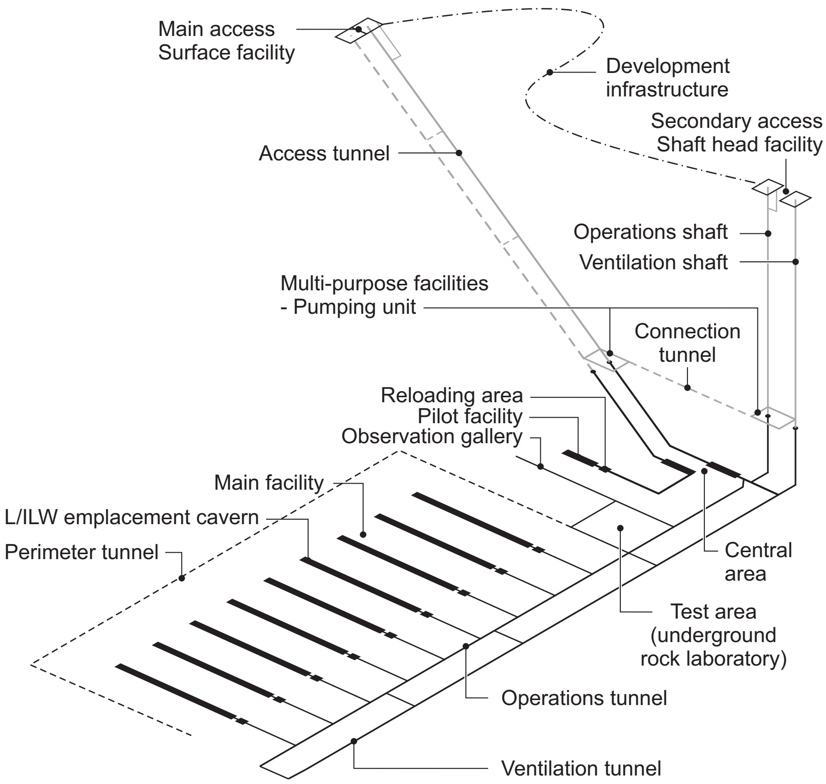

Fig. 2.1-1: Schematic plan-view layout of a generic concept for a L/ILW repository.

The number and dimensions of the caverns corresponds to a waste volume (conditioned and packaged) of approximately 75'000 m^3 (scenario with wastes from the existing nuclear power plants with an assumed operation time of 50 years). A design variant for an enlarged waste volume ("umhüllendes Abfallinventar" with 200'000 m^3 of L/ILW, referred to in this report as "bounding inventory"; as used for the evaluation of siting regions), is described in Nagra (2008c).

Specific components of the repository system that are of special relevance for the assessment of gas release are described in the subsequent chapters.

2.1.2 Emplacement caverns

The disposal containers are emplaced in caverns with a cross section of approximately 11.0 × 13.2 m as shown in Fig. 2.1-2 (design variant K09)[9]. The length of the caverns is approximately 200 m but can be longer or shorter. The caverns need to be supported with rock bolts and sprayed concrete lining including reinforcement (steel wire mesh). Each cavern is connected to the operations tunnel via a branch tunnel. The disposal containers are transported to the branch tunnels by rail. At the transition to the emplacement cavern, the branch tunnel is enlarged to provide sufficient space for the transfer of the disposal containers from the railway wagon to the deposition overhead crane. The lower part of the cavern ("cavity") is partitioned into disposal sections of approx. 28 m length by reinforced concrete walls ("bulkheads"). The void space between the disposal containers with cementitious mortar and the void space between the crane columns and between the disposal containers in the upper part of the cavern ("top heading") are both filled with cementitious mortar.

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[9] Several cavern size options have been considered by Nagra for L/ILW caverns (Nagra 2010). Because of stability considerations and concerns about excavation disturbance having a negative impact on characteristics of the Opalinus Clay, the large diameter cavern concepts, K12, K16 and K20, are considered much less suitable than K04, K06 and K09.

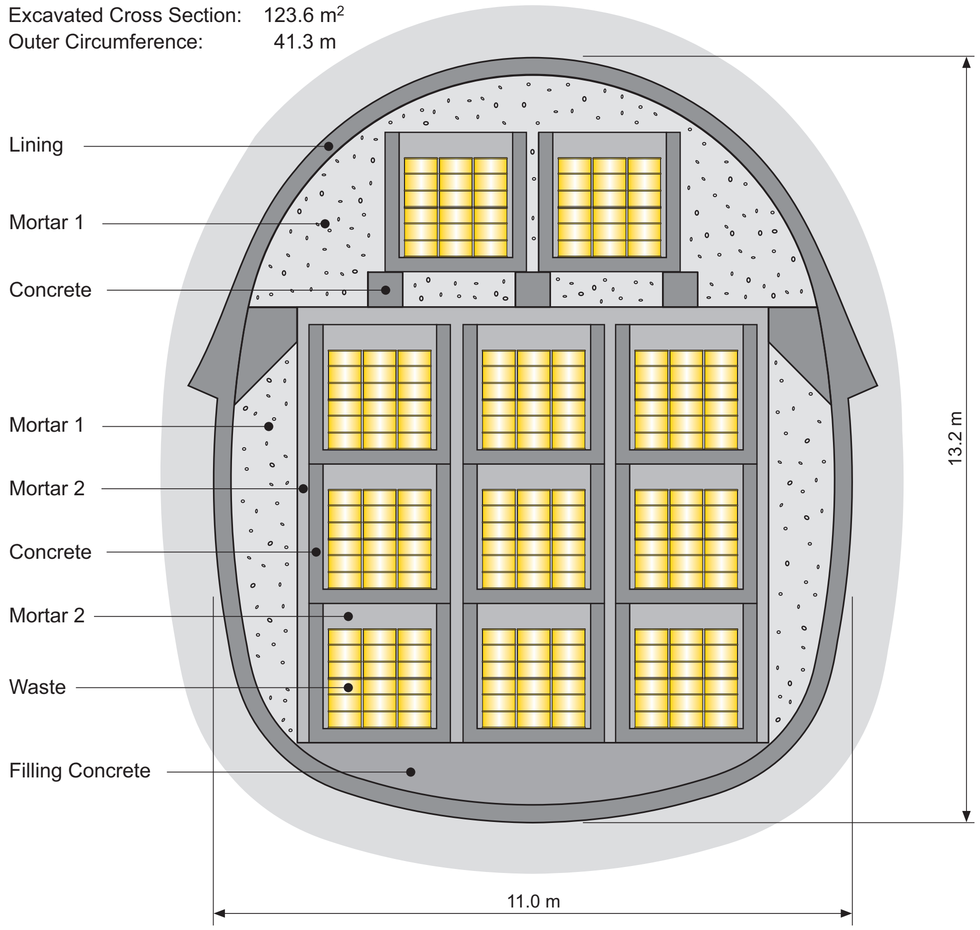

Fig. 2.1-2: Cross section of a L/ILW emplacement cavern after closure (K09).

2.1.3 Backfilling and sealing systems

As soon as the emplacement of disposal containers in one section of a cavern is completed, the voids between the containers and the cavern lining are backfilled with cementitious mortar. Once all sections of the cavern and the top heading are backfilled the enlarged section of the branch tunnel at the caverns entrance is also backfilled with mortar. Each cavern is closed with a concrete plug (see Fig. 2.1-3). At the end of the operational phase, both the operations 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 with 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 operations 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 from the seal section.
2. A ring of Opalinus Clay is excavated to a depth of approximately 1 m to remove the excavation damaged zone (EDZ), 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).

An engineered gas transport system (EGTS) is foreseen which allows the release of gas from the emplacement caverns into the overlying more permeable rock formations. The gas path follows from the caverns through the branch tunnels into the operations tunnel and then along the access tunnel into more permeable units. Fig. 2-1.4 shows the concept with the expected engineered gas transport path on the basis of the reference project (Nagra 2002a and 2008d).

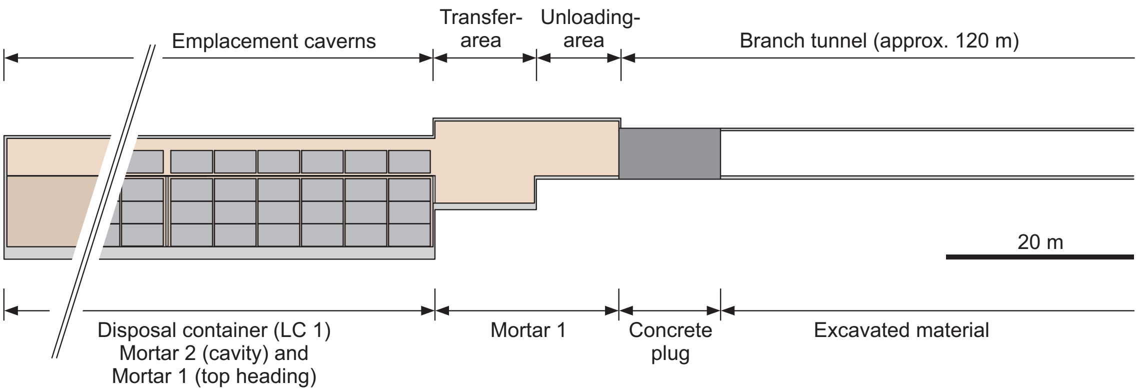

Fig. 2.1-3: Longitudinal section of L/ILW emplacement cavern after closure.

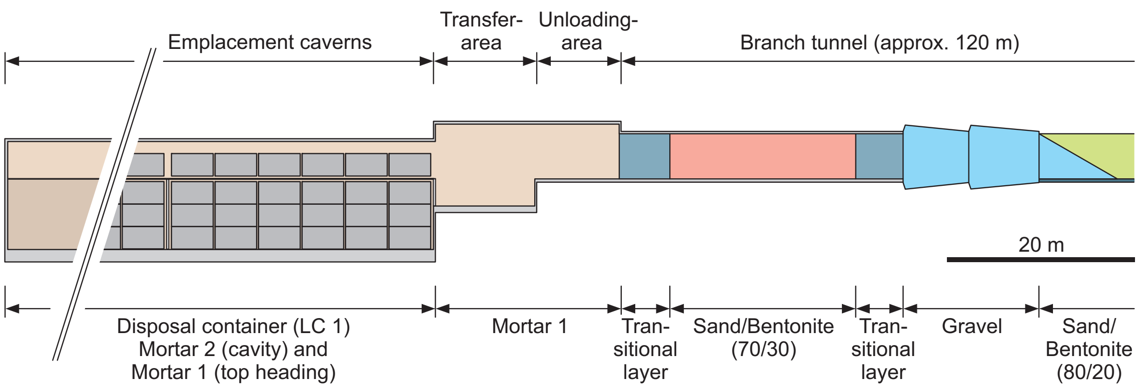

Fig. 2.1-4: Longitudinal section of a possible seal/plug variant for L/ILW described in Nagra (2008d).

2.2 Safety concept and safety function indicators

Each element of the barrier system performs one or several long-term safety functions, which are (Nagra 2008c, Nagra 2010):

- physical isolation of the wastes from the human environment and long-term stability of the barrier system
- confinement of radionuclides
- retarded release of radionuclides
- retention of radionuclides in the near field and geosphere
- attenuated release of radionuclides to the environment

The overall geological situation should ensure the long-term stability of the barrier system over the so-called *time frame for safety assessment*, which is the main period of concern from the perspective of post-closure safety and which was first defined in Nagra (2008c) based on the decrease in radiological toxicity that occurs over time. It extends to 100'000 years for the L/ILW repository.

The various elements of the barrier system that are key to providing these safety functions are (Nagra 2008c):

- **the deep underground location of the emplacement caverns** that provides physical isolation of the wastes from the human environment over the time period to be considered
- **the geological setting** that is not prone to geological events and processes affecting the long-term stability of the barrier system over the time period to be considered, and that is unlikely to attract human intrusion due to the absence of resources considered viable today or in the near future
- **the host rock and – where present – the confining units** that provide low water flows, a fine and homogeneous pore structure and favourable geochemical conditions, thus providing strong retention and attenuated release of radionuclides to the environment as well as a suitable hydrogeological, geochemical and geomechanical environment for the engineered barrier system over the time period to be considered
- **the cementitious near field** that provides a contribution to the overall retention of radionuclides and an environment that ensures low microbial activity and low corrosion rates
- **the backfill and sealing elements of the underground facility** that prevent human access to the disposed wastes and that ensure mechanical stability of the underground structures, thus providing controlled conditions compatible with the favourable conditions in the host rock, as well as strong retention and attenuated release of radionuclides to the environment
- **the waste forms** retain their initial properties for a long period of time in the expected environment, with low corrosion and degradation rates, and thus contribute to the confinement and retardation of releases for those radionuclides that are incorporated in the waste matrices

These elements and the safety functions they provide must be shown to be robust with respect to repository-induced thermal, rock-mechanical, gas-related and chemical effects. In practice, this means that:

- The temperature rise due to heat generated by the waste should be insufficient to adversely affect the transport and retention properties of the host rock and EBS.
- The excavation damaged zone (EDZ) formed around underground openings should be of limited radial extent and not lead to transport pathways with unacceptable properties.
- Gas should be able to migrate without permanently damaging the transport and retention properties of the host rock.
- The effects of corrosion products, the high-pH plume from cementitious materials and trapped oxygen on the host rock and on the EBS should be insignificant, and the materials used to stabilise underground openings should not be used in amounts that could compromise long-term safety.

These claims are substantiated by the qualitative and quantitative assessments given in Chapters 3 and 4, which show, for example, that the EDZ formed around the emplacement caverns will not exceed one to two tunnel diameters, thus the extent of intact host rock above and below the repository is not greatly reduced. The thickness of the undisturbed host rock is an example of a safety function indicator, and the corresponding criterion is that this should always exceed 20 m (see Section 4.1). As noted in Chapter 1, the criteria specify how high (or low) the indicators need to be before certain adverse consequences could potentially arise. If the criteria can be shown to be satisfied for all plausible paths of evolution, then the corresponding adverse consequences can be excluded.

Other safety function indicators considered in the following chapters include:

- maximum temperature-induced pore-fluid pressure
- maximum gas pressure
- EDZ effective hydraulic conductivity
- the extent of host rock above and below the repository that is not damaged by excavation

Criteria for these and other indicators are developed and applied in Chapter 4. In terms of the Safety Case, robustness is also enhanced by the fact that, if needed, design options are available to ensure that the safety function indicator criteria are met, e.g. by reducing the impact of the EDZ or by reducing the gas-pressure build-up in the repository tunnel system. These options are discussed further in Chapter 5.

3 Qualitative description of the repository-induced effects

This chapter provides a qualitative description of the identified processes related to the four broad repository-induced effects (i.e. processes related to temperature, processes related to rock-mechanical effects, processes related to pressure and gas generation, and processes related to chemical interactions; see Fig. 3.1-1). This chapter provides also an overview of the safety-relevance and degree of available understanding of these processes and of how the processes are treated within models.

Fig. 3.1-1 shows the main relevant processes that are currently believed to influence the geochemical evolution in Opalinus Clay. The colour intensity indicates in a non-quantitative way their expected importance over time. Most of these processes are described in more detail in this report.

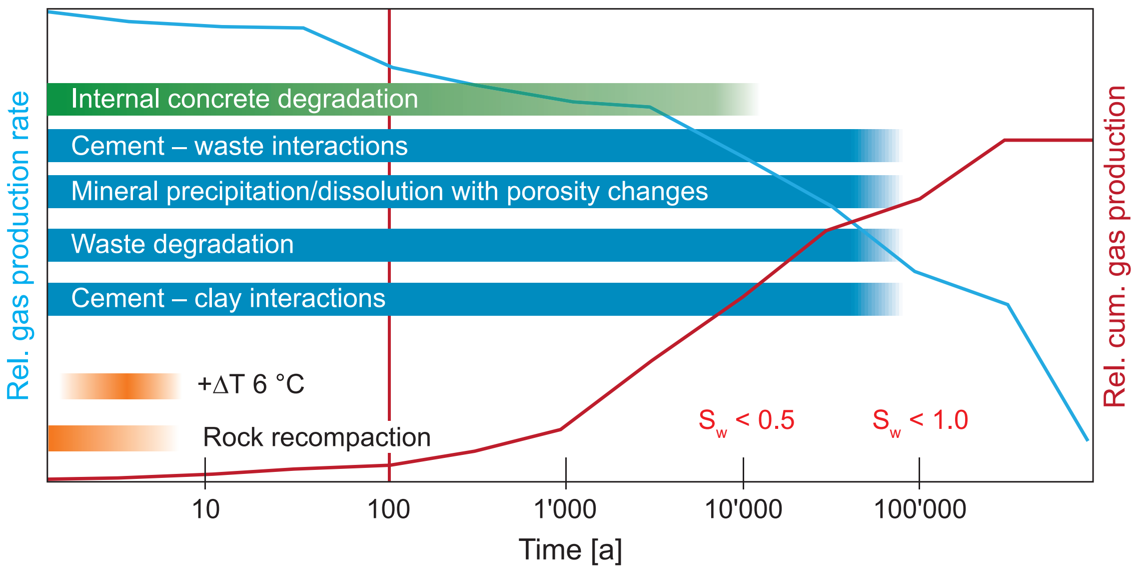

Fig. 3.1-1: Overview of the expected evolution of main processes in a L/ILW repository.

The red vertical line indicates repository closure at 100 years and S_w indicates the degree of saturation of the emplacement cavern.

3.1 Processes related to temperature evolution and its effects on the repository system

Heat in the L/ILW emplacement caverns is produced by setting cement (hydration processes) (Poller et al. 2014) and by radioactive decay of the waste. By the time of repository closure, the cement will be completely set (i.e. hydrated). The release of hydration heat from mortar used in plugs to close the repository and/or shotcrete used to stabilise underground structures would occur within a few months, leading to a relatively short-term temperature increase within and around the repository. It is expected that the temperature increase in the host rock will be limited to around 5 to 10° C, because only low heat emitting waste is present (see Section 4.2). The ambient temperature may range from about 36 – 50° C depending on the location (depth of the host rock) of the finally selected site. As discussed in Section 4.2, a temperature rise in the host rock in the range of 5 to 10° C is expected to have a negligible effect on any chemical or physical processes.

The expected temperature rise is too small to have any impact on the repository evolution other than a potential increase in degradation kinetics of organic compounds in the waste. A higher degradation rate is taken into account by attributing high degradation rates to organics and assuming a "bounding" rate of gas generation. The corrosion rate of steel under repository conditions is not expected to be affected by such a temperature increase (Diomidis 2014).

The short duration and small rise of the temperature peak will unlikely greatly increase the depth of the de-saturated zone and thus will be expected to have no significant impact.

3.1.1 Summary of potentially detrimental effects due to couplings between temperature evolution and other processes

The potentially detrimental temperature-related effects identified in the preceding sections are summarised in Tab. 3.1-1, together with an assessment of their relevance, coupling to other rock-mechanical, gas-related or chemical processes and their treatment in, or omission from, the quantitative analyses in Chapter 4.

Tab. 3.1-1: Potentially detrimental temperature-related (T) effects, assessment of their relevance, coupling to other rock-mechanical (RM), gas-related (G) or chemical (C) processes and treatment in, or omission from, the quantitative analyses in Chapter 4.

Temperature-related effects	Relevance/couplings	Treatment
Increased kinetics of degradation of organics	Degradation of organics (T $\rightarrow$ G)	Taken into account in analyses of gas production and transport by assuming higher degradations rates and a "bounding" rate of gas generation (Section 4.4)

3.2 Processes related to rock mechanics and its effects on the repository system

Excavation of caverns and tunnels in the host rock leads to stress redistribution that results in micro- and macro-scale fractures within an excavation damaged zone (EDZ). The formation of an EDZ[10] alters the properties of the host rock adjacent to the emplacement caverns, sealing zones and other underground structures. In particular, damage to the host rock results in an increased porosity, thus leading to a higher hydraulic conductivity and gas permeability.

The EDZ will become partially desaturated as a result of evaporation due to ventilation during the construction and operation phase (as noted in Section 3.1, it is unlikely that the additional heat from the radioactive decay of L/ILW waste material will greatly increase the depth of the de-saturated zone). Desaturation will also result in stiffening of the host rock (Nagra 2002a).

The EDZ around the backfilled underground structures of a geological repository represents a potential release path for radionuclides as well as a possible escape route for corrosion and degradation gases. The efficiency of this release path depends on the shape and extent of the EDZ (see Fig. 3.2-1), as well as on the driving forces for solute and gas transport.

[10] The excavation damaged zone is conceptualised in the rock-mechanical model (see Fig. 4.3-2) as simulated fracture patterns around the cavern and referred to as plastified zone in terms of tensile and shear failure around the excavation.

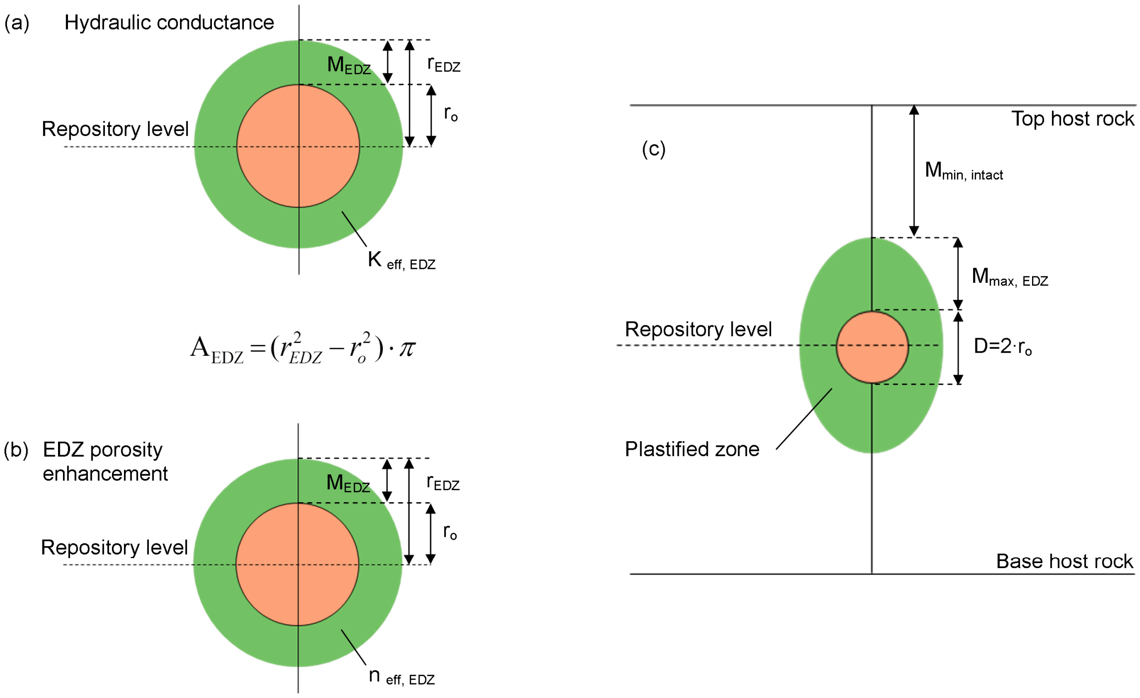

Fig. 3.2-1: EDZ indicator criteria related to long-term safety.

(a) hydraulic conductance of the EDZ ($K_{eff,EDZ} \times A_{EDZ}$), (b) effective porosity enhancement of the EDZ and (c) minimum thickness of the intact host rock ($M_{min,\ intact}$) in a non-isotropic stress field.

The hydraulic conductivity of the excavation damaged zone after the closure of the repository mainly depends on the size, geometry and orientation of the excavation, as well as on rock-mechanical parameters, the in-situ stress conditions, and the self-sealing capacity of the host rock.

In the case of the Opalinus Clay, evidence from experimental work at the Mont Terri underground rock laboratory and from modelling studies indicate that the self-sealing capacity of the rock will eventually limit the hydraulic conductivity and gas permeability of the EDZ; the evolution of the EDZ is thus potentially affected by chemical processes that could clog the EDZ (see Section 3.4) and impact the swelling pressure in tunnel sections where bentonite or bentonite – sand mixtures are used as backfill materials. Furthermore, tunnel support (e.g. anchors etc.) will be used during construction of the emplacement caverns to limit the radial propagation of EDZ fractures. Temperature effects on EDZ development in an L/ILW repository are expected to be relatively minor for Opalinus Clay.

The EDZ around the emplacement caverns is not expected to affect the overall radionuclide transport along the caverns because of the high porosity of the mortar that is used as cavern backfill which has a higher permeability than the EDZ. The EDZ around the sealing zones is, however, relevant to the repository safety functions because, if sufficiently conductive, it could provide a pathway for groundwater flow, gas flow and radionuclide transport, by-passing both the sealing zones and the undisturbed host rock. However, the EDZ around the caverns is also potentially safety-relevant because a large radial extent of the EDZ may lead to a significant reduction of the thickness of the intact host rock.

Another potentially safety-relevant effect related to the EDZ is that microorganisms may also be locally active within it. Microbiological effects are discussed in Section 3.3.3. A positive effect of the EDZ is that it may provide a reservoir for repository-generated gas and thus contribute to a reduction of peak gas pressures (see Section 3.3).

The potentially safety-relevant rock-mechanical effects related to the EDZ are summarised in Tab. 3.2-1, together with an assessment of their relevance, coupling to other temperature-related, gas-related or chemical processes and their treatment in, or omission from, the quantitative analyses in Chapter 4.

Tab. 3.2-1: Potentially safety-relevant rock-mechanical (RM) effects[11], assessment of their relevance, coupling to other temperature-related (T), gas-related (G) or chemical (C) processes and treatment in, or omission from, the quantitative analyses in Chapter 4.

Note: chemical effects of H_2 dealt with in Section 3.4.

Rock-mechanical effects	**Relevance/couplings**	**Treatment**
EDZ creation, fracture creation and rock-mechanical reactivation during the thermal period	EDZ around the seals provides a potential pathway for ground-water flow, gas flow and radio-nuclide transport (RM $\rightarrow$ G)	Taken into account in analyses of gas production and transport in Section 4.4
	Various chemical and micro-biological processes may occur within the EDZ (RM $\rightarrow$ C)	See Sections 3.3 and 3.4
	EDZ reduces the thickness of the undisturbed host rock	Taken into account in hydro-mechanical calculations in Section 4.4

3.3 Processes related to the gas pressure build-up and its effect on the L/ILW repository system

The accumulation and release of repository-generated gases may affect a number of processes that influence long-term safety. The specific issues highlighted in the following are:

- gas production in the backfilled repository emplacement caverns
- impacts of gas accumulation on the repository near field
- role of the EDZ as a gas release path, and
- impacts of gas accumulation and gas release on the host rock

[11] The long-term safety criteria according to Tabs. 4.1-4 and 4.1-5 are illustrated in Fig. 3.2-1:

- The maximum hydraulic conductance of the EDZ after backfilling of the repository: Dose calculations in Nagra (2014) suggest that the radionuclide transport in the EDZ of the backfilled repository structures is not significant when the effective hydraulic conductance of the EDZ remains below 10^{-8} m^3/s (corresponding to an equivalent thickness of the EDZ of 1 m).
- The extent and shape of the plastified zone (EDZ): From a long-term safety perspective (Nagra 2014), the plastified zone may not reduce the thickness of the intact host rock to less than 20 m, in which case its safety function as a transport barrier for radionuclides would be markedly reduced.

3.3.1 Gas production in the backfilled emplacement caverns

Gases are generated in an L/ILW repository as a result of anaerobic corrosion of metals (which produces H_2), microbial and chemical degradation of organic matter (which may produce gaseous compounds CO_2, CH_4, which may incorporate ^{14}C) and radiolysis of water (which principally produces H_2). The sources of gas generation comprise the contributions directly related to the waste inventory, whereby gas generation from degradation of organic waste amounts to typically less than 20 % of gas production from metal waste. In addition, structural materials used for tunnel construction and repository operation (rock support: anchors, bolts, arches, steel mats, steel fibres; waste emplacement: rails, track beds, lifting devices) produce further volumes of H_2 that are small compared to gas production from the waste. Gas production takes place preferentially on the surface of the waste materials and at the interface between backfilled caverns and host rock. Gas production rates are largely determined by the nature of the structural materials and wastes to be disposed, as well as by the environmental conditions and the porewater chemistry at the loci of interaction.

Because the backfill material (mortar) is highly porous, the L/ILW emplacement caverns will saturate relatively slowly and water saturation will begin in the bottom part of the cavern. Anaerobic conditions will develop while the caverns are still only partially saturated due to the consumption of O_2 by aerobic corrosion and other processes. As gas is produced, it will mix with the remaining air and accumulate at the top of the cavern in the porous mortar.

A balanced assessment of the aforementioned processes associated with gas generation requires a detailed evaluation of the environmental conditions for a given repository configuration. Not only the type of repository, but also the site-specific hydraulic conditions (rock permeability, formation pressure) and the porewater chemistry are governing the impact of the relevant processes on the long-term evolution of the repository system (see Section 3.4).

3.3.2 Gas accumulation on the repository near field

As noted above, localised anaerobic conditions can occur during the early post-closure period as the cementitious backfill and the EDZ resaturate. The saturation distribution will be controlled by the capillarity of the different backfill materials, as well as by gravity. That is, the construction concrete in the cavern base, which has small pores, will be saturated earlier than the mortar in the cavern roof and the cavern sides, which has large pores and therefore a low capillarity. H_2 generation due to the anaerobic corrosion of metals can potentially affect resaturation. As the gas pressure increases in the cavern, the porewater in the backfill can be displaced. This will depend on the extent to which effective gas permeability of the cavern seal and adjacent EDZ allows the release of the accumulated gas from the repository caverns. Thus, depending on the assumed gas generation rate, host rock properties, and on the design of the engineered barrier system, the de-saturation regime may last between a few thousand years and more than hundred thousand years.

Gas generated by the disposal containers migrates mainly in an upward direction towards the ceiling and laterally towards the cavern seal. Volatile radionuclides (mainly ^{14}C) will be dispersed in the gas phase, which accumulates in the ceiling of the cavern.

Pore blocking that potentially prevents outward gas flow could occur along the contact between the caverns and the surrounding host rock and along the contact between the cementitious backfill and the sand/bentonite seal of the EGTS. This is due to the hydrochemical self-sealing processes associated with chemical reactions of high-pH porewater with clay minerals (backfill/seal interface) and clay porewater with cement (host-rock/liner interface; see Section 3.4). These reactions typically occur under fully saturated conditions, which are more likely to occur at the outer cavern interface with the host rock rather than at the inner interface between the caverns and seal.

Various transport mechanisms control the combined flow of gas and porewater in the backfill surrounding the L/ILW containers. These include advection and diffusion of dissolved gas, visco-capillary displacement of porewater and dilatancy-controlled gas flow at an elevated gas pressure (Senger et al. 2013). In contrast and independent of the actual gas transport mechanism, combined flow of gas and water through the sand/bentonite seal is associated with localisation phenomena such as capillary fingering and pathway dilation.

The EGTS seal, composed of a mixture of 80 % sand and 20 % bentonite, is designed to allow preferential flow of gas, while restricting liquid flow and transport of dissolved radionuclides (Nagra 2008d). The sand/bentonite mixture has relatively low water retention, but gas can still be trapped in irregular patterns in the inter-granular pore space of the sand/bentonite. Trapped gas facilitates easier gas migration through the sand/bentonite mixture creating continuous gas paths through the cavern seal. The percolation of a gas phase through an initially saturated sand/bentonite seal is a subject of recent studies within Nagra's RD&D programme (Rüedi et al. 2012).

3.3.3 The role of the EDZ as a gas release path

As discussed in Section 3.2, an EDZ develops around all underground structures during repository construction and subsequent ventilation during the repository operation. After backfilling of the underground structures, the EDZ will re-compact partially according to the local stress conditions and the swelling capacity of the sealing materials and of the near-field host rock.

The EDZ around the sealing sections will play a significant role in the release of gas from the emplacement caverns because of the preferential flow paths in the EDZ that are created at the time of EDZ formation or are reactivated as a result of an increase in gas pressure along the fractures. Furthermore, the gas-filled pathways in the EDZ could host sulphide-producing microbes, which could increase corrosion rates of metals used in engineered structures. The effect of this process is accounted for by the pessimistic evaluation of the steel corrosion rate and H_2 gas generation rates. At late times, when the gas production rate has diminished, the gas pressure declines and the effective stress on the EDZ fractures increases, resulting at least partly in their closure.

The EDZ around the sealing sections will also potentially affect radionuclide release and transport. Poller et al. (2014) compare two variants for the main access route to the underground facilities of a deep geological repository (a ramp and shafts vs. shaft access only) using flow and radionuclide transport calculations. The results show that, for realistic parameter values, radionuclide release along the access routes of a deep geological repository is extremely low. Thus, they confirm the reference assumption that radionuclide release occurs predominantly through the host rock. Furthermore, even for highly unfavourable parameter values including a highly conductive EDZ around the seals, the calculated dose rates are several orders of magnitude below the regulatory safety criterion of 0.1 mSv per year, since water flow along the underground tunnel system is ultimately limited by the low hydraulic conductivity of the host rock.

3.3.4 Impacts of gas accumulation and gas release on the host rock

Gas migration into the intact host rock can occur when the gas pressure exceeds the gas entry pressure of the intact formation and overcomes the resistance to flow due to the relatively low effective gas permeability of the host rock. As gas accumulates in the EDZ, displaced porewater could enter the host rock and increase the porewater pressure in the intact host rock. The increase in pressure causes a decrease in the effective stress in the host rock which can create localised deformation and changes in pore volume by reopening pre-existing, tight fractures or by the creation of new pathways (pathway dilation). This can produce preferential pathways for the generated gas which self-seal when pressure drops. In addition, because of the relatively large surface area of the emplacement cavern, heterogeneity in host rock properties and potential fractures may be encountered that could also provide pathways for gas migration.

Although these effects make the entry of a gas phase into the intact rock matrix less likely, the relatively large surface area of the potential radial gas propagation front allows for diffusive transport of dissolved gas into the intact host rock. As the pore pressure declines away from the emplacement caverns, the solubility limit decreases and exsolution of dissolved gas can occur[12].

In principle, a sufficiently large gas pressure build-up could lead to gas pressures that exceed the shear strength of the rock, of which the lithostatic pressure is an indicator (Nagra 2008d). The possibility of this situation occurring in reality has been evaluated in the simulations in Section 4.4.

3.3.5 Summary of potentially detrimental effects due to couplings between gas-related processes and other processes

The potentially detrimental gas-related effects identified in the preceding sections are summarised in Tab. 3.3-1, together with an assessment of their relevance, coupling to other temperature-related, rock-mechanical or chemical processes and their treatment in, or omission from, the quantitative analyses in Chapter 4.

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[12] Gas exsolution may enhance the overall gas transport capacity of the host rock formation (its effect can be represented in terms of residual gas saturation in the relative permeability relationship).

Tab. 3.3-1: Potentially detrimental gas-related (G) effects, assessment of their relevance, coupling to other temperature-related (T), rock-mechanical (RM) or chemical (C) processes and treatment in, or omission from, the quantitative analyses in Chapter 4.

Note: chemical effects of H_2 are dealt with in Section 3.4.

Gas-related effects	**Relevance/couplings**	**Treatment**
Gas pressurisation and gas-induced porewater displacement	Could lead to delayed resaturation and uncertainty regarding hydraulic evolution of the near field	Accounted for in gas migration analyses in Section 4.4
Gas can be trapped in irregular patterns in the inter-granular pore space of the sand/bentonite seal	May delay the consolidation process and delay the homogenisation of the seal during the resaturation process and affect gas transport.	Favourable: trapped gas lowers the gas entry pressure and increases gas transport capacity Consolidation and homogenisation takes place with decreasing gas generation rates
Gas-filled pathways in the EDZ could host sulphide producing microbes	May affect metal corrosion ($G \rightarrow C$)	Accounted for by pessimistic evaluation of H_2 gas generation rates in Section 4.4
Gas pressure decreases the effective stress in the host rock	Pathway dilation ($G \rightarrow RM$)	Accounted for in gas migration analyses in Section 4.4

3.4 Processes related to chemical interactions and their effects on the repository system

Chemical interactions between repository barriers (engineered and natural) are driven by chemical, thermal, and hydraulic gradients, which evolve in space and time in the repository system. The use of contrasting materials, such as clay (natural and engineered), cement/concrete, and steel leads to sharp chemical gradients at interfaces. The interactions of the materials are influenced by various chemical reactions and transport processes and moreover, will be strongly coupled in a non-linear fashion. Dissolution and precipitation processes, as well as ion exchange reactions, might alter the pore space with accompanying changes in material characteristics (transport, flow, and mechanical properties). In terms of transport, saturation state, water flow and diffusion of solutes across the various material interfaces will strongly influence the extent and timescale over which chemical processes occur. The temperature pulse originating from the hydration of cement or from radioactive decay (though the latter is less important for a L/ILW repository than for a HLW repository) may also accelerate chemical transformations, change the stability of mineral phases, and accelerate diffusive transport. However, these effects will be minor for the likely peak temperature increase in the host rock of 5 – 10° C above ambient temperatures.

Detailed descriptions of the chemical evolution of the near field of a L/ILW repository in Opalinus Clay have been produced (Nagra 2002c, Kosakowski et al. 2014). The L/ILW emplacement caverns contain waste solidified mainly with cement grout, surrounded by a relatively high permeability cement-based mortar with a porosity of ~ 25 %. About 75 % of the mass in the L/ILW tunnels is concrete (~ 80 % aggregate and 20 % cement) with about 17 % steel, present both in the waste and as structural material (Kosakowski et al. 2014). Other materials present in smaller quantities include other metals (e.g. Al, Zn and Zircaloy) and organic waste components such as bitumen. These materials, together with the porewater from the host rock, determine the chemical conditions in the near field.

Chemical conditions in the repository, as well as their temporal changes, are driven by the interactions between hydrated cement, steel, concrete aggregates and clays. Considering the chemical nature of the major materials involved, two basic processes take place: an acid – base reaction (aggregate/clays – alkaline cement) and the corrosion of iron. The chemical reactions only proceed if a sufficient amount of water is present, either as a (stagnant or mobile) aqueous phase or as a humid atmosphere.

Timescales for some of these processes are illustrated in Fig. 3.1-1. Here, the following issues have been highlighted as being potentially safety-relevant:

- effects of construction
- effects of degradation of concrete and cement matrices
- degradation of organic materials
- metal corrosion
- colloid generation and migration

These issues are described in more detail, below.

3.4.1 Effects of construction and operational phase

During repository operation and for some time after closure, the geochemical processes in the repository will be dominated first by de-saturation of the rock in the vicinity of the tunnels. As discussed in Section 3.3.2, after repository closure, resaturation will be affected by gas production due to the degradation of organic materials and the anaerobic corrosion of steel (Sections 3.4.3 and 3.4.4). The period of gas generation might be very long and a complete resaturation of the near field might require more than hundred thousand years (Nagra 2008c). The oxidising conditions prevailing during the operational phase and immediately thereafter will change to reducing conditions once the oxygen in the entrapped atmosphere is consumed.

During repository construction and before closure, tunnels and vaults will be connected to the surface atmosphere, which will influence the pressure, humidity and oxidation state of the tunnels and vaults. These conditions will lead to the following processes occurring in the Opalinus Clay:

- evaporation of water, and
- oxidation, especially of chemically-reduced minerals such as pyrite (FeS_2)

Evaporation

Evaporation during the ventilation phase could promote effects such as an increase in salinity of the pore fluid close to the disposal containers, as well as in the EDZ. However, the porewater salinity may only be slightly increased (~ 2 %) as a result of evaporation during the operating phase (Gribi & Gautschi 2001), so any changes are expected to be transient. Additionally, the effect of an increase in ionic strength on the radionuclide retention properties of the cementitious barrier seems to be limited (Cloet et al. 2014).

Oxidation of pyrite

Opalinus Clay contains roughly 1 wt. % pyrite (Table 4 in Mazurek 2011). Other sources, such as Traber & Blaser (2013), give a range between 1 – 3 % pyrite in Opalinus Clay. The oxidation of this pyrite would lead to a decrease in pH of pore fluids in the host rock, the dissolution of solid carbonate minerals and the precipitation of sulphate minerals (e.g. gypsum, jarosite).

Estimates of the extent of oxidation in Opalinus Clay have previously been derived from various field studies (Nagra 2002b). Results indicate that gypsum formation in the EDZ is limited to open fracture surfaces. Calculations based on field studies of tunnels open from a few years (Mont Terri) to over 100 years (Hauenstein railway tunnel) permit bounds to be placed on the extent of oxidation. For SF/HLW emplacement rooms, only about 1 % of the pyrite originally present in the EDZ will be altered, thus long-term impacts will be insignificant (Mäder & Mazurek 1998, Nagra 2002c, Mäder 2002).

3.4.2 Effects of degradation of concrete and cement matrices on the repository system

Concrete consists of aggregates and cement paste. Cement paste is thermodynamically metastable and can therefore be altered by the porewater of the host rock. Initially, the alkali metal hydroxides (NaOH, KOH) are leached ("degradation phase I"). Experiments and modelling have shown that, after about 10 exchanges of the porewater, the pH is reduced from > 13 to 12.5, where it is stabilised because of buffering by dissolution of portlandite, $Ca(OH)_2$ ("degradation phase II"). During this second degradation phase, which may continue for more than 1'000 water exchange cycles, portlandite, is dissolved and secondary minerals, mainly calcium carbonate, are formed (Kosakowski et al. 2014). In terms of time, Phase I of cement degradation (pH > 13) may continue for thousands of years and phase II (pH ca. 12.5) is expected to continue for hundreds of thousands of years (Kosakowski & Berner 2013). The internal degradation of cement includes the interaction between aggregates and cement minerals. This reaction, also known as alkali silica reaction is fast and dependent on the dissolution of quartz (Kosakowski et al. 2014)

Sharp chemical gradients between the host rock and the cement/concrete mean that dissolved sodium, potassium, calcium and hydroxyl ions will diffuse out of the L/ILW near field, while bicarbonate ions in the rock porewater will diffuse towards the near field. Carbonates (e.g. vaterite, calcite) are expected to precipitate at the interface of the cement and rock. This self-sealing process will further slow transport of chemical species and cement degradation.

Diffusive solute exchange across the host rock/concrete interface may cause dissolution of significant amounts of portlandite in hundred thousand years (Kosakowski et al. 2014). The results of reactive transport calculations show that the portlandite might be dissolved up to a distance of two meters from the cavern walls (Kosakowski & Berner 2013). Portlandite dissolution is followed by temporal decrease in the Ca/Si ratio of C-S-H phases, which proceeds more rapidly near the interface, leading to lower Ca/Si values towards the interface. The mechanical strength after closure of the repository is due to the incompressibility of the aggregates, thus there is no long-term safety requirement for the mechanical strength of the concrete backfill as a whole (i.e. the cement minerals can degrade as long as the aggregates remain intact).

The impact of cementitious leachates from the concrete and cement matrices, i.e. the high-pH plume, on the Opalinus Clay and on the EGTS is considered in the following paragraphs.

Impact on Opalinus Clay

Diffusion of solutes is the dominant transport mechanism in Opalinus Clay and therefore governs the spatial extent of the high-pH plume. Observations from natural analogues (e.g. Tournemire; Tinseau et al. 2006, Techer et al. 2012), as well as reactive transport calculations (e.g. Kosakowski & Berner 2013) indicate porosity clogging on a centimeter scale for clay – cement interfaces in diffusion-controlled transport regimes. The extent of mineralogical changes which do not significantly change the porosity in the host rock is limited to a few centimeters to decimeters. The pH of the host rock porewater may increase to values between 8 and 9 over several meters within 100 ka. For Opalinus Clay, Kosakowski & Berner (2013) predict that major mineralogical changes are restricted to less than 0.4 m after 100 ka.

It is expected that locally the porosity close to clay/concrete interfaces will decrease significantly with time, which will decrease the water flow and diffusive mass fluxes across the interface (including radionuclide fluxes). Partial self-sealing of the gas transport paths along the interface between the emplacement caverns and the surrounding host rock and between the caverns and the cavern seals would influence the evolution of gas pressure in the repository near field. Reactions that could lead to sealing typically occur under fully water-saturated conditions, which is more likely to occur at the outer emplacement cavern interface with the host rock rather than along the inner interface between the emplacement caverns and seal. Spatial heterogeneity, such as mineralogy, porosity and fracturing may prevent the complete sealing of clay – cement interfaces, but since the Opalinus Clay is rather homogeneous, it is considered that such features will not cause significant deviations from the expected geochemical evolution of the system.

Despite potential mineral transformations due to the limited influence of the high-pH plume and changes in porewater chemistry, sorption properties of the Opalinus Clay are insignificantly affected (Wieland 2014).

Kosakowski et al. (2014) identified the following process and time couplings:

- Diffusive exchange between the cementitious near field and the host rock is expected to cause minor concrete degradation within the first 100 ka after closure.
- Diffusive exchange across concrete/clay interfaces might cause local pore clogging that could inhibit solute and mass transport across the interface within relatively short times (hundred(s) to thousands of years).

The waste – cement reactions and the degradation of metals will consume water and generate hydrogen gas that will delay saturation of the emplacement cavern (see Section 3.3.2). Depending on the host rock properties, and on the design of the engineered barrier system, the de-saturation regime may last between a few thousand years and more than 100 ka. This will slow down diffusive transport (of solutes and water) in the repository and delay associated concrete degradation.

Impact on the EGTS

Assuming resaturation starts mainly in the construction and operations tunnels and moves towards the emplacement caverns, water would first be conditioned by reaction with the sand / bentonite backfill and the gravel used as abutment material in the EGTS to then react with the mortar of the cavern backfill. Simulations demonstrate that SiO_2 containing materials (quartz sand or gravel) will cause changes at the interface to concrete materials. High-pH solution from the concrete will enhance dissolution of SiO_2 near the interface. The dissolved Si will diffuse towards the concrete and form C-S-H together with Ca from cement minerals (portlandite and

Ca-rich C-S-H). C-S-H precipitation is localised at the interface and might reduce the porosity. However, simulations reported in Kosakowski & Smith (2014) do not reveal any loss of the functionality of the EGTS as porosity changes are minor and far less than would be required for full clogging. Nevertheless, these detrimental processes could be effectively mitigated by using gravel with a low SiO_2 content (e.g. carbonate gravel).

3.4.3 Degradation of organic materials

As described in Nagra (2008c), some of the L/ILW contains substances that could reduce the chemical containment of radionuclides because they:

- form complexes with the latter and thus can increase their mobility (cyanide, cellulose degradation products etc.), or
- release CO_2 during their decomposition (e.g. organic materials such as bitumen), which will lead to the degradation of cement and to changes in the retention properties of the cementitious near field

Kosakowski et al. (2014) differentiate between low molecular weight (LMW) and high molecular weight (HMW) organic materials. These waste components can degrade via biotic, abiotic or radiolytic processes. Kosakowski et al. (2014) report that abiotic decomposition under alkaline conditions is observed in the case of cellulose, while the radiolytic decomposition of bitumen could generate LMW organic compounds. They conclude that, in general, hydrolysis or abiotic degradation of HMW organics is the first step for the subsequent microbial degradation of HMW organic compounds. Biotic degradation is expected to be slow under the hyperalkaline conditions of the cementitious near field.

The decomposition of L/ILW organic materials is expected to take place mainly during the early oxic and anoxic stages of the repository, and might be completed within a time span of less than 1'500 years. The timescale for the decomposition of the slowly degrading HMW organic materials under anoxic conditions is estimated to range from several thousand years to some tens to hundreds of thousands of years. The effects of complexation of radionuclides with organic species are addressed by the pessimistic choice of sorption and solubility coefficients.

The generation of CO_2 could have an impact on the mineral composition of the cement matrix and consequently on the retention properties of the cementitious near field as it is expected to locally transform portlandite into calcium carbonate and AFm[13] phases into monocarboaluminate. Carbonation of the cement matrix due to the decomposition of organic matter is expected to be a local process, and the temporal evolution is determined by microbial activity. According to Kosakowski et al. (2014) the effect of carbonation on the retention of metal cations is expected to be negligibly small since the main sorbing cement phase (C-S-H) will not be affected as long as portlandite is present in the cement matrix.

3.4.4 Corrosion of metals

Several waste types will consist of, or contain, metallic materials, in particular steel. Steel is used for waste packaging (e.g. steel drums etc.), in the reinforced disposal containers (e.g. reinforcement with bars, fibres etc.) and in the construction materials (e.g. anchors, bolts etc.), all of

[13] The general composition of an AFm phase can be written as: $C_3(A,F) \cdot CX_2 \cdot nH_2O$ where X represents an anion with a single negative charge (e.g. Cl^-, OH^-) or half an anion with double negative charge (e.g. SO_3^{2-}, CO_2^{2-}); n indicates that the amount of water is variable e.g. n = 12 for monosulphate (from Winter 2009).

which are susceptible to corrosion (oxic and anoxic) over time (Wersin et al. 2003). Consumption of the residual oxygen in the near field is expected to occur after repository closure due to the aerobic corrosion of metals, which generates no hydrogen gas, the degradation of easily degradable organic matter and oxidation of pyrite (Nagra 2002c). Thus, redox conditions are expected to be oxidising only during the early evolution of an L/ILW repository. Wersin et al. (2003) estimated that the oxic stage would last much less than 1'000 years, depending on the state of saturation of the near field.

After depletion of dissolved oxygen from pore fluids, the near field will remain anoxic. Redox conditions will be determined by various reactions between dissolved and solid redox-active species in the alkaline environment of the near field. The redox potential will largely be determined by the anaerobic corrosion of steel (Wersin et al. 2003). The latter process produces a thin film of magnetite on the steel surface and the redox-active species are considered to be magnetite and dissolved Fe(II).

The anaerobic corrosion of metals in the near field will produce hydrogen (see Section 3.3 on gas pressure build-up). For each mole of H_2 produced, one mole of H_2O is consumed. That is, H_2O in the form of water (liquid) or vapour (gas) is required to maintain the corrosion reaction. The consumption of water by the corrosion process may locally reduce the saturation and increase the capillary pressure gradient for water flow from the surrounding host rock to the backfill next to the containers. At the same time, the dissociation of water might lead to increased salinity in the near field, leading to increased steel corrosion rates. This effect is accounted for by the pessimistic evaluation of the steel corrosion rate.

Hydrogen can be an energy source for bioreduction of aqueous species such as SO_4^{2-}, Fe^{3+} etc. (Libert et al. 2011) and could thus be consumed by such processes. Utilisation of hydrogen will, in the long-term, decrease the gas pressure build-up as long as sulphate is amended to the hydrogen in an environment viable for microorganisms such as sand – bentonite backfilled tunnels and seals.

Microbial production of sulphide could enhance steel corrosion. On the other hand, H_2 oxidation would reduce H_2 concentrations in the porewater. These effects are accounted for by the pessimistic evaluation of the steel corrosion rate and H_2 gas generation rates.

Anaerobic corrosion of iron is accompanied by a volume increase (Pilling-Bedworth ratio for Fe_3O_4: 2.1). The volume increase could create stresses acting on the backfill and on the concrete container. The steel corrosion may lead to cracking of the concrete container which has no long-term safety functions. However, the effect of corroding steel mesh and rods in the tunnel liner will only have a limited effect on the compression of the cement backfill (due to the grain to grain contact). Some pore clogging may occur and this is addressed by simple mass balance considerations in Appendix A, and it is estimated that corrosion of the carbon steel may decrease the overall porosity by around 12 %. A complete clogging of the pore space in the cementitious environment does not – based on these mass balance considerations – seem very likely and enough pore space remains for the storage of gases. These volume changes are thus not deemed to have any safety-relevant impact.

The anaerobic corrosion rate of steel in a cementitious environment depends on the degree of water saturation. A large number of studies exist in the literature for corrosion in saturated cement or in cement porewater, and they tend to suggest that the long-term corrosion rate of steel under such conditions is around 20 nm/year (Diomidis 2014). On the other hand, only one study in unsaturated cement exists (Newman & Wang 2010 and 2013), and the preliminary results indicate a corrosion rate of 5 nm/a or less.

3.4.5 Colloid generation and migration

Wieland (2001) has shown that, for a porewater composition representative of an L/ILW cementitious near field, the concentration of colloids is very low (≤ 100 µg/L). In addition, it is expected that, during migration from the near field (high pH) to the lower, near-neutral pH in the undisturbed Opalinus Clay, such colloids would flocculate, since they are not stable in such an environment. Consequently, the influence of near-field colloids for long-term safety is negligible according to current knowledge.

3.4.6 Summary of potentially detrimental effects and couplings between chemical and other processes

The following potentially detrimental chemical effects identified in the preceding sections are summarised in Tab. 3.4-1, together with an assessment of their relevance, coupling to other temperature-related, rock-mechanical or gas-related processes and their treatment in, or omission from, the quantitative analyses in Chapter 4.

Tab. 3.4-1: Potentially detrimental chemical (C) effects, assessment of their relevance, coupling to other temperature-related (T), rock-mechanical (RM) or gas-related (G) processes and treatment in, or omission from, the quantitative analyses in Chapter 4.

Chemical effects	**Relevance/couplings**	**Treatment**
Degradation of organic materials and corrosion of steel, including elevated metal corrosion rates due to (i) pyrite oxidation and/or (ii) sulphide produced by microbial activity	Gas production affects gas pressure build-up, evolution of saturation ($C \rightarrow G$)	Accounted for in gas generation rates assumed in Section 4.4, discussed in Diomidis (2014)
	Volume increase creates stresses acting on the backfill and on the concrete container, which may lead to cracking of the concrete container; may also lead to compaction of the cement backfill thereby decreasing the porosity and limiting gas release from the waste and liquid flow towards the waste ($C \rightarrow G$)	Discussed in Section 3.4.4 and in Appendix A: no relevance
Water uptake by waste – cement reactions and the corrosion of metals	Affects evolution of saturation and thereby temperature evolution ($C \rightarrow T$, $C \rightarrow G$)	Discussed in Section 4.2: no relevance
Pore blocking due to (i) dissolution/precipitation zones of sulphates and carbonates caused by evaporation, (ii) pyrite oxidation and/or (iii) high-pH plume	Pore blocking leading to reduction in hydraulic conductivity, affecting gas pressure evolution, and saturation ($C \rightarrow G$)	Taken into account in Section 4.5; further discussions in Kosakowsi & Smith (2014) and Kosakowski & Berner (2013)
Sulphate attack of cementitious backfill due to (i) sulphate inflow resp. enrichment, (ii) pyrite oxidation	Interaction with sulphate might lead to the formation of ettringite in the cementitious backfill. Due to the large molar volume of ettringite, this may lead to stresses acting on the concrete container and backfill which could result in cracking of the concrete container and compaction of the cement backfill thereby decreasing the porosity and restricting gas release from the waste and liquid flow towards the waste ($C \rightarrow G$)	Cement can be designed to handle this issue. Not relevant
Complex formation with organic degradation products and/or development of locally oxidising conditions in the near field due to organic materials; release of CO_2 due to degradation of organic materials	May affect radionuclide retention and solubility	Handled by assigning geochemical parameters to radionuclide transport in safety assessment (Nagra 2014c)
Chemical plume of organic substances	May reduce radionuclide sorption in the host rock.	Handled by assigning geochemical parameters to material transport in safety assessment (Nagra 2014c)
Colloids	May impact radionuclide transport	Discussed in Section 3.4.5 and shown to be insignificant

4 Quantitative assessment of the repository-induced effects

4.1 Safety function indicator criteria for the assessment of processes

The purpose of this section is to formulate safety function indicator criteria for key parameters describing the site-specific evolution of the host rock in response to the processes considered. If the parameter values can be shown to meet these criteria, then potentially important detrimental effects related to the process can be excluded (see Section 1.2.2 for the methodology).

The hereby listed safety function criteria are based on the current understanding of the repository system and host rock behaviour and might be subjected to adjustments when site specific parameters are known or progress is made that allows for a better understanding of the system evolution. The scientific robustness of the safety function criteria listed below varies but continuous efforts are made to constrain uncertainties.

The scope of the safety function indicator criteria is limited to repository-induced effects on the host rock and engineered barriers (see Tab. 4.1-1). The criteria will vary to some extent according to the chosen site (which affects repository depth), as will the calculated values of the parameters. Safety function indicators relevant for the assessment of the repository safety and repository-induced effects were derived from Nagra (2008c), Appendix A.

Tab. 4.1-1: Safety function criteria for the assessment of processes.

Effects	**Relevant process**	**Potential safety function indicator criteria**	**Table**
Thermal	Thermal effect on the host rock	Maximum temperature	4.1-2
Mechanical	Thermally-induced increase of porewater pressure	Pressure maximum	4.1-3
	Formation of EDZ	Radial extent and hydraulic conductance of the EDZ	4.1-4
	Vertical propagation of faults related to the formation of EDZ	Extent of the vertical propagation of faults related to the formation of the EDZ	4.1-5
	Effect of the EDZ – convergence interaction	Advective water flow (convergence-induced water flow)	4.1-6
Gas	Gas pressure build-up	Gas pressure (threshold for pathway dilation and gas fracking)	4.1-7
	Gas-induced porewater displacement through host rock	Porewater displacement	4.1-8
Chemical	Degradation of cementitious backfill and liner (host rock)	Chemically disturbed zone: radial extent and hydraulic conductance	4.1-9
	Degradation of cementitious backfill (EGTS)	Chemically disturbed zone: longitudinal extent and hydraulic conductance	4.1-10

Safety function indicator criteria for the assessment of processes related to the thermal effects on the host rock

The criterion for host-rock temperature is that it should remain below the maximum paleotemperature experienced by the host rock (Tab. 4.1-2), i.e. the maximum temperature to which the rock has been subjected throughout its geological history. In the case of the Opalinus Clay from the drill core at Benken, the criterion is thus that the maximum temperature should be < 85° C, and is applicable to both the HLW and L/ILW repository (although it is most relevant to the former; Nagra 2002c). If the temperature meets this criterion, significant thermally-induced mineralogical alterations can be excluded.

Tab. 4.1-2: Criteria for the thermal effect on the host rock.

Issue	**Definition and description**	**Reference**
Relevance to safety functions	Precautionary criterion to avoid significant changes in the safety-relevant properties of the host rock	Nagra (2002c)
Safety function indicator	Temperature [° C]	
Safety function indicator criterion	Maximum rock temperature < paleotemperature maximum (80 – 90° C)	
Application of criterion	The criterion applies to the host rock at any location	
Justification	Heating of the host rock above its paleotemperature maximum engenders an inherent uncertainty regarding chemical and mineralogical evolution (Nagra 2002b)	

Safety function indicator criteria for the assessment of processes related to pore fluid pressure

The thermal output of the waste is too low to greatly increase porewater pressures in the rock, but the pressures will potentially be influenced by the presence of gas (Tab. 4.1-3). The criterion for fluid pore pressure (gas or liquid) should be set such that the possibility can be excluded that a rock fracture will be generated and will propagate to a feature that could form a preferential release pathway (fractures, sedimentary architectural elements, faults/fault zones, and combinations of these features). Such a criterion excludes any seismicity by the aforementioned repository-induced effects. Site- and repository-specific values of the respect distance to such features will be set to specify the acceptable range for fluid pore pressure more accurately.

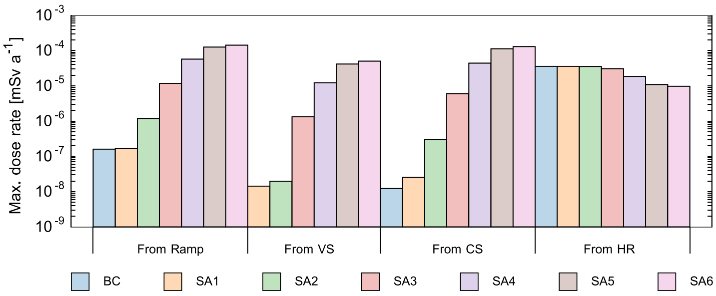
Tab. 4.1-3: Criteria for the gas and thermally-induced porewater pressures.

Issue	**Definition and description**	**Reference**
Relevance to safety functions	Reactivation of existing or creation of new water-conducting pathways would affect the safety functions: (i) retention of radionuclides in the near field and geosphere and (ii) attenuated release of radionuclides to the environment	See Section A1.32 in (Nagra 2008c)
Safety function indicator	Porewater pressure	
Safety function indicator criterion	$p < \sigma$ i.e. the porewater pressure p is below the lithostatic pressure σ	Criterion is dependent on depth
Application of criterion	The criterion applies to the host rock surrounding the backfilled and sealed emplacement caverns of the main and pilot repository	
Justification	Reactivation of existing or creation of new water-conducting pathways are avoided if the effective stress remains positive, i.e. if the porewater pressure or gas pressure is below the lithostatic pressure	

Safety function indicator criteria for the assessment of processes related to EDZ formation

The formation of EDZs could potentially lead to preferential transport pathways along the repository tunnel system and along the access tunnel and/or shafts to the surface. The resultant flows and the consequences in terms of doses have been, and are being, investigated and can be shown to be small, since the low hydraulic conductivity of the rock limits inflow to the tunnel system (even if the repository seals are less effective than expected and the EDZ conductivities are very high). Nevertheless, a criterion for the EDZ hydraulic conductance around the backfilled and sealed access routes should remain below 10^{-8} m^3/s for all times beyond 100 years (Tab. 4.1-4). No criterion is set for the EDZ conductance around the emplacement caverns (in axial direction) due to the fact that the hydraulic conductivity of the interior of the emplacement caverns is in any case high (hydraulic conductivity ~ 10^{-6} m/s) and is expected to exceed that of the EDZ.

Tab. 4.1-4: Criteria for the EDZ formation.

Issue	Definition and description	Reference
Relevance to safety functions	EDZ along the access routes, if sufficiently large and conductive, could provide a flow and transport pathway that would by-pass the transport barrier provided by the host rock and – where present – the confining units. As a result, the safety functions: (i) retention of radio-nuclides in the near field and geosphere, and (ii) attenuated release of radionuclides to the environment, would be affected.	See Section A1.29 in Nagra (2008c)
Safety function indicator	Hydraulic conductance, i.e. the product of EDZ cross-sectional area (A_{EDZ}) and effective hydraulic conductivity of the EDZ ($K_{EDZ,eff}$).	
Safety function indicator criteria	$K_{EDZ,eff} \times A_{EDZ} < 10^{-8}$ m^3/s $A_{EDZ} = (r_{EDZ}^2 - r_0^2)\pi$ where r_{EDZ} is the radial extent of the EDZ with its origin along the tunnel axis and r_0 is the tunnel radius.	
Application of criterion	EDZ along the access routes. No criterion specified for EDZ around the caverns.	
Justification	Calculations reported in Poller et al. (2014) indicate that, at hydraulic conductance values of around 10^{-8} m^3/s or above (cases SA4, SA5 and SA6 in the figure, below), and for an EDZ thickness of 1 m, the repository tunnel system and access structures with their attendant EDZs can provide more significant pathways contributing to peak dose rates (esp. via the construction and ventilation shafts, CS and VS in the figure below) compared to the host rock. Similar findings have been made for a HLW repository. It should be noted that the regulatory guideline of 0.1 mSv/a is not exceeded in the calculations reported in Poller et al. (2014) even for higher values of K, since the flows along the repository tunnel system and access structures remain limited by the low hydraulic conductivity of the host rock. 	

Safety function indicator criteria for the assessment of processes related to the vertical extent of the EDZ

The EDZ, if it were sufficiently large, could in principle approach the upper or lower boundaries of the effective containment zone (host rock and confining units), reducing the extent of the undisturbed geological barrier. Calculations indicate that the geological barrier remains sufficiently effective provided a hydraulic conductivity of 10^{-12} m/s or less is maintained over a distance of at least 20 m (Tab. 4.1-5). Thus, the extent of the EDZ should not be such that it increases the hydraulic conductivity above this value at distances less than 20 m from the upper or lower boundaries of the effective containment zone.

Tab. 4.1-5: Criteria for the effects for the vertical extent of the EDZ.

Issue	Definition and description	Reference
Relevance to safety functions	The EDZ will diminish the extent of undisturbed host rock and, if sufficiently large, could hence compromise the host rock safety functions	
Safety function indicator	T [m] – thickness of undisturbed host rock (with $K < 10^{-12}$ m/s)	
Safety function indicator criteria	T > 20 m	
Justification	The required minimum thickness of undisturbed Opalinus Clay is 20 m in order to comply with legal and regulatory guidelines for the dose maxima (Nagra 2008c)	

Safety function indicator criteria for the assessment of processes related to the convergence-induced porewater displacement through host rock

It is possible that tunnel convergence occurs after resaturation of the caverns, i.e. possibly after the start of radionuclide release, resulting in possible expulsion of porewater and dissolved radionuclides. In order to fulfil the safety functions related to the retention and attenuated release of radionuclides (Tab. 4.1-6), the convergence-induced specific porewater displacement rate in the host rock should not exceed 10^{-11} m/s.

Tab. 4.1-6: Convergence-induced porewater displacement through the host rock.

Issue	Definition and description	Reference
Relevance to safety functions	Excessive convergence-induced porewater displacement rates would affect the safety functions: (i) retention of radio-nuclides in the near field and geosphere, and (ii) attenuated release of radionuclides to the environment	See Nagra (2002c)
Safety function indicator	Convergence-induced specific porewater displacement rate	Specific flow rate = Darcy flow rate
Safety function indicator criterion	$q \leq 10^{-11}$ m/s i.e. the convergence-induced specific porewater displacement rate in the host rock, q, does not exceed 10^{-11} m/s	
Application of criterion	The criterion applies to the backfilled and sealed emplace-ment caverns of the main and pilot repository	
Justification	Figure A5.2-1 in Nagra (2008c) shows that the dose criterion of 0.1 mSv/a can be fulfilled for all waste types if $K \leq 10^{-10}$ m/s (assuming a hydraulic gradient of I = 0.1 m/m), i.e. for $q = K \times I \leq 10^{-11}$ m/s	

Safety function indicator criteria for the assessment of processes related to the gas pressure build-up

Repository-generated gas will enter the rock by diffusion and, as the gas pressure increases beyond the gas entry pressure, by advection (two-phase flow) through the existing pore space in the rock. If the gas pressure increases still further, a critical pressure may be reached at which pathway dilation occurs. This process is not thought to lead to permanent damage to the favourable properties of the rock, since the microscopic dilated pathways are expected to close again once the gas pressure declines. However, if the process can be excluded, then this simplifies the analysis of the system and excludes some uncertainties. Thus, a gas criterion for the exclusion of pathway dilation will be defined.

At still higher pressures (if reached at all), the formation of macroscopic gas fractures cannot be ruled out a priori. If this were to occur, irreversible changes to the favourable properties of the rock cannot be excluded. Thus, a gas pressure criterion for the exclusion of gas fractures is defined in Tab. 4.1-7.

Tab. 4.1-7: Gas pressure build-up and pathway dilation.

Issue	**Definition and description**	**Reference**
Relevance to safety functions	Reactivation of existing or creation of new water-conducting pathways would affect the safety functions: (i) retention of radionuclides in the near field and geosphere, and (ii) attenuated release of radionuclides to the environment	See Section A1.31 in Nagra (2008c)
Safety function indicator	Gas pressure P_g	
Safety function indicator criteria	$P_g < P_{dilation}$ ($< P_{gasfrac}$) i.e. the gas pressure P_g is below the threshold pressure for pathway dilation ($P_{dilation}$) and also below the threshold pressure for tensile fractures ($P_{gasfrac}$)	The threshold pressures, and hence the criteria, are dependent on repository depth
Application of criteria	The criteria apply to the host rock surrounding the backfilled and sealed emplacement caverns of the main and pilot repository	
Justification	The onset of pathway dilation is assumed to take place if gas pressure is above about 80 % of the lithostatic pressure (Table 3-3 in Nagra 2008c) at repository depth: HLW repository: $P_{dilation}$ = 13 MPa for a depth of ca. 650 m (p. 47 in Nagra 2004) ILW repository: $P_{dilation}$ = 6.5 MPa for a depth of ca. 325 m (Table 3-3 in Nagra 2008c)	

Safety function indicator criteria for the assessment of processes related to the gas-induced porewater displacement through host rock

Excessive gas production in a repository might lead to the displacement of porewater in the near field and far field, thus potentially affecting the retention properties of the Opalinus Clay. A criterion is set such that the potential displacement of the porewater does not imply any increase in the dose rate (Tab. 4.1-8).

Tab. 4.1-8: Gas-induced porewater displacement through host rock.

Issue	**Definition and description**	**Reference**
Relevance to safety functions	Excessive gas-induced porewater displacement rates would affect the safety functions: (i) retention of radionuclides in the near field and geosphere, and (ii) attenuated release of radionuclides to the environment	See Section A1.31 (Nagra 2008c)
Safety function indicator	Gas-induced specific porewater displacement rate	Specific flow rate = Darcy flow rate
Safety function indicator criterion	$q \leq 10^{-11}$ m/s i.e. the gas-induced specific porewater displacement rate in the host rock, q, does not exceed 10^{-11} m/s	See p. 125 (Nagra 2008c)
Application of criterion	The criterion applies to the backfilled and sealed emplacement caverns of the main and pilot repository	
Justification	Figure A5.2-1 in Nagra (2008c) shows that the dose criterion of 0.1 mSv/a can be fulfilled for all waste types if $K \leq 10^{-10}$ m/s (assuming a hydraulic gradient of $I = 0.1$ m/m), i.e. for $q = K \times I \leq 10^{-11}$ m/s	

Safety function indicator criteria for the assessment of processes related to the alkaline disturbed zone (ADZ) in host rock and EGTS

A potentially important safety-relevant issue in the context of chemical interactions involving the rock are the effects of a high-pH plume generated by cementitious materials (Tabs. 4.1-9 and 4.1-10). No specific criteria have yet been defined for parameters related to the high-pH plume. However, a number of detrimental effects associated with such a plume have been identified that could provide a basis for such ranges, namely:

- clogging of pore spaces (host rock, backfill/seals), which could be detrimental if it led to (a) a build-up of excessive gas pressures within and around the repository, and (b) a reduction or prevention of matrix diffusion along advective pathways through the rock (relevant only if such advective pathways exist and do not themselves become clogged)
- loss of swelling capacity of bentonite used as backfill or sealing material
- loss of self-sealing capacity (host rock, backfill/seals)

Tab. 4.1-9: Alkaline disturbed zone (ADZ) in host rock.

Issue	Definition and description	Reference
Relevance to safety functions	Degradation of cement and concrete backfill could potentially alter the host rock by dissolving aluminosilicate minerals and re-precipitating less dense, non-swelling silicates such as zeolites and C-S-H. These processes could cause changes in hydraulic conductivity and porosity (thereby affecting gas pressure), which could affect the safety functions of the host rock	
Safety function indicator	Extent of ADZ, ADZ_{rock}	
Safety function indicator criteria	$ADZ_{rock} \leq 2$ m (suggested value)	See Kosakowski et al. (2014) and Nagra (2014c)
Justification	A maximum extent (lateral and vertical) of the ADZ in the host rock should be defined over long timescales to preserve safety functions such as hydraulic conductivity and sorption properties	

Tab. 4.1-10: Alkaline disturbed zone (ADZ) in EGTS.

Issue	Definition and description	Reference
Relevance to safety functions	Degradation of cement and concrete backfill could potentially alter the bentonite in the EGTS by dissolving aluminosilicate minerals and re-precipitating less dense, non-swelling silicates such as zeolites and C-S-H. These processes could cause changes in hydraulic conductivity, porosity and gas permeability (thereby affecting gas pressure), which could affect the safety functions of the EGTS	
Safety function indicator	Extent of ADZ, ADZ_{EGTS}	
Safety function indicator criteria	$ADZ_{EGTS} \leq 0.5$ m (suggested value)	Kosakowski & Smith (2014)
Justification	A maximum extent (lateral and vertical) of the ADZ in the EGTS should be defined over long timescales to preserve EGTS safety functions such as hydraulic conductivity and porosity	Kosakowski & Smith (2014)

4.2 Effects related to temperature evolution

4.2.1 Overview

The temperature of the repository will evolve over time primarily due to the local geothermal gradient but also to the cement hardening and, to a lesser extent, the heat output from the disposed waste. In the near field, heat will be transferred from the waste packages and cementitious mortar by thermal conduction, and also, to some extent, by convection and radiation. The temperature of the surrounding media will first rise due to heat production, and then eventually fall as heat production diminishes. If it can be ensured that the peak temperature of the rock does not significantly exceed the maximum value attained during its burial history, which is around 80 to 90° C in the case of Opalinus Clay (Nagra 2002b), no irreversible structural changes are expected. Thus, the aim of the analyses from the perspective of the present chapter is to test whether temperatures of this order could be attained or exceeded. The methodology and analysis results are presented in Darcis et al. (2014) and summarised in the following sections.

The results show that the criterion given for the maximum temperature in the host rock (Tab. 4.1-2) is satisfied.

4.2.2 Methodology

Modelling approach and general assumptions

A numerical model has been developed using the code VPAC (Nagra 2008c). VPAC was developed for modelling radionuclide transport in saturated geological media. The governing equations for the thermal evolution of the repository are sufficiently similar to those for radionuclide transport that the code can be applied to both types of problems, with suitable redefinitions of parameters. The main heat transfer process explicitly included in the model is thermal conduction. Heat transfer by convection and radiation is included implicitly by means of effective thermal conductivity values that are adjusted for the effects of these processes. The governing equations are solved in a 3D finite-element grid, a cross section covering an emplacement cavern and the immediately surrounding host rock is illustrated in Fig. 4.2-1. The modelled volume extends to the upper and lower boundaries of the host rock. The confining units are not modelled explicitly since scoping calculations have shown that the heat from the repository does not reach as far as the host rock boundaries within the modelled time period. Only a single, generic emplacement cavern is modelled; in the lateral direction, symmetry boundary conditions are imposed to represent the effects of identical, parallel caverns, with an assumed separation of 85 m.

In the Reference Case, the host rock is represented as an isotropic, homogeneous, porous medium. Host rock heterogeneity, either naturally occurring or associated with the EDZ, is not represented. The partially saturated part of the host rock shown in Fig. 4.2-1 is, however, differentiated from the bulk of the host rock in a variant case (see matrix of calculation cases in Tab. 4.2-1). All other material types, represented by different colours in Fig. 4.2-1, are also represented as homogeneous and isotropic, e.g. the interiors of the disposal containers. Neither saturation state nor temperature is assumed to affect the heat-transfer parameter values. However, the main part of the emplacement cavern (termed "Wanne" *in German*) is distinguished in the model from the upper part of the cavern (termed "Kalotte" *in German*) to facilitate the modelling of the different phases of repository operation.

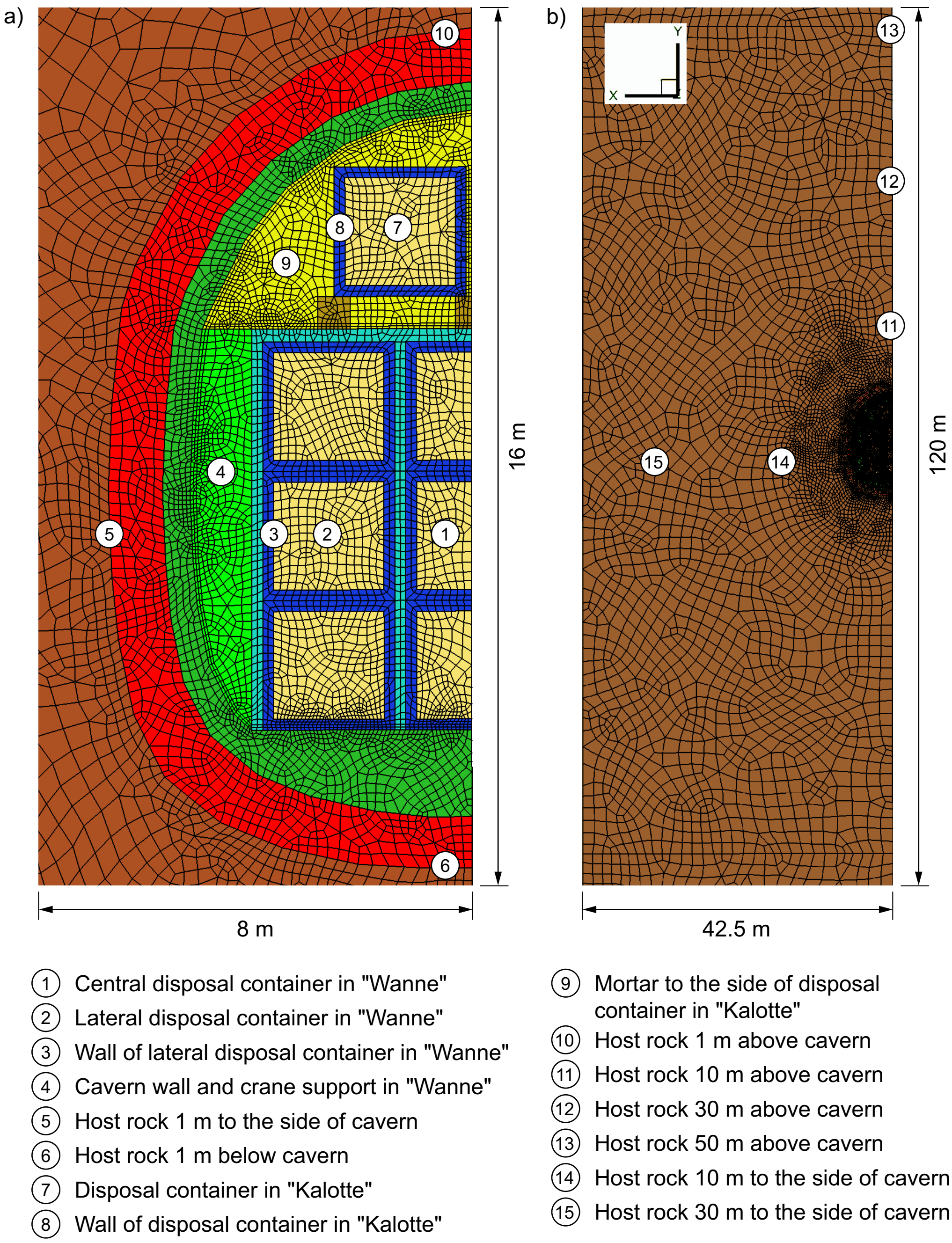


Fig. 4.2-1: Detail of the finite-element mesh covering an emplacement cavern and the adjacent host rock.

From Figure 6.1 of Darcis et al. (2014). Locations for which temperature time histories have been calculated are numbered. The partially saturated part of the host rock shown in the figure is differentiated from the bulk of the host rock only in a variant case (see matrix of calculation cases, Tab. 4.2-1).

The operation of the repository is simplified in such a way that the modelled period comprises three discrete phases, in each of which the amounts of waste and mortar are considered to be constant, as illustrated in Fig. 4.2-2:

- Phase 0 (3 years): during this phase, the excavated emplacement cavern remains empty, with no emplaced waste. The cavern is ventilated.
- Phase 1 (2 years in the Reference Case): during this phase, the main part of the cavern is filled with waste packages and cementitious mortar, whereas the upper part of the cavern remains empty and is ventilated.
- Phase 2 (100 years): during this phase, the upper part of the cavern is also filled with waste packages and mortar.

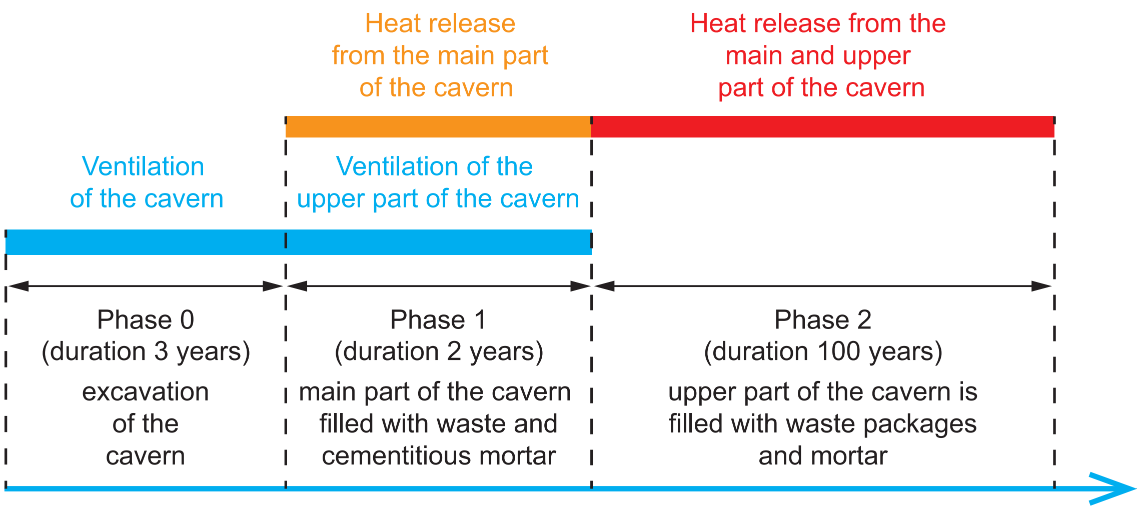


Fig. 4.2-2: Schematic illustration of the phases covered by the modelled period.

From Figure 4.5 of Darcis et al. (2014).

Geoscientific database

The main heat-transfer parameter values for Opalinus Clay (thermal conductivity and heat capacity) are taken from the study of SF/HLW disposal in the HLW repository (Leupin et al. 2016). In the Reference Case, the initial temperature profile across the model and the temperature boundary conditions are based on a geothermal gradient for Opalinus Clay of 43° C/km, with an ambient temperature of 36° C at the repository horizon, under the assumption of a 600 m repository depth. A variant case considers a geothermal gradient for Opalinus Clay of 44° C/km, with an ambient temperature of 50° C at the repository horizon, under the assumption of a 900 m repository depth. This depth is clearly an extreme value which lies outside the envisaged depth range for an L/ILW repository, but which is useful for analysing the sensitivity for thermal evolution of the model.

Heat generation

Heat production by the waste is based on a representative waste package with, in the Reference Case, an average time-dependent heat-production rate, based on the inventory for radioactive materials MIRAM 12 (Nagra 2013). In a variant case, the maximal heat production rate from the base scenario of MIRAM 12 is used. Heat production by hydration of the cementitious mortar is assumed to take place at a specified variable rate, based on VDZ (2008).

Matrix of calculation cases

In the Reference Case, the Opalinus Clay is assigned properties representative of typical, average values for the siting regions. A repository depth of 600 m is assumed. The waste properties (porosity, permeability) also represent typical, average values for the waste inventory.

The matrix of variant calculation cases that explore the impact of alternative assumptions and parameter values is summarised in Tab. 4.2-1.

Tab. 4.2-1: Matrix of calculation cases.

Calculation case	**Changed parameters with respect to the reference values**
V2	Partially saturated zone in the host rock
V3	Influence of ventilation
V4	Upper bounding value for in-situ temperature (50° C at the repository horizon, corresponding to 900 m depth)
V5	Maximal release rate of hydration heat
V6	Bounding values for heat-transfer parameters resulting in high temperatures in the near field
V7	Bounding values for heat-transfer parameters resulting in high temperatures in the host rock
V8	Maximal rate of heat release from the waste packages
V9	Rapid waste emplacement, Phase 1 = 0.5 a

4.2.3 Impacts for the Reference Case

The evolution of temperature at various points within and around an emplacement cavern is shown in Fig. 4.2-3 (see Fig. 4.2-1 for locations of numbered points). At the start of phase 1, a short temperature peak occurs within the mortar that reaches up to 72° C. At the start of phase 2, a second short temperature peak within the mortar occurs that reaches 76° C. These peak temperatures affect the rock immediately at the near-field/geosphere interface, but decline rapidly with distance into the host rock (see, e.g. the results for Point 5, at 1 m into the rock). Heat from cement hydration is primarily responsible for these peaks; the heat produced by the waste itself is far less significant (Darcis et al. 2014).

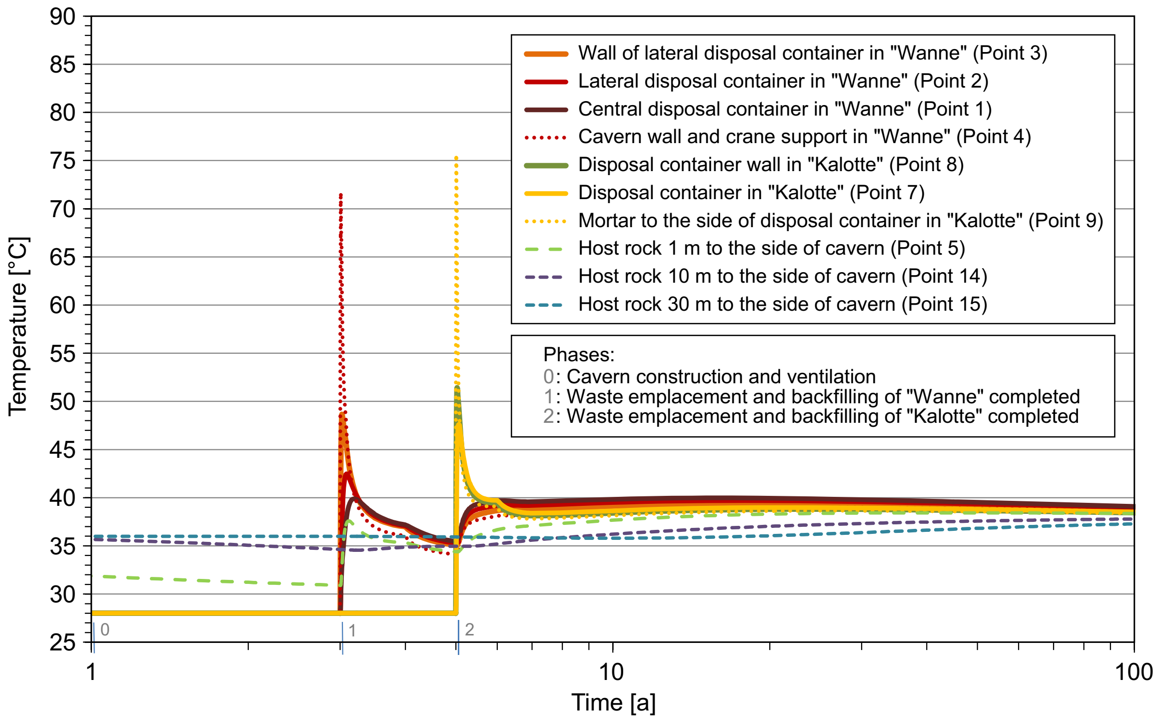


Fig. 4.2-3: Evolution of temperature in the waste packages, mortar and host rock at selected points within the repository system (see Fig. 4.2-1).

From Figure 6.4 of Darcis et al. (2014).

4.2.4 Impacts for variant cases

The peak temperatures reached at selected locations in the repository system in the Reference Case and in the variant cases are shown in Fig. 4.2-4.

In each case, the highest peak temperatures occur in the mortar (and at the near-field/geosphere interface). They are associated with the hydration of cement and are of short duration (a few months). The highest peak temperatures in the mortar are similar in all cases except V5 (maximal release rate of hydration heat), and are below 80° C, and hence below the maximum value attained during the burial history of Opalinus Clay (Nagra 2002a). In Case V5, the short-lived pulse at the start of Phase 2 reaches 88° C (the pulse at the start of Phase 1 reaches about 84° C). It is, however, noted that engineering measures to reduce these peaks can be taken if deemed necessary (see Chapter 5).

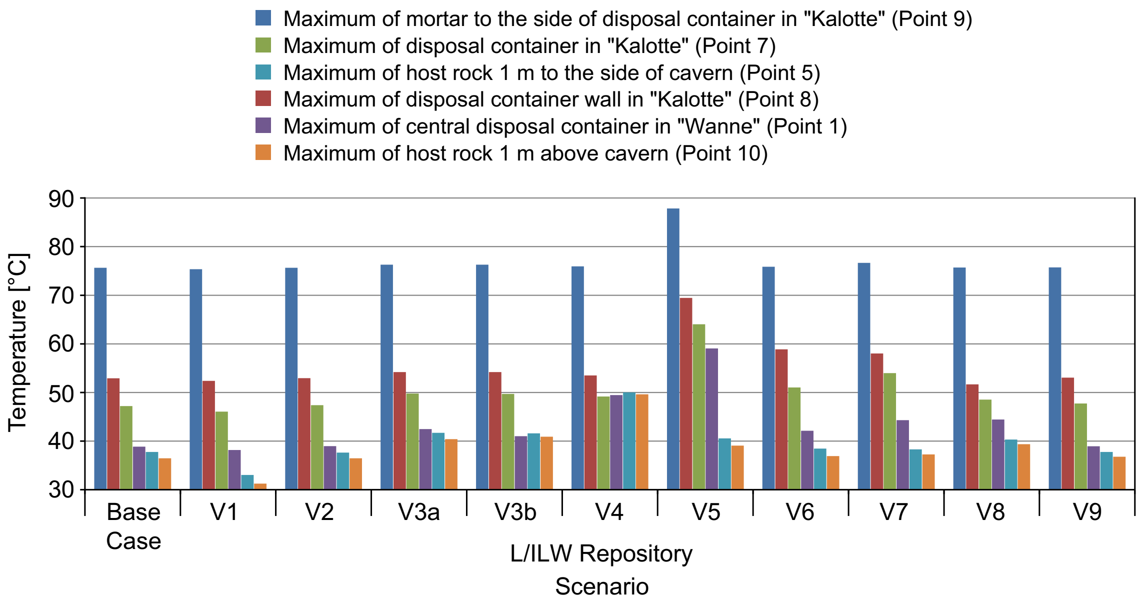


Fig. 4.2-4: Peak temperatures in the waste packages, mortar and host rock at selected points within the repository system (see Fig. 4.2-1) for all calculation cases.

From Figure 6.1 of Darcis et al. (2014).

In all cases, at a short distance into the rock (Point 5, 1 m into the rock), temperatures remain near or below 40° C, except in Case V4, where a higher ambient rock temperature is assumed, and, even in this case, the temperature remains close to 50° C.

Thus, the results show that the criterion given for maximum temperature in the host rock in Tab. 4.1.2 is clearly satisfied.

4.2.5 Concluding remarks on the significance of thermal effects

It is expected that the temperature increase in the host rock will be limited to around 5 to 10° C, because only low heat emitting waste is present. The ambient temperature may range from about 36 – 50° C depending on the location (depth of the host rock) of the finally selected site. A temperature rise in the host rock in the range of 5 to 10° C is expected to have a negligible effect on any chemical or physical processes.

4.3 Effects related to rock mechanics

4.3.1 Overview

Hydromechanical sensitivity analyses have been conducted to assess the extent and the shape of the EDZ around the underground structures of a L/ILW repository. The emphasis is on the following components of the repository system: (i) an L/ILW emplacement tunnel, (ii) a horizontal repository seal section, and (iii) a vertical shaft seal section.

Geomechanical simulations (Geomechanica 2013) provided discrete fracture networks representing the EDZ around the disposal structures for a wide range of possible repository configurations in the Opalinus Clay. The discrete fracture networks derived from the geomechanical simulations have been used to evaluate the hydraulic significance of the EDZ (Alcolea et al.

2014). For this, a sequential modelling procedure has been developed, aimed at converting the discrete fracture networks into hydraulic continuum models with heterogeneous porosity and hydraulic conductivity distributions. The complex shape of the EDZ has then been abstracted to provide a simplified representation that is amenable to handling with, for example, radionuclide transport modelling tools.

The results of the simulations can be summarised as follows:

- In no case did the vertical extent of the EDZ around the L/ILW emplacement caverns exceed a thickness of one cavern or sealing-section diameter (the diameter of the K09 cavern is around 10 m). Thus, the required minimum thickness of the intact host rock (see Tab. 4.1-5) was not undercut for any of the assessed repository configurations.
- In no case did the hydraulic conductance of the EDZ around shafts and seals exceed a value of 1×10^{-8} m^3/s (see Tab. 4.1-4).

Thus, the safety function indicator criteria given in Tabs. 4.1-4 and 4.1-5 are clearly satisfied.

4.3.2 Methodology

Conceptual framework for the creation and closure of the EDZ fracture network in Opalinus Clay

Drawing on empirical and experimental evidence regarding the hydraulic significance of the EDZ during tunnel construction, its evolution during operational times and after backfilling of tunnels (Lanyon et al. 2014), and the conceptual framework for a quantitative EDZ evolution model can be formulated as follows (see Fig. 4.3-1):

- The creation of the EDZ is a brittle process, i.e. the increase of the void volume of the plastified rock zone around the excavation is solely attributed to fracture opening, whereas the porosity of non-fractured rock domains remains essentially unchanged during early times.
- Initially, the newly created EDZ fractures are unsaturated and exposed to atmospheric pressure, whereas the non-fractured rock domains remain saturated and exhibit high matrix suction as a consequence of the high gas entry pressure of the Opalinus Clay. The initial transmissivity of the unsaturated EDZ fractures is controlled by the fracture aperture and can be very high. The matrix hydraulic conductivity remains essentially unchanged, i.e. it is the same as the conductivity of the intact rock.
- The matric suction in the rock matrix diminishes with time, due to the uptake of porewater[14] from outer rock zones and the fractures start to resaturate.
- Porewater uptake in the non-fractured rock zones in response to the reduction of effective stress (drained response) is associated with swelling and consequently with an increase of matrix porosity. This porosity increase of the rock matrix happens at the expense of fracture aperture, i.e. the fractures start to close and fracture transmissivity reduces drastically, whereas the hydraulic conductivity of the non-fractured matrix zones increases slightly as a consequence of the porosity increase.

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[14] Note, in low permeability rocks such as Opalinus Clay, vapour diffusion in the air-filled EDZ fracture network is the dominant transport process. Assuming a relative humidity < 1 in the ventilated tunnel sections, a radial gradient in relative humidity is the driving force for vapour flux.

- This process of matrix porosity and hydraulic conductivity increase associated with the decrease of fracture aperture and transmissivity progresses until a state of effective stress equilibrium is reached. This is essentially the case when pore pressure reaches the static formation pressure.

In the subsequent paragraphs, a heuristic EDZ model is described that simulates the afore-mentioned phenomenological features in a simplified manner. In a first step, the size and extent of the EDZ in response to the excavation process is simulated with an uncoupled fracture mechanics code. In a second step, a simplified hydromechanical modelling approach is used to model the evolution of the hydrological properties of the EDZ over a period starting with the early post-excavation phase and ending with static formation pressure recovery.

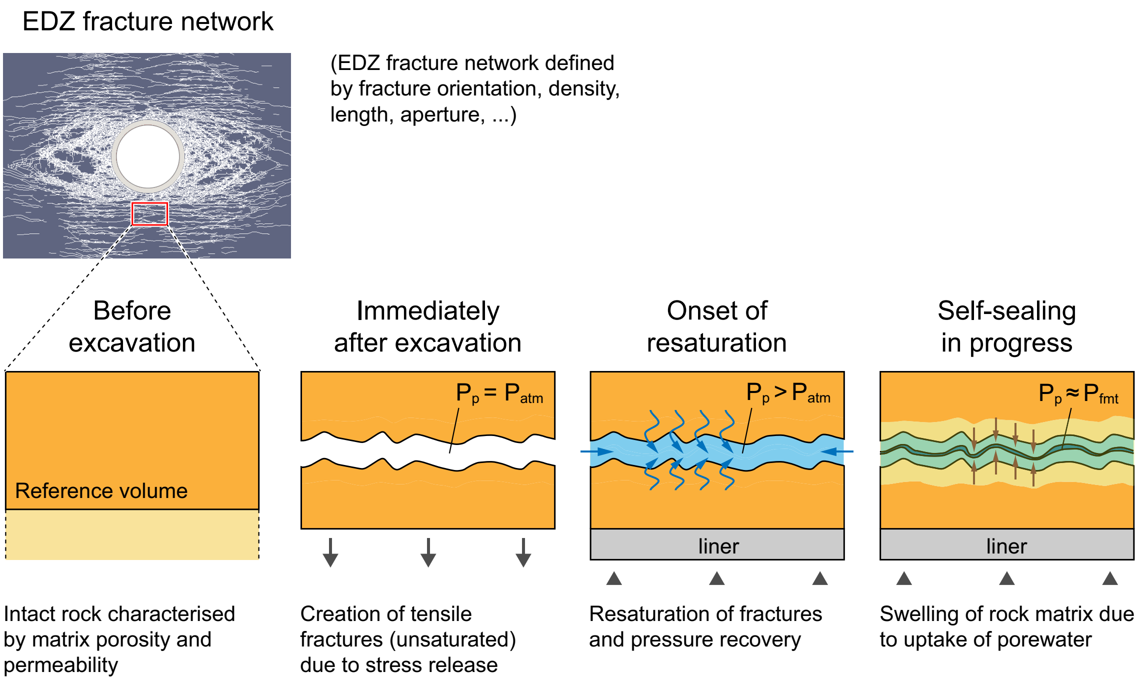

Fig. 4.3-1: A conceptual framework for EDZ fracture closure in Opalinus Clay, covering the key phenomena and features from the early post-excavation phase until static formation pressure recovery.

After Figure 2-17 of Alcolea et al. 2014. P_p: pore pressure, P_{atm}: atmospheric pressure, P_{fmt}: formation pressure.

Modelling approach

A fracture mechanics code (Geomechanica 2013) was used to simulate the brittle behaviour of the host rock around the repository structures in response to the excavation process. The modelling study provided discrete fracture networks representing the EDZ around the cavities for a wide range of possible repository settings representing the geological conditions in the candidate siting regions in Northern Switzerland. The simulations were based on the robust assumption of a maximum acceptable convergence of the structures which is limited to a value < 4 % (note: according to the engineering design requirements, the maximum convergence shall not exceed 2.5 %; see Lanyon et al. 2014).

Fig. 4.3-2 shows the simulated fracture patterns around a K09 cavern at a repository depth of 800 m under different in-situ stress conditions. The plastified zone is shown in terms of tensile (blue) and shear failure (orange), respectively. Tensile fractures, representing the most permeable hydraulic features, are located only in the immediate vicinity of the tunnel surface.

The simulations of the EDZ around the L/ILW emplacement cavern K09 were conducted for vertical stresses corresponding to burial depths between 450 and 800 m bgl. The EDZ fracture patterns of the cavern models were governed by the geomechanical properties of the Opalinus Clay but also by the stress ratio K_o. The simulations with low rock strength exhibit unrealistically high fracture densities. The extension of the EDZ ranged between 1 and 2 tunnel diameters for the different sensitivity runs, indicating that the required minimum thickness of the intact host rock (see Tab. 4.1-5) was not undercut in any of the simulation cases. Notably, in all cases a high density of tensile features was observed in a 1 – 2 m thick zone around the tunnel wall.

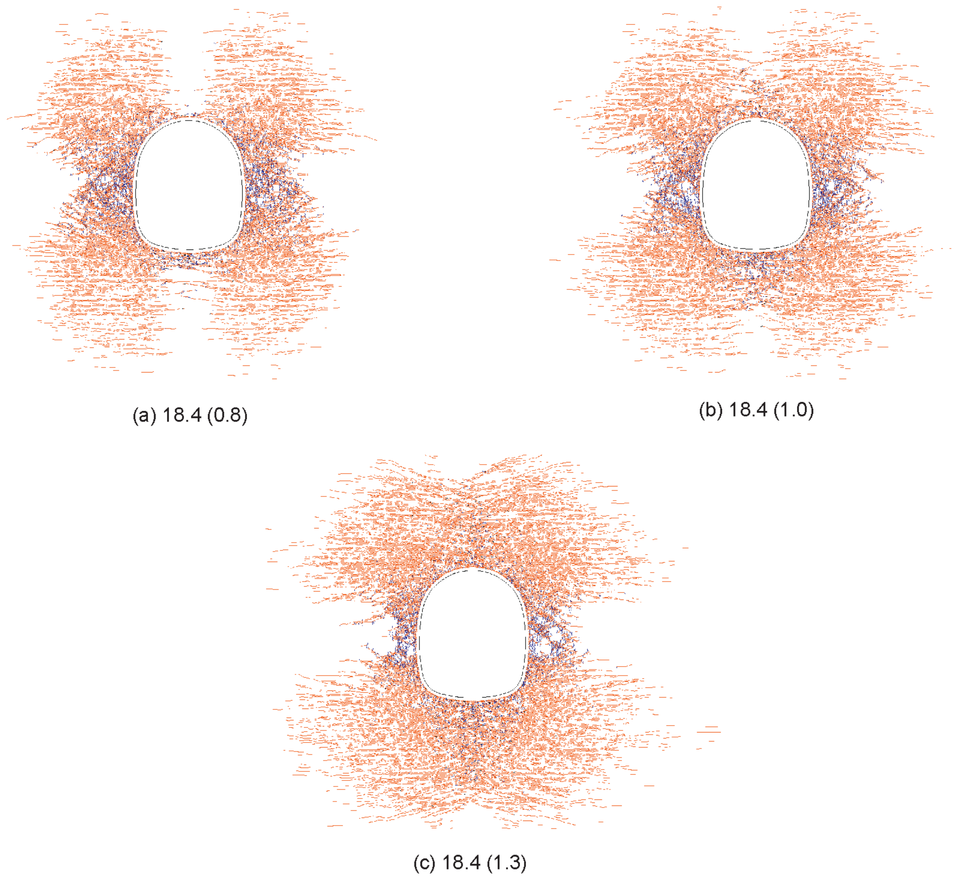

Fig. 4.3-2: Typical fracture patterns around a K09 cavern under different in-situ stress conditions (S_v = 18.4 MPa, stress ratio K_o = 0.8, 1.0, 1.3).

Tensile and shear failure are indicated in blue and orange, respectively (from Geomechanica 2013).

Evolution of the hydraulic conductance of the EDZ along horizontal / vertical seal sections

The EDZ discrete fracture networks consist of thousands of fractures, each characterised by its orientation, length and aperture. To study the hydraulic significance of the EDZ around the sealing sections (note that the criterion of the hydraulic conductance of the EDZ given in Tab. 4.1-4 does not apply to the caverns), Alcolea et al. (2014) derived hydraulic EDZ abstractions for cylindrical tunnel cross sections by carrying out the following steps, also illustrated in Fig. 4.3-3:

- a box counting approach was applied to convert the fracture networks into cell-based porosity distributions
- an empirical porosity-permeability relationship (Kozeny-Carman) was applied to convert cell porosities in hydraulic conductivities
- cell-based porosity and hydraulic conductivity distributions were used to define a simplified representation of the EDZ consisting of a homogeneous annular region around the tunnel with elevated porosity and hydraulic conductivity compared with the undisturbed host rock

Resaturation of the EDZ causes two hydromechanical effects (see also Fig. 4.3-1), essentially controlling the evolution of its hydraulic conductance:

- Pressure increase in the fractures from atmospheric to nearly hydrostatic pressure conditions causes a reduction in the effective normal stress. This reduction leads to mechanical fracture closure. Fracture closure leads to a reduction in fracture porosity and hydraulic conductivity.
- The high percentage of clay materials makes the rock matrix swell at low pressures (< 2 MPa), causing both matrix porosity and conductivity to increase with time.

Early stages of the resaturation process are controlled by the high transmissivity of the EDZ fracture network. Resaturation is initially very fast, but slows considerably at mid and late times, when a certain degree of resaturation has already taken place.

The resaturation process and the response of the EDZ to resaturation is simulated using the finite element mesh presented in Fig. 4.3-3. Boundary conditions are zero drawdown at the outer model boundaries. Initial conditions are the hydrostatic pressure (which varies with the assumed repository depth) at elements not intersected by fractures. At elements intersected by fractures and within the buffer zone, atmospheric pressure conditions are imposed.

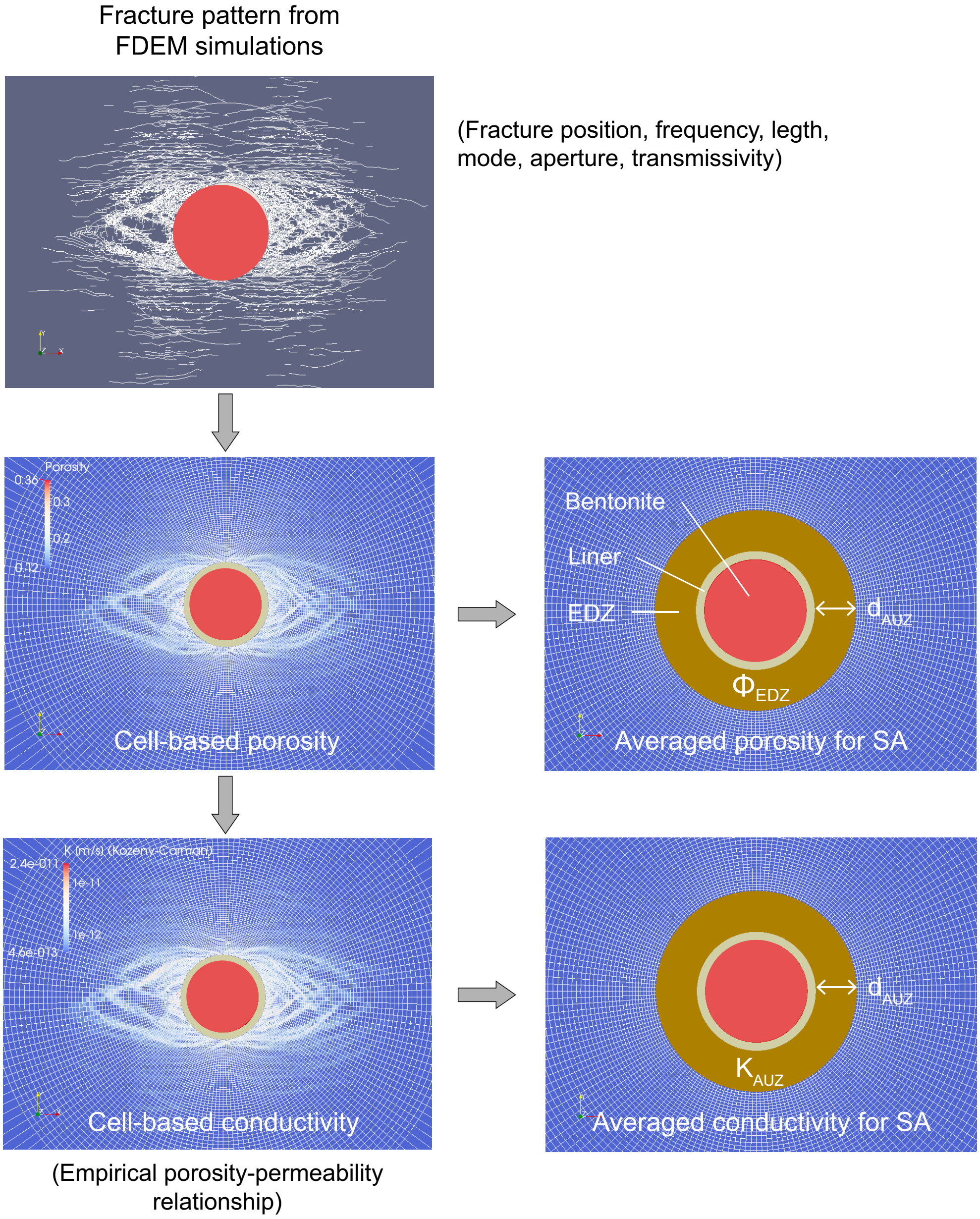

Fig. 4.3-3: Basic features of the EDZ abstraction process for a circular tunnel: representative fracture patterns are simulated for relevant repository configurations with a discrete fracture network model.

The resulting fracture patterns are converted into heterogeneous porosity and conductivity distributions. In a final abstraction step, the heterogeneous porosity / permeability distributions are converted to an annular shell of uniform porosity / conductivity defined by a radius $r_{EDZ} = r_{tunnel} + d_{EDZ}$.

4.3.3 Impacts for the Reference Case

The heterogeneous distribution of hydraulic properties in the EDZ at any given time can now be spatially integrated and averaged. For example, the average total specific flux[15]along the EDZ around the seal at early times is in the order of 0.1 m/s and drops dramatically to values smaller than 10^{-12} m/s at late times, when all fractures are closed (Alcolea et al. 2014). Note that the equivalent hydraulic conductivity multiplied by the area of the EDZ is equal to the hydraulic conductance, for which a criterion is given in Tab. 4.1-4 that it should be below 10^{-8} m^3/s. As observed, the hydraulic conductance of the EDZ drops approximately 11 orders of magnitude due to mechanical closure of fractures and swelling of the clayey materials of the matrix, easily satisfying the criterion.

The late time value of equivalent hydraulic conductivity is in good agreement with experimental values obtained at Mont Terri (Lanyon et al 2014).

4.3.4 Impacts for variant cases

A total of 9 variant cases for the shaft seal section was analysed, comprising sensitivity analyses of the in-situ stress conditions, the impact of rock strength and the effect of the tunnel support. The compilation of all radial profiles of effective porosity and hydraulic conductivity at late times (i.e. after recovery of static formation pressure) reveals a low variability despite the significant differences in the assumed geological conditions (Fig. 4.3-4). Close to the tunnel/shaft wall, the porosities range between 0.13 and 0.16. The corresponding hydraulic conductivities are increased by less than one order of magnitude with respect to the intact rock matrix. At a distance of 2 tunnel radii (at 12 m), the rock properties are indistinguishable from the intact rock matrix.

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[15] In Alcolea et al. (2014) the average value of total flux $< Q_{edz} >$ of the EDZ is calculated by integration of total specific flux $q_{EDZ}(r)$:

$$< Q_{edz} >= \int_{r_o}^{\infty} (< q_{EDZ}(r) > - q_{matrix}) \cdot r \cdot dr$$

were r_o represents the radius of the unlined tunnel. Eventually, the average total flux $< Q_{edz} >$ is used to define homogenised properties of the abstracted EDZ in terms of a relationship between the equivalent hydraulic conductivity $K_{EDZ,equiv}$ and the associated equivalent EDZ radius r_{equiv}:

$$K_{EDZ,equiv} = K_{matrix} + \frac{< Q_{edz} >}{(r_{equiv}^2 - r_0^2) \cdot \pi}$$

The homogenised EDZ properties are reported in Fig. 4.3-3 for the shaft and seal sections.

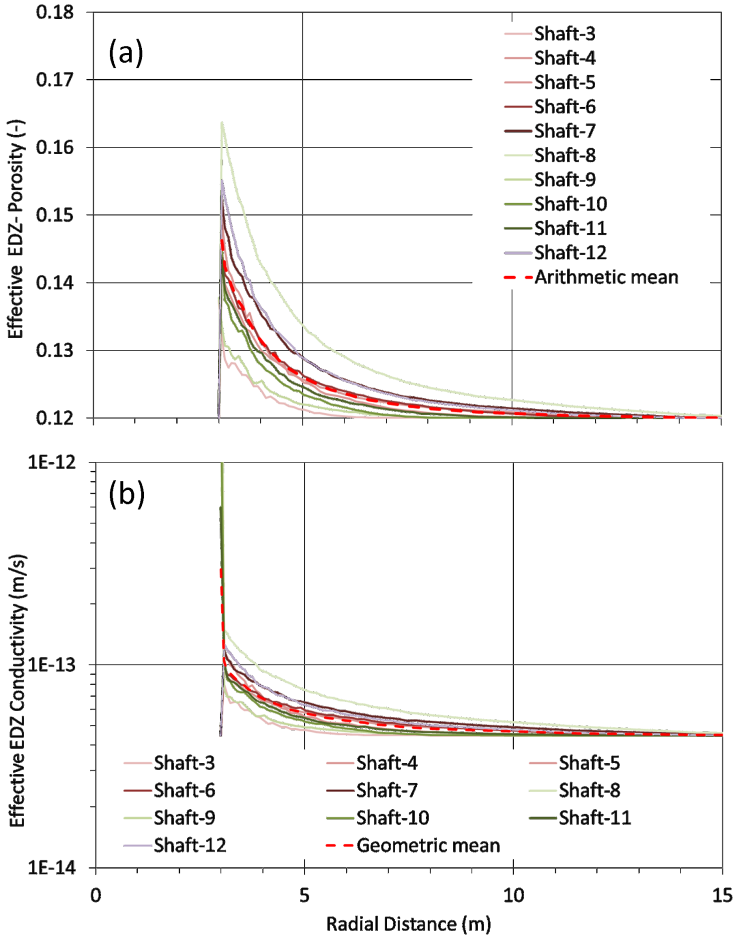

Fig. 4.3-4: Radial profiles of effective porosity $\phi_{EDZ,Shaft-i}$ (r) and effective hydraulic conductivity $K_{EDZ,Shaft-I}$ (r) of 9 variants of the seal section model after recovery of static formation pressure (late times).

Average profiles of < ϕ_{EDZ} (r) > (arithmetic mean) and of < K_{EDZ} (r) > (geometric mean) were derived from the effective porosity and conductivity profiles. The moderate spread of the individual profiles around the average profiles suggests that the average profiles can be regarded as representative ensemble means. The averaged profiles were used for calculating the average void volume < V_{EDZ} > and total axial flux < Q_{EDZ} > along the seal section / shaft. In a final step, the homogenised EDZ properties were derived. Fig. 4.3-5 shows the corresponding relationship between the equivalent EDZ radius r_{equiv} and the equivalent porosity $\phi_{EDZ,equiv}$ and between the equivalent radius and the equivalent hydraulic conductivity $K_{EDZ,equiv}$. The equivalent hydraulic conductance of the EDZ is about 5×10^{-12} m^3/s, indicating that the safety criteria in Tab. 4.1-4 are undercut by several orders of magnitude.

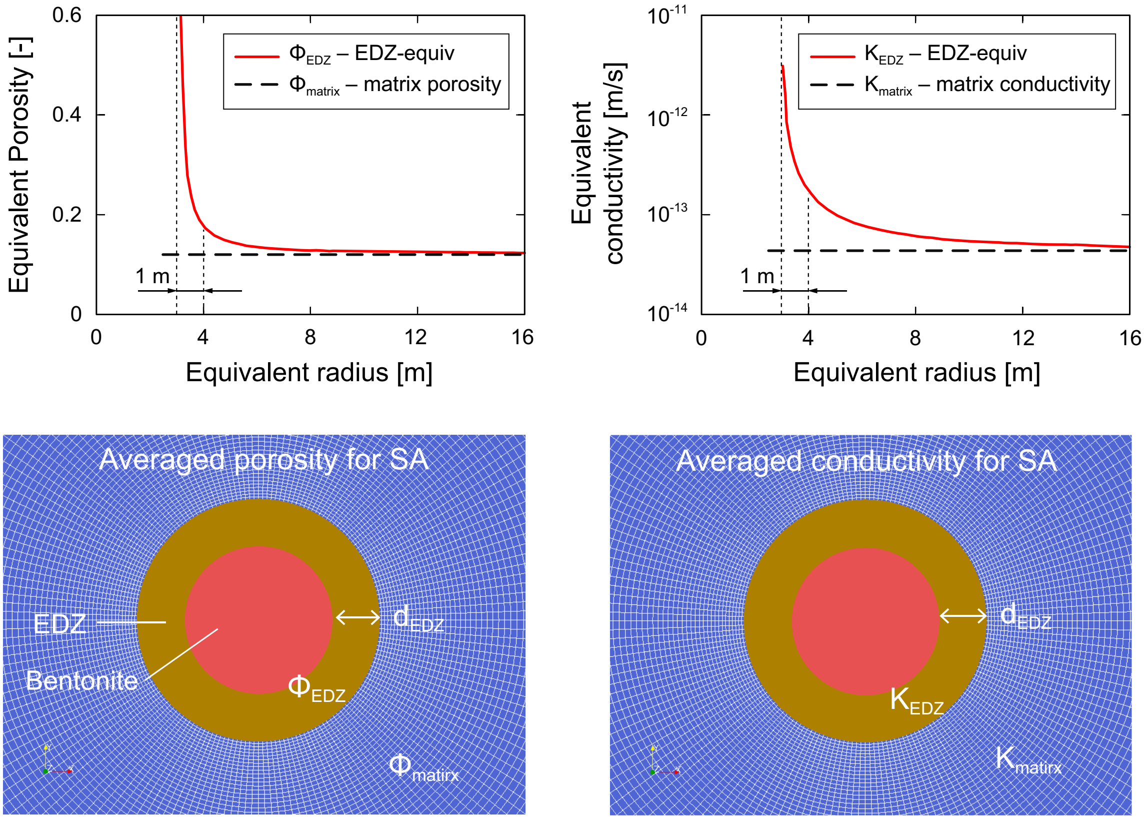

Fig. 4.3-5: Relationship between equivalent EDZ radius and homogenised porosity (upper left) and hydraulic conductivity (upper right), representative for the shaft configuration.

The corresponding hydraulic conductance of the EDZ is in the range of 5×10^{-12} m^3/s.

The extension of the EDZ around the seal sections ranged between 1 and 2 tunnel diameters for the different sensitivity runs, indicating that the required minimum thickness of the intact host rock (see Tab. 4.1-5) was not undercut in any of the simulation cases.

4.3.5 Concluding remarks on the hydraulic significance of the EDZ

Evaluations of the extent and hydraulic properties of the EDZ around the seal sections and shafts were conducted for a wide range of repository settings, covering sensitivity analyses with regard to repository depth, stress state, rock strength, tunnel shape and design of the lining. The overall assessment of the simulations indicates a marked change in hydraulic conductance of the EDZ after repository closure, which is controlled by the evolution of pore pressure in the vicinity of the backfilled underground structures. During the early times, between the first hundreds of years, the EDZ conductance is dominated by the high transmissivity of the fractures. As the pore pressure recovers, the EDZ fractures close progressively and the non-fractured rock matrix swells by water uptake, leading to an increase of porosity and decrease of hydraulic conductivity.

At late times, the hydraulic conductance of the EDZ decreases by many orders of magnitude compared with its early-time values. When comparing the different simulation cases, the variability of specific flux is very modest with a spread of less than an order of magnitude. Furthermore, the radial extent of the EDZ at late times is very similar for all cases.

The key conclusions can be summarised as follows:

- At late times (i.e. after recovery of static formation pressure) the EDZ around the backfilled underground structures of a deep geological repository in the Opalinus Clay is restricted to a radial zone with a thickness of less than 2 tunnel diameters (note that this criterion is even met at early times). Hence, the safety function criteria in Tab. 4.1-6 (vertical extent of EDZ) are met at all times.
- Significant enhancement of hydraulic conductivity is observed only in a zone with a thickness of less than half of a tunnel diameter. As late times (corresponding to the resaturation time of the repository), the corresponding enhancement of effective hydraulic conductivity in this zone is less than 1 order of magnitude with respect to the intact rock matrix. The effective hydraulic conductance is approximately 10^{-12} m^3/s Tm[16] and thus several orders of magnitude lower than the corresponding safety function criteria (Tab. 4.1-4).
- The increase of the EDZ porosity is less than 50 % of the porosity of the intact rock matrix. An average value of around 0.2 m^3/Tm for the normalised void volume has been calculated, meaning that the corresponding safety function criteria (Tab. 4.1-4) can be met. For the great repository depth and for low rock strength (e.g. strong tectonic overprint of the rocks), significant efforts may be needed with regard to the design of the tunnel support to ensure that the corresponding safety criteria are satisfied.

4.4 Effects related to gas pressure build-up and transport

4.4.1 Overview

Anaerobic corrosion and degradation of waste materials in the emplacement caverns of a L/ILW repository is associated with the formation and accumulation of a free gas phase and the build-up of gas pressures in the backfilled repository structures.

The EGTS is designed to provide the principal exit route for gas from the caverns, limiting gas pressure build-up. Furthermore, as described in Section 3.3, the EDZ around the sealing sections can play a significant role in the release of gas from the caverns. Gas and liquid pressure increase will occur over time, causing a decrease in the effective stress in the host rock and EDZ. This can lead to localised deformation and to changes in pore volume by the re-opening of pre-existing, tight fractures or by the creation of new pathways (pathway dilation) for the generated gas through the EDZ or the previously unperturbed host rock. Pore blocking which may affect the gas flow due to chemical – mineralogical reactions leading to precipitates are considered in the sections on chemical effects (Sections 3.4 and 4.5).

An important feature of the deformation behaviour of argillaceous materials is their self-sealing capacity (e.g. Nagra 2002b). Permeability enhancement due to pathway dilation at elevated gas pressures tends not to be permanent; when the gas pressure is reduced, the material reconsolidates and the hydraulic and mechanical properties of the porous medium approach the values which are characteristic for the undisturbed stress state. Nevertheless, if pathway dilation can be excluded, this simplifies the analysis of the system and excludes some uncertainties.

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[16] [Tm] stands for tunnel meter.

Pathway dilation may occur once gas pressure reaches about 80 % of the lithostatic formation pressure at the repository level[17]. If gas pressure rises further, such that lithostatic pressure is exceeded, then gas fracturing may occur (lithostatic pressure is used in the oil and gas industry as an indicator for the fracture pressure) on the decameter scale, which could be more detrimental to the performance of the host rock barrier.

To examine whether such situations could occur in practice, numerical modelling studies have been conducted that examine the evolution of gas pressure in an L/ILW repository. After closure of the repository, the evolution of gas pressure will be affected by numerous factors related to geology (hydrogeological and hydromechanical conditions, formation depth, hydraulic properties, confining formations) as well as aspects of the repository design (pathways through the EGTS, gas generation rates, properties of backfill materials, seals and EDZ). Thus, a range of calculation cases has been evaluated to explore the sensitivities to relevant parameter values. The modelling studies are reported in detail in Papafotiou & Senger (2014) and summarised in the following sections of the present report.

Measures can be taken if needed to reduce the gas production rate (e.g. melting of the metallic waste). In addition, the gas-forming materials can be significantly reduced in the L/ILW caverns (e.g. pyrolysis of organics). Chapter 5 also describes options to increase the gas storage volume and increase the gas transport capacity of the backfilled underground structures.

4.4.2 Methodology

Modelling approach and general assumptions

A 3D model of a generic L/ILW repository system (Fig. 4.4-1) has been used to simulate gas release through the host rock and along the backfilled underground structures. The potential effects of pore blocking due to chemical – mineralogical precipitation reactions on gas transfer properties of the EGTS and host rock are discussed in the chapter on chemical effects and are not considered in the gas simulations. In most model calculations, it has been assumed that waste-generated gas has the properties of hydrogen in terms of viscosity, density and solubility. The model was implemented using the TOUGH2 equation-of-state module EOS5 for water and hydrogen (Pruess et al. 1999). Dissolution of gas in the porewater is taken into account. Diffusive transport of dissolved gas is, however, neglected, providing a conservative approach with respect to gas pressure build-up. Some additional simulations were also carried out for water and air as a conservative approach with respect to gas properties, since the solubility of air in water is smaller than that of hydrogen in water, and the viscosity of air is greater than the viscosity of hydrogen.

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[17] Benson et al. (2002) reviewed the safety results of underground storage in the United States as part of a comprehensive study considering CO_2 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/cm^3), where the lithostatic pressure gradient represents a lower limit for the initiation of macroscopic fractures. 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 rock mass is assumed to behave as an elastic medium. The propagation of the gas phase through the porous medium is controlled by the gas entry pressure, 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. Once the gas entry pressure has been exceeded, the gas mobility is controlled mostly by the intrinsic permeability of the formation, the permeability – saturation relationship (commonly known as relative permeability), and the relationship between the capillary pressure and the water saturation (also known as 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, such as that by van Genuchten (1980). In calculations where the process of pathway dilation is considered, this is implemented by an approach that involves the use of a pressure-dependent permeability function (Senger et al. 2008). As noted above, the onset of pathway dilation is assumed to occur once gas pressure reaches 80 % of the lithostatic formation pressure at the repository level.

The detailed geometry of the disposal container with the different backfill materials of the L/ILW emplacement cavern is shown in Fig. 2.1-4. Due to computational constraints the emplacement caverns were represented by a single backfill material having uniform properties in terms of average porosity and permeability. All other underground structures in the host rock formation were assumed to be backfilled with sand/bentonite mixtures or with crushed Opalinus Clay. The 3D model geometry (Fig. 4.4-1) is discretised using a rectangular nested grid (Integrated Finite Differences IFD) with refinement in and around the underground structures and coarsening away from the repository. The cross sections of all repository elements are rectangular and do not precisely represent the actual cross sections of the repository (see Fig. 2.1-2). Discrepancies in cross-sectional areas and volumes are compensated through scaling of the hydraulic properties assigned to the repository elements in the model. The details of the model implementation and assumptions are described in Papafotiou & Senger (2014).

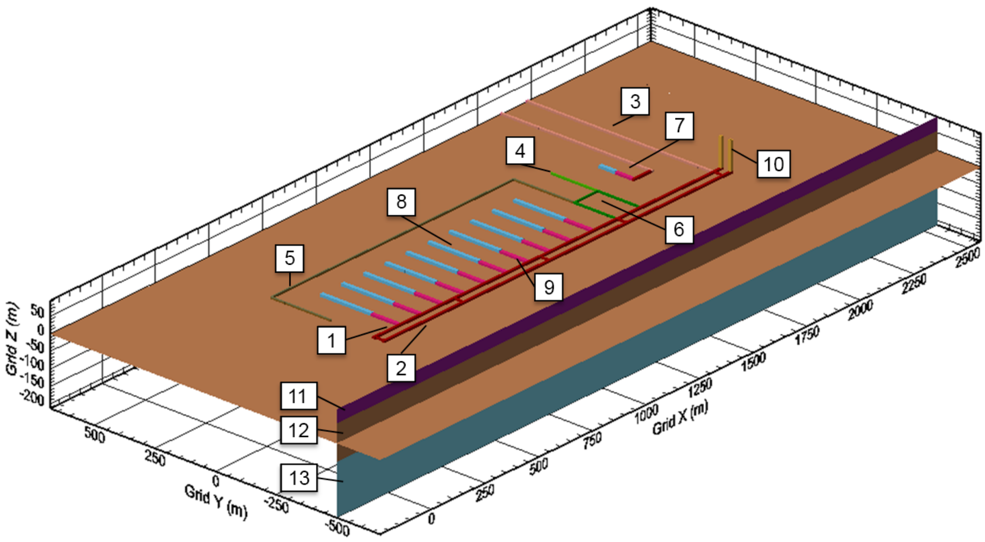

Fig. 4.4-1: 3D representation of the L/ILW repository model geometry with the various underground structures: (1) operations tunnel; (2) ventilation tunnel; (3) access tunnel; (4) control tunnel; (5) perimeter tunnel; (6) test facility; (7) pilot cavern; (8) L/ILW emplacement caverns; (9) branch tunnels; (10) shafts; (11) Upper confining unit; (12) Opalinus Clay; (13) Lower confining unit.

The calculations take into account the phased construction, operation, monitoring and closure of the repository, for which the assumed timeline is shown in Tab. 4.4-1. The model domain is assumed to be initially fully water-saturated and hydrostatic pressures are assigned to the model nodes prior to the repository construction. Gas generation is assumed to begin at the start of the post-closure phase. Prior to this, ventilation of open structures is taken into account.

The hydraulic and two-phase properties for the repository components are based on the compilations in Nagra (2008d) and summarised in Papafotiou & Senger (2014). Of particular importance are the different seals representing the EGTS, which is designed to limit gas pressure build-up in the repository. To examine the effects of the properties assigned to the EGTS on the gas pressure build-up, various sets of intrinsic permeabilities are assumed for the EGTS components, as shown in Tab. 4.4-4 for different simulation cases.

Tab. 4.4-1: Repository timeline and corresponding timeline of a cavern in the centre of the main repository facility.

Data have been subjected to Nagra's data clearance procedure.

Phase	**Repository timeline**	**Timeline of cavern in the centre of the main repository**
Construction of facility for underground geological investigations	Years 0 – 4	Not existing
Operation of facility for underground geological investigations	Years 4 – 9	Not existing
Construction of main repository	Years 9 – 12	Cavern construction (years 10.5 – 11.5)
Operation / emplacement period	Years 12 – 27	Cavern operation / waste emplacement and backfill (years 20 – 22)
Monitoring of main repository	Years 27 – 37	Cavern monitoring (years 22 – 37)
Observation of entire repository	Years 37 – 77	Cavern monitoring (years 37 – 77)
Post-closure phase	Years 77+	Cavern monitoring (years 77+)

Geoscientific database

The results of the recent laboratory and field studies that provide the gas-related database for gas calculations were compiled and evaluated in the report of Senger et al. (2013) for SGT Stage 2. The main data sources are linked to the following programmes and research platforms:

- *WLB:* a total of 10 gas threshold pressure tests were conducted in the investigation boreholes SB2, SB3, SB4 and SB4a/v and SB4a/s. A synopsis of all gas-related studies within the WLB project are given in Nagra (1997).
- *OPA/Entsorgungsnachweis:* Characterisation of gas-related properties of the Opalinus Clay by laboratory tests and Packer Test O7 (Nagra 2002b).
- *Mont Terri URL:* A series of gas-related laboratory and in-situ experiments were conducted (Marschall et al. 2005, Croisé et al. 2006).
- *EU-Projects:* Laboratory tests and field experiments performed in various URLs in argillaceous formations (NFPRO, FORGE).
- Complementary desk studies comprising evidence from elsewhere (CO_2, natural gas storage, reservoir engineering, shale gas).

Furthermore, additional gas-related studies have been initiated in the context of SGT Stage 2 to complement the existing gas-related database of the candidate host rock formations (Nagra 2010, Marschall et al. 2013, SHARC Consortium 2012), the results of which are also taken into account in Senger et al. (2013) and in the modelling summarised in the present report.

The interpretation and synthesis performed for the Opalinus Clay indicated that:

- The intact rock matrix of the Opalinus Clay is characterised by a very low hydraulic conductivity, typically in the range between 10^{-14} and 10^{-13} m/s.
- Variability of rock matrix conductivity is low.
- Discrete water-conducting features (WCF) or faults in the Opalinus Clay are not hydraulically active.

The compilation of reference hydraulic properties for gas transport comprises four different sets of values, i.e. reference and alternative values for both shallow (300[18] – 500 m bgl) and deep (500 – 900 m bgl[18]) repository configurations as summarised in Tab. 4.4-2.

Tab. 4.4-2: Gas-related parameters for the undisturbed Opalinus Clay for a L/ILW repository in Northern Switzerland.

RV = reference values; AV = alternative values.

Repository depth	**Host permeability** k [m^2] (normal to bedding)		**Capillary strength parameter** Van Genuchten: P_0 [MPa]	
	RV	**AV**	**RV**	**AV**
Shallow (300 – 500 m)	10^{-20}	5×10^{-20}	18	4.6/12
Deep (500 – 900 m)	2×10^{-21}	1×10^{-21}	34	18/60

Treatment of the EDZ

In the framework of SGT Stage 2, Alcolea et al. (2014) have developed a methodology for the abstraction of complex EDZ fracture networks to simplified representations with equivalent flow and transport characteristics (see Section 4.3). This was implemented in the 3D model assuming an EDZ of 1m width around the underground opening and scaling the permeability by the cross-sectional area of the EDZ along the tunnel axis and by the width of the EDZ perpendicular to the tunnel, as described in detail in Papafotiou & Senger (2014).

Gas generation rates

Gas generation rates are investigated based on metal corrosion and the degradation of organic materials in the L/ILW. Based on preliminary assessment calculations, the contributions of gas generated from the corrosion of tunnel installations (i.e. cavern lining, concrete, rock anchors etc.) are assumed negligible.

[18] This depth is clearly an extreme value which lies outside the envisaged depth range for a L/ILW repository but which is useful for analysing the sensitivity for gas pressure evolution of the model.

The assumed gas generation rates (in m^3 of gas per year per m^3 of waste) are shown in Fig. 4.4-2:

- A Reference Case evolution is defined based on a typical time-dependent gas generation rate for average L/ILW. The evolution of the rate shows the gradual decrease of gas generation with time, based on the different material groups included in the inventory and their corrosion rates.
- To illustrate parameter sensitivities for stylised, steady-state rates of gas generation, two further cases are defined.
  - A "realistic" rate of gas generation of 0.1 m^3 of gas per year per m^3 of waste. The "realistic" steady-state rate corresponds to the (upwardly rounded) initial rate of gas generation in the Reference Case.
  - A "bounding" rate of gas generation of about 1 m^3 of gas per year per m^3 of waste. This "bounding" steady-state rate is thus one order of magnitude greater than the already conservative "realistic" rate, and is defined in order to test the robustness of the system to a hypothetical, high rate of gas generation.

Fig. 4.4-2 shows gas generation rates up to one million years in the future. Note, however, that the so-called *time frame for safety assessment*, which is the main period of concern from the perspective of post-closure safety and which was first defined in Nagra (2008d), extends to 100'000 years for the L/ILW repository. 100'000 years are also the time period considered in the following calculations.

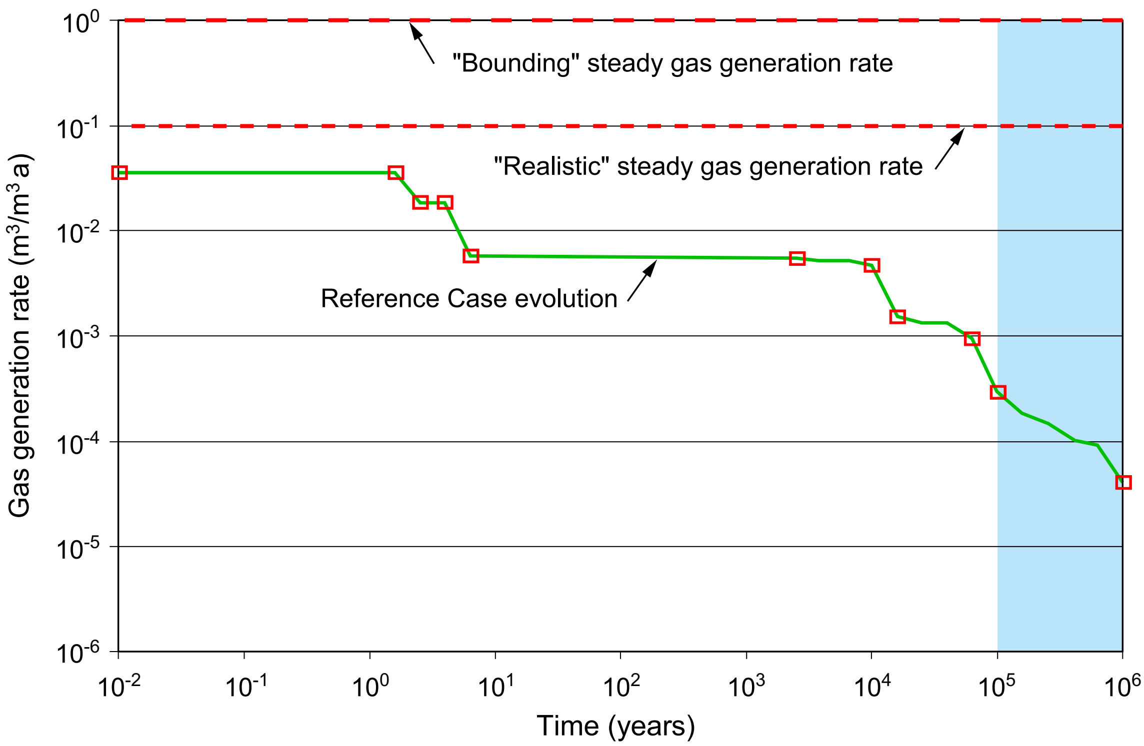

Fig. 4.4-2: Time-dependent gas generation rates in the Reference Case and steady gas generation rates in the "realistic" and "bounding" cases.

Blue shading shows times beyond the time period under consideration for a L/ILW repository.

It should be noted that, in the context of Nagra's current RD&D programme, comprehensive studies have been initiated to reduce the uncertainties in the expected gas generation rates. Other research projects deal with the biogenic conversion of hydrogen into methane, which may lead to a significant volume reduction of the accumulated gas volumes.

Matrix of calculation cases

The matrix of calculation cases is shown in Tab. 4.4-3. The calculations are based on the parameter variants noted in the previous paragraphs (variants of the EGTS properties are defined in Tab. 4.4-4). Note that only case SMA07dil includes the impact of pathway dilation on pressure evolution.

The cases are grouped as follows:

- A Reference Case is defined that makes use of the typical time-dependent gas generation rate for average L/ILW shown in Fig. 4.4-2. The repository is assumed to be at a depth of 500 m bgl. Hydraulic properties assigned to the host rock correspond to the reference parameters derived for shallow Opalinus Clay. The gas phase has the physical properties of hydrogen. This simulation accounts for an EDZ, but pathway dilation is not taken into account. The case thus focuses on the pressure build-up associated with the advective transport of H_2 through the EGTS and host rock in both the gas and liquid phase.
- A set of "realistic cases" were analysed in which physical properties of the repository, the host rock and the gas itself are considered realistic. The cases are, however, stylised in that a fixed gas generation rate is assumed for the entire calculation period, based on the initial rate in the Reference Case. The analysis of this set of cases addresses primarily: (i) the impact of the geological and hydrogeological conditions on gas pressure build-up in a L/ILW repository, including the associated conceptual and parametric uncertainties in the proposed siting regions, and (ii) the assessment of the role of the engineered gas transport system (EGTS) as a gas release path and the optimisation of the design thereof.
- Two "bounding cases" are also analysed that are stylised, one with a fixed gas generation rate, this time set to the "bounding" rate of gas generation shown in Fig. 4.4-2, and one with no gas generation in the repository.

Tab. 4.4-3: Matrix of calculation cases, highlighting in light red those for which 80 % of lithostatic pressure is exceeded and in darker red where 100 % of lithostatic pressure is exceeded.

Case i.d.	**Repository**		**Host rock**	**Gas**	
	Depth [m]	EGTS properties		Generation rate	Properties
Reference Case					
SMA10	500	*high-k*	Reference values/shallow repository	Reference (time-dependent)	Based on hydrogen
"Realistic" cases					
Base case, SMA01, SMA12	500	*high-k* (3 variants; see Tab. 4.4-2)	Reference values/shallow repository	"Realistic" (steady)	Based on hydrogen
SMA02, SMA 03	500	*low-k* (2 variants; see Tab. 4.4-2)	Reference values/shallow repository	"Realistic" (steady)	Based on hydrogen
SMA04	As base case, but with low-*k* upper confining units				
SMA07	500	*low-k*	Reference values/shallow repository	"Realistic" (steady)	Based on air
SMA07dil	As SMA07, but with pathway dilation included in model				
SMA08	300	*high-k*	Reference values/shallow repository	"Realistic" (steady)	Based on hydrogen
SMA09	700	*low-k*	Reference values/deep repository	"Realistic" (steady)	Based on hydrogen
SMA11	300	*high-k*	Alternative values/shallow repository	"Realistic" (steady)	Based on hydrogen
"Bounding" cases					
SMA06	500	*high-k*	Reference values/shallow repository	None	Based on air
SMA05	500	*high-k*	Reference values/shallow repository	"Bounding" (steady)	Based on hydrogen

Tab. 4.4-4: Sets of intrinsic permeabilities for EGTS components considered in the calculation cases.

V2 seals are placed in the construction and operations tunnels, the V4 seal (repository plug) along the access ramp at the top of the Opalinus Clay the V5 seals and the ends of the emplacement caverns. The V3 seal corresponds to the backfill of the shaft.

Parameter set (see Tab. 4.4-3 for use in calculation cases)	**Permeability k** [m^2]			
	V2 seal	V4 seal	V5 seal	Shaft (V3)
high-k	10^{-16}	5×10^{-18}	10^{-16}	5×10^{-18}
high-k (SMA01 variant)	as above	10^{-16}	as above	as above
high-k (SMA12 variant)	as above	10^{-16}	as above	10^{-16}
low-k	10^{-17}	10^{-18}	10^{-17}	10^{-20}
low-k (SMA03 variant)	as above	5×10^{-18}	as above	5×10^{-18}

4.4.3 Impacts for the Reference Case

The simulated gas saturations for the Reference Case (Case SMA10) are shown in Fig. 4.4-3. After 1'000 years, a large portion of the repository structures (except emplacement caverns and parts of the operations/ventilation tunnels) are entirely saturated with porewater from the surrounding host rock. Gas saturations in the repository caverns and tunnels increase until 10'000 years with some of the waste-generated gas migrating into the immediate vicinity of the host rock. However, the extent of the gas front into the host rock is limited. Gas saturations in the host rock next to the emplacement caverns reach maximum values of approximately 0.001 after 10'000 years. Afterwards, gas saturations decrease to the end of the simulation after 100'000 years.

The time history of pressures in the selected repository locations is shown in Fig. 4.4-4. The plot shows that pressures are calculated to peak before 10'000 years and subsequently gradually decline to the hydrostatic value in all locations. It is also indicated that pressures in different locations of the repository reach the hydrostatic pressure (about 5 MPa at an assumed repository depth of 500 m) after 50'000 years. The time history plot of gas saturations shows that part of the access tunnel near the repository seal (Access2) saturates entirely with water (zero gas saturation) after a few hundred years, and that gas saturation at all locations within the repository decreases to 20 % or less by 2'000 years, due to the inflow of porewater from the surrounding host rock. During this time, waste-generated gas dissolves in porewater. Later, the ongoing generation of gas increases the amount of dissolved gas until the gas phase forms again in the tunnels and gas saturations increase again up to 10'000 years. Thereafter, due to the declining gas generation rate, gas saturation decreases in the access tunnel by about 50'000 years and in part of the operations tunnels and in the caverns by 100'000 years, when nearly fully water-saturated conditions are reached.

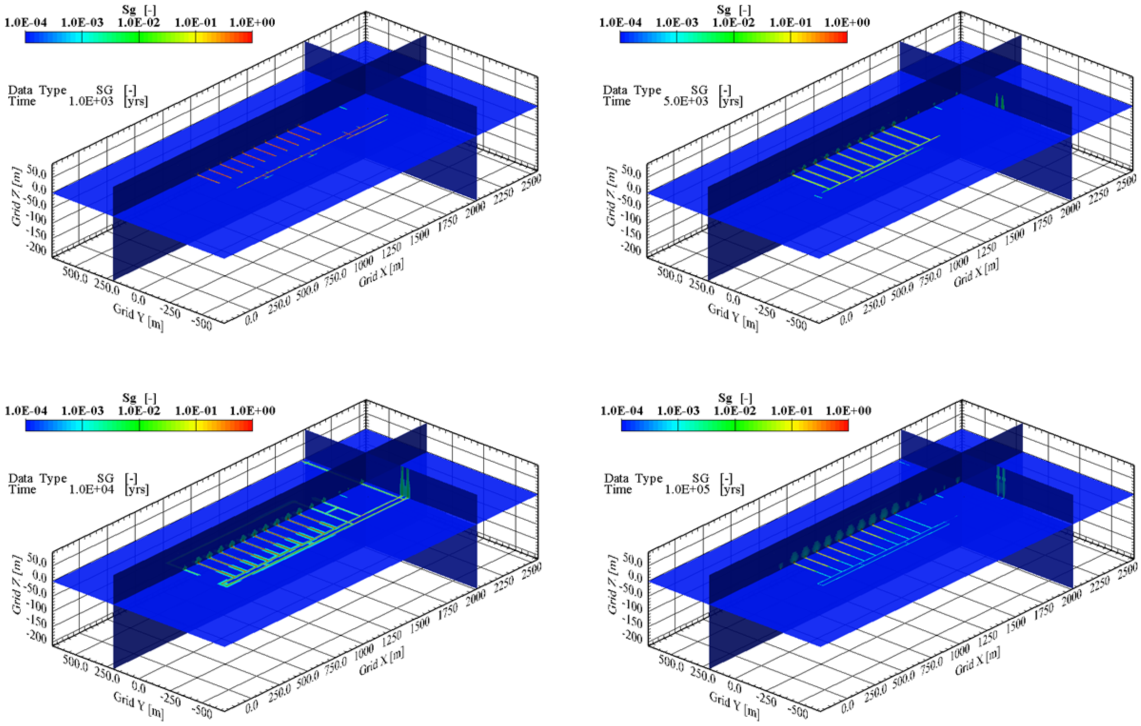

Fig. 4.4-3: Reference Case (SMA10): distribution of gas saturation after 1'000, 5'000, 10'000, and 100'000 years.

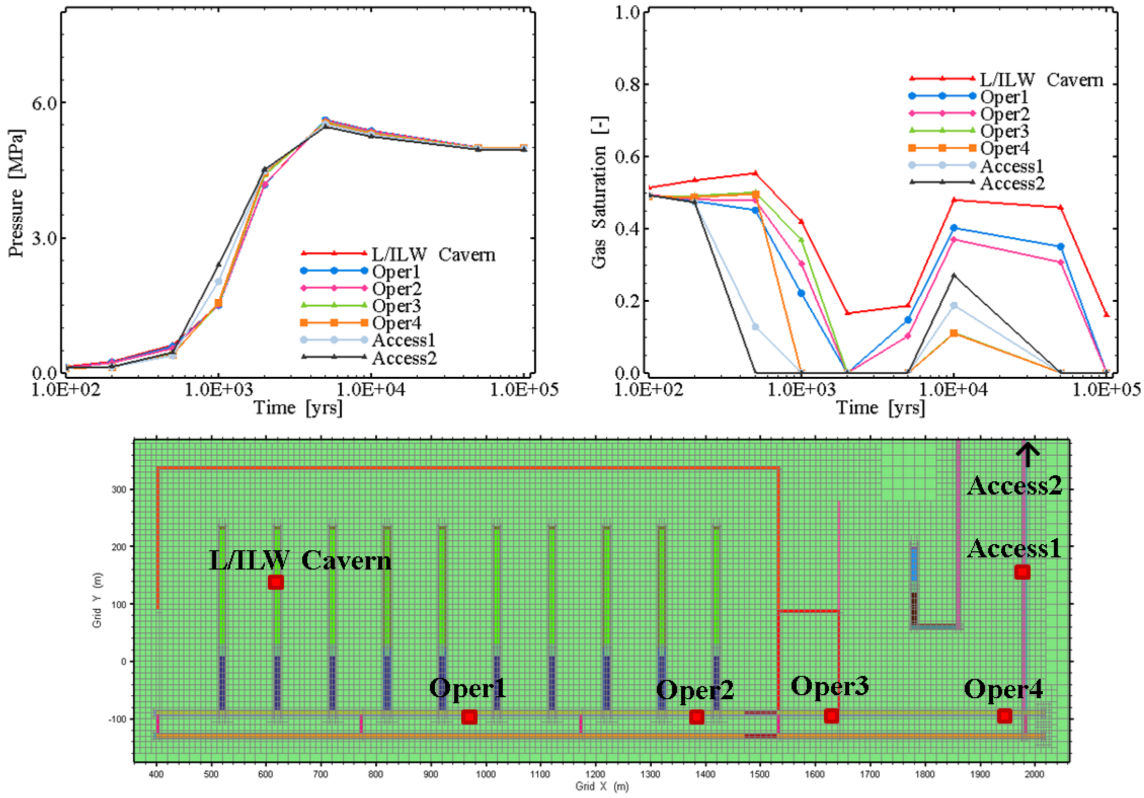

Fig. 4.4-4: Reference Case (SMA10): pressure (left) and gas saturation (right) time history in different locations of the repository shown in the plan view of the model (bottom).

Note: hydrostatic pressure at repository level is around 5 MPa.

4.4.4 Impacts for realistic cases

Fig. 4.4-5 shows the time history of the cavern pressure in the Reference Case (SMA10) and in all of the realistic cases (fixed gas generation rate is assumed for the entire calculation period, based on the initial rate in the Reference Case), normalised to the level of lithostatic stress. The threshold pressure for the on-set of pathway dilation, assumed to correspond to 80 % of the lithostatic stress, is also shown.

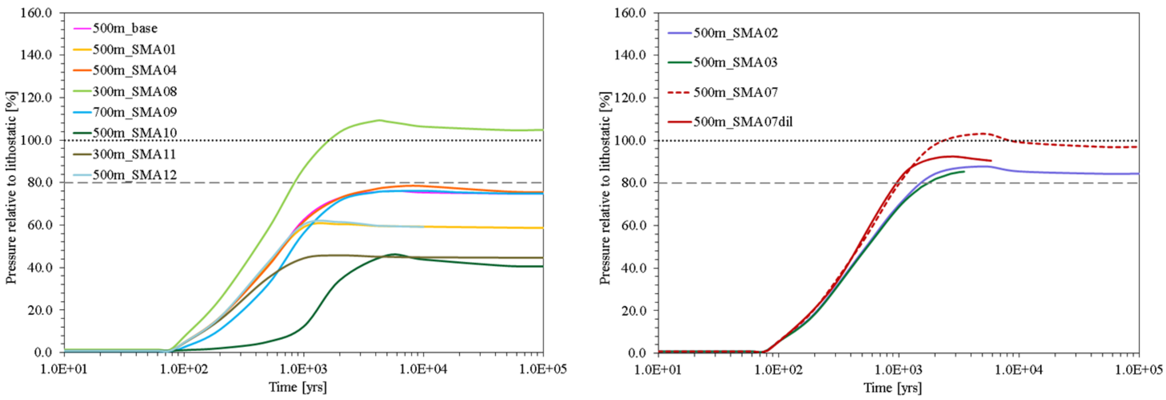

Fig. 4.4-5: Time history of gas pressure in the cavern in the Reference Case (SMA10) and in all of the realistic cases, relative to the lithostatic pressure for the corresponding depths (300 m, 500 m, and 700 m bgl), in %.

The left figure shows cases with *high-k* EGTS gas transport capacity and the right figure shows cases with *low-k* EGTS gas transport capacity.

Peak gas pressures are consistently higher than in the Reference Case, since the initial gas generation rate assumed in the Reference Case is (hypothetically) maintained throughout the entire calculation period in these cases. However, the figure clearly shows that only in a small number of cases 80 % of the lithostatic pressure is exceeded. Referring to Tab. 4.4-3, these are the cases where:

1. a relatively shallow repository depth (300 m), and so a relatively low lithostatic pressure, is assumed (SMA08 only), indicating that the depths of 500 and 700 m bgl are less sensitive with respect to gas pressure build-up than the shallow 300 m depth, or
2. unfavourable (*low-k*) properties are assigned to the EGTS (SMA02, SMA03, SMA07 and SMA07dil), highlighting the important role of the underground structures and EGTS as gas release pathways and, in particular, the importance of selecting materials that will provide adequate gas release

100 % of lithostatic pressure is exceeded only in Cases SMA07 and SMA08. Pathway dilation is not included in these calculations. Comparing the results for SMA07 with SMA07dil, where pathway dilation is included, illustrates how this process reduces further gas pressure build-up above 80 % of lithostatic pressure, such that 100 % of lithostatic pressure is not exceeded in SMA07dil.

Comparing the Reference Case, where a *high-k* is assigned to the V2 seals in the construction and operations tunnels, V5 seals and the ends of the emplacement caverns, with SMA01, where a *high-k* is also assigned to the repository plug (V4 seal), indicates the importance of an adequate permeability of the repository plug in reducing gas pressure build-up. Case SMA12, where a *high-k* is also assigned to the shaft (V3 seal) gives similar results to SMA01. Overall, it can be concluded that pressure build-up directly relates with the capacity of the pathways for gas transport between the main repository and the repository ramp and shaft and that pressure build-up can be limited through the selection of EGTS materials with suitable hydraulic properties.

4.4.5 Impacts for "bounding" cases

"Bounding" case SMA06 aims at estimating the saturation times and associated porewater pressure recovery in the absence of waste-generated gas. The simulated gas saturations and pressures after 500, 1'000, 2'000 and 5'000 years are shown in Fig. 4.4-6. After 500 years, the gas phase is still present in all of the repository structures and in some parts of the host rock around them. After 1'000 years, the access tunnels, branch tunnels, perimeter tunnel, and large portions of the facility for underground geological investigations and ventilation tunnel are entirely saturated. After 2'000 years, the repository structures have saturated entirely, with the exception of some residual air that remains trapped in the emplacement caverns.

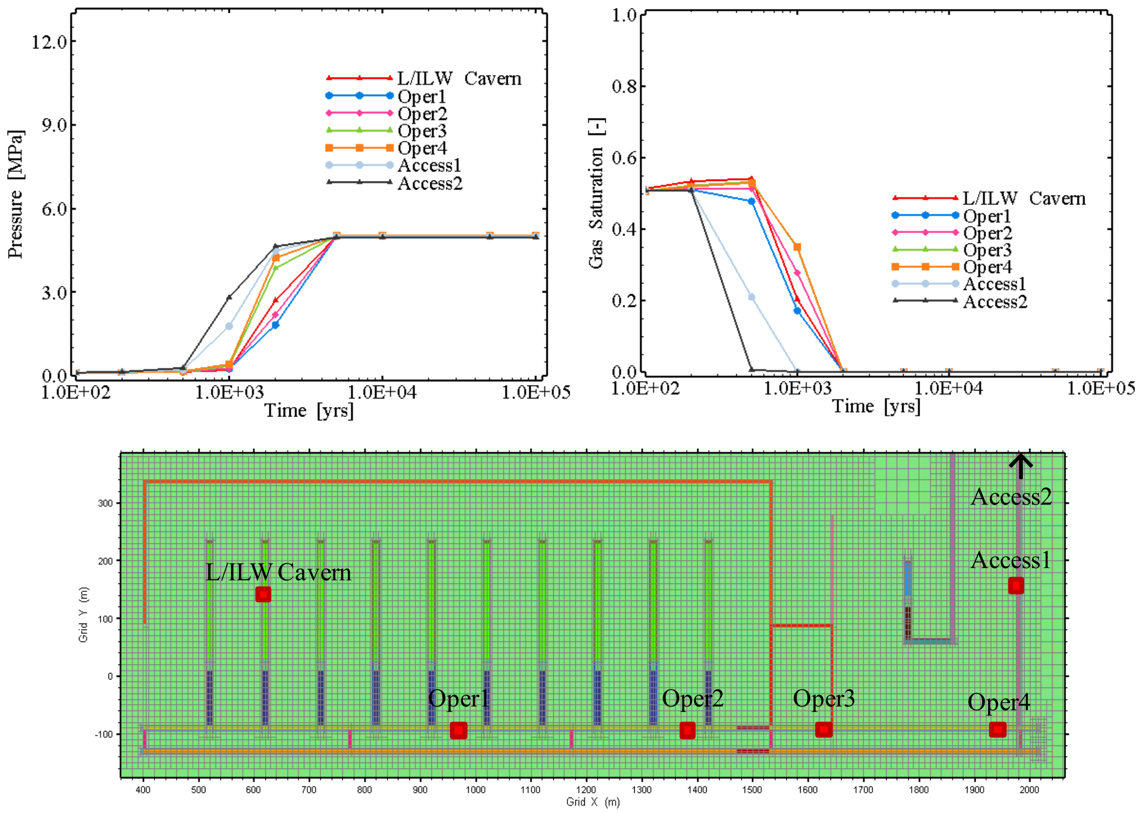

Fig. 4.4-6: "Bounding" case (SMA06): pressure (left) and gas saturation (right) time history in different locations of the repository shown in the plan view of the model (bottom).

Note: hydrostatic pressure at repository level is around 5 MPa.

The second "bounding" case, SMA05, adopts a highly conservative gas generation rate of 1 m^3 of gas per year per m^3 of waste (and disregards pathway dilation), which is assumed to be maintained for 10'000 years. Thereafter, gas generation stops and the gas phase continues to expand into the host rock, however, with decreasing saturation values due to the gradual dissolution of gas in the porewater. In this case, Fig. 4.4-7 shows that gas migrates relatively rapidly through the repository structures and into the surrounding host rock. After 1'000 years, the gas front has already reached the upper model boundary. After gas generation stops, the gas phase continues to expand into the host rock, however, with decreasing saturation values due to the gradual dissolution of gas in the porewater.

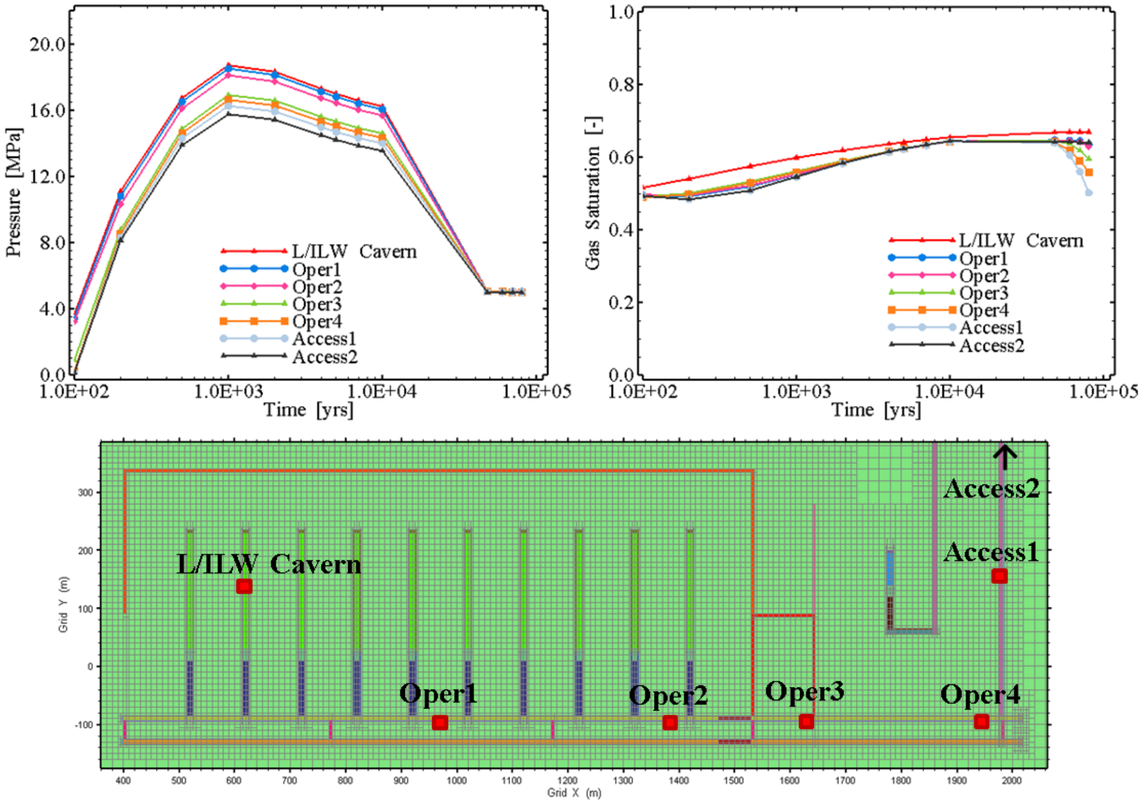

Fig. 4.4-7: "Bounding" case (SMA05): pressure (left) and gas saturation (right) time history in different locations of the repository shown in the plan view of the model (bottom).

Peak cavern pressure in this second "bounding" case exceeds lithostatic pressure by some 50 %, indicating that such high gas generation rates could, if they were to occur, lead to perturbations (fracturing) of the rock. It is stressed, however, that such rates are not expected in a real setting and that these gas generation rates were chosen to explore the robustness of the repository system.

4.4.6 Concluding remarks on gas pressure build-up and transport

The model analyses by Papafotiou & Senger (2014) provide evidence for the temporal evolution of the gas release paths from the backfilled L/ILW caverns along the Engineered Gas Transport System (EGTS; see also Nagra 2008d) and through the host rock, respectively. The sensitivity study with the 3D model of a generic L/ILW repository reveals a pronounced sensitivity of gas pressure build-up to the variations of parameters associated with the geological conditions, the configuration of the EGTS, and the uncertainty in gas generation rates. In the case with the reference values for the gas generation rates, the safety function criteria for maximum gas pressure in the L/ILW caverns are met (Tab. 4.1-7), whereas for the upper bounding gas generation rates, gas pressures exceeded lithostatic pressures. The results indicate that the depths of 500 and 700 m bgl are more suitable with respect to gas pressure build-up. Furthermore, pressure build-up directly relates to the length of the pathways for gas transport between the main repository and the repository ramp. Results obtained with the sensitivity cases for a repository depth at 500 m bgl indicate that pressure build-up can be optimised through the engineering design of the repository layout and the hydraulic properties of the EGTS. It can be concluded, that the issue of gas pressure build-up can be addressed through the appropriate configuration of the L/ILW repository design.

A detailed discussion of the safety function indicator related to gas-induced porewater displacement (Tab. 4.1-8) has been conducted in Nagra (2008d). Accordingly, in the early post-closure phase (< 1'000 a) the maximum specific flux from the L/ILW caverns into the host rock may slightly exceed the safety indicator criteria ($q < 1 \times 10^{-11}$ m/s) by less than half an order of magnitude[19]. On the other hand no significant displacement of contaminated porewater will occur as a result of gas release after the maximum of the overpressure. Thus, after 100'000 years the value of specific water flux through the host rock formation is in the order of magnitude of 1×10^{-13} m/s, so that one can expect diffusion-dominated radionuclide transport in this time period.

4.5 Effects of chemical interactions

4.5.1 Overview

Quantitative effects relating to the migration of concrete pore fluids from the repository vaults have been assessed. Saturation of concrete with groundwater leads to the development of a hyperalkaline (pH > 12.5) pore fluid. The pH value decreases with time in accordance with the leaching of progressively less-soluble solids, such that initial fluids with pH > 13 correspond to leaching of readily soluble NaOH and KOH (e.g. Atkinson 1985). The removal of portlandite, $Ca(OH)_2$, buffers pH at 12.5, with Ordinary Portland Cement (OPC) pastes typically containing 20 – 25 % of this solid. In the long-term, pH in concrete pore fluids is defined by the incongruently soluble calcium silicate hydrate gel (C-S-H), with pH progressively decreasing from 12.5 to < 10. Predictive models for C-S-H gel behaviour are now focused on solid – solution mechanisms (e.g. Walker et al. 2007) rather than the variable solubility product type relationships used earlier (e.g. in Berner 1992).

Karlsson et al. (1999) estimated that some 8'000 moles of OH^- may be liberated by each cubic metre of concrete through such processes. Although some of this alkalinity may be neutralised by reactions with dissolved carbonate species in groundwater, pore fluids of pH > 10 can destabilise silicate and carbonate minerals in the host rock. In some instances, this reactivity between concrete and the host rock may be manifested in increased bonding between the OPC paste and the minerals within the host rock. Calcite in the host rock will be initially destabilised, but will re-precipitate as pH decreases. Dolomite is unstable in the presence of cement pore fluids, such that irreversible 'dedolomitisation' occurs with the precipitation of brucite ($Mg(OH)_2$) and calcite.

In this regard, it is likely that there will be a difference between the alteration of the host rock at pH > 12 and that at lower pH values. Mineralogical alteration at pH > 12 is dominated by the growth of calcium silicate hydrate (C-S-H) solids, whereas alteration at pH < 12 is typified by zeolites, such as phillipsite, clinoptilolite, and analcime (Savage et al. 2007). Secondary mineral formation at pH < 11 (i.e. at pH conditions typical of low-pH cement) will therefore tend to be zeolitic.

The degree of rock alteration is sensitive to a number of factors, such as the precise rate and mechanism of mineral dissolution close to equilibrium, the variation of physical properties (porosity, permeability) with time, the composition of cement pore fluids, and the assumed

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[19] During the early post-closure phase the water displaced from the host rock into the surrounding rock units cannot be contaminated with radionuclides.

crystallinity and types of secondary minerals (Savage et al. 2007). Essentially, a front of alteration will move through the rock (Opalinus Clay) as reactants diffuse through it, controlled by the changing physical properties (porosity, permeability) with time. Secondary solids are likely to include minerals such as calcium (aluminium) silicate hydrates (C-(A)-S-H), zeolites, feldspars, hydroxides, carbonates, polymorphs of silica, and some sheet silicates (Savage et al. 2007). These processes are usually accompanied by a decrease in porosity and permeability, such that the spatial scale of alteration is self-limiting.

4.5.2 Methodology

Migration of the alkaline plume through the host rock has been simulated using 1D reaction transport modelling (Kosakowski & Berner 2013). In this modelling, transport is assumed to occur either solely by diffusion (Fig. 4.5-1) or by advection and diffusion (Fig. 4.5-2). It is a simplification to assume that one or other of these transport mechanisms occurs alone, but modelling of the isolated processes provides an insight in the extreme bounding cases. The cases that are relevant for a repository in Opalinus Clay are mainly dominated by diffusive transport, with advective transport often being very limited. The hydraulic parameters controlling advective transport are also relatively poorly defined. Consequently, purely diffusive models have been employed in situations where sufficient confidence exists that transport is diffusion-dominated. These cases have been calculated in a realistic way, with full coupling between porosity changes, mineral precipitation and dissolution, together with changes in effective diffusion coefficients.

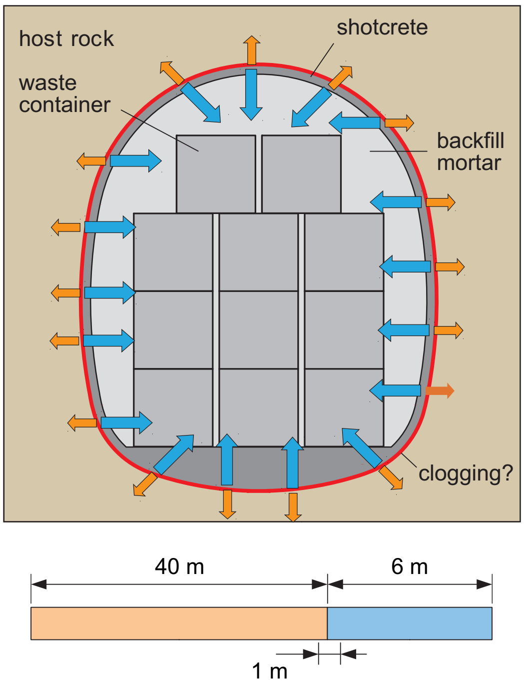

Fig. 4.5-1: Cross section through a generic emplacement cavern (type K09, upper picture) and its simplifications into a one-dimensional model (lower part with clay in orange and cement in blue) for diffusive transport.

The cement compartment is coloured in grey and the host rock compartment in brown. The arrows indicate the directions in which alteration and reaction fronts progress. Red colours indicate possible zones of porosity clogging. The cavern is assumed to have an equivalent radius of 6 m. From Kosakowski & Berner (2013).

In other situations, advection can dominate in the long-term. The rate of flow will, in reality, vary with time, in response to the variations in the gradient driving the flow, and also due e.g. to permeability changes resulting from mineral precipitation and dissolution. However, for simplicity, advective models were used in which the Darcy flux was held constant during the course of the simulation, and the coupling between mineral precipitation/dissolution and porosity and permeability changes was 'switched off' (Kosakowski & Berner 2013). The long-term behaviour of these simulations shows a linear relation between the progress of reaction fronts in flow direction and the amount of water flowing through the system. The geometry for this system is shown in Fig. 4.5-2.

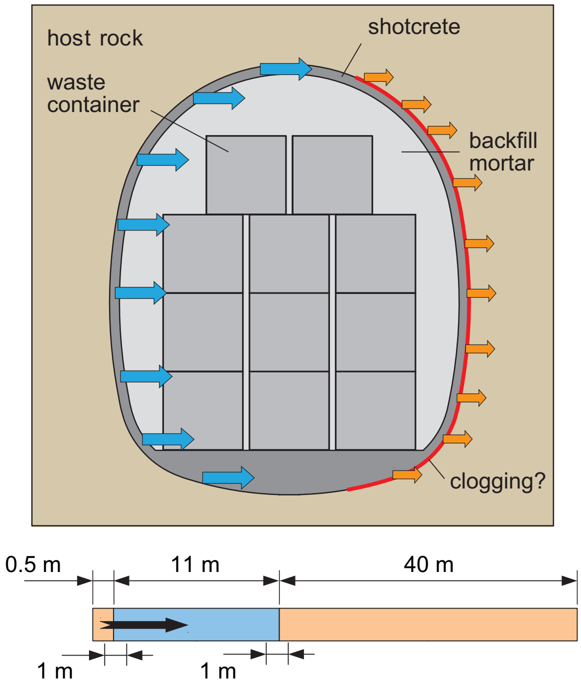

Fig. 4.5-2: Cross section through a generic emplacement cavern (type K09, upper picture) and its simplifications into a one-dimensional model (lower part with Opalinus Clay in orange and cement in blue).

The cement compartment is coloured in grey and the clay material (host rock) compartment in brown. The cavern is assumed to have an equivalent diameter of 11 m[20]. The arrows indicate the directions in which alteration and reaction fronts progress. Red colours indicate possible zones of porosity clogging. From Kosakowski & Berner (2013).

The calculations assume chemical equilibrium rather than kinetic control of mineral reactions. From previous studies and from test calculations, it can be shown that, for the investigated systems of diffusion-dominated transport in low permeability rocks, most reactions are con-

[20] For these calculations Kosakowski & Berner (2013) assumed an emplacement cavern that has a width of 10 m, a height of 11 m, a length of 200 m and a resulting cross-sectional area of 110 m^2. Figs. 4.5-1 and 4.5-2 provide the model setup and dimensions for cases with diffusive and advective transport respectively. In order to minimise the code execution time, the 3D tunnel geometry was simplified into 1D setups. For the diffusive calculations the complex cavern cross section was transformed into a circular area with approximately 6 m radius (Fig. 4.5-1). As reactions take place near the interface a simple linear 1D setup instead of a rotationally symmetric model was chosen. A sensitivity study comparing linear and axisymmetric setups showed that for the investigated cases the differences between both conceptualisations are very small. For the advective scenarios the geometry was converted into a rectangle of 10 m × 11 m (Fig. 4.5-2) where the flow direction is parallel to the longer side.

trolled by local equilibrium rather than by kinetic constraints. These test calculations revealed that the principal mineral precipitation sequences and even the spatial extent of mineral alterations are the same when assuming thermodynamic equilibrium instead of kinetics. The timescale associated with the occurrence of certain mineral phases (e.g. zeolites) might differ, but the overall system characteristics are unchanged. Timescales for porosity clogging are only slightly shorter in the equilibrium case, as the major precipitates are not primarily controlled by kinetic constraints.

All the different concrete materials were represented by a typical concrete, based on 'CEM I 52.5 N HTS' sulphate-resistant Portland cement. This represents a typical chemical composition and matches the currently defined porosity of 0.2 used in L/ILW near-field radionuclide release and transport calculations (Nagra 2010). The starting points for modelling concrete were the studies of Lothenbach & Wieland (2006), the cement database CEMDATA07 (Kosakowski et al. 2014), Version 1b, the Nagra/PSI chemical thermodynamic database 01/01 (Nagra 2010), and the geochemical modelling code GEMSPSI, version v3.0.0 (http://gems.web.psi.ch/).

The aim of the models was to simulate the evolution of porewaters and mineralogical compositions, and to simultaneously produce reasonable values for water content, anion accessible porosities and cation exchange capacities (CEC). The main model assumption for the host rock is that cation exchange properties of the rock were those of a montmorillonite solid solution comprising Na, K, Ca, and Mg end-members.

4.5.3 Impacts for the Reference Case

The Reference Case considers diffusion-controlled transport. Simulation results for this case from Kosakowski & Berner (2013) are summarised in Fig. 4.5-3. Due to the precipitation of secondary minerals near the interface between the host rock and the concrete, mass fluxes occurring across the interface decrease with time. The simulations were terminated after porosities reduced to less than 0.002. Such a value was considered to be sufficiently low that mass transport over the interface is negligible. Major mineralogical changes are restricted to less than 5 centimeters on both sides of the interface when porosity clogging occurs. In the host rock compartment, changes are characterised by precipitation of Na- and K-phillipsite (zeolite) and calcite, and by dissolution of clay minerals. In addition, kaolinite is transformed into illite and montmorillonite. It is not possible to deduce the integrity and mechanical strength of such an interface, but a reduced porosity is likely to inhibit fluid transport. In the concrete compartment, portlandite and monocarbonate dissolution fronts develop. Additional C-S-H with a low Ca/Si ratio is precipitated near the interface, and ettringite gradually replaces monocarbonate.

Modelling investigations have shown that host rocks with lower initial porosities generally clog earlier and show narrower mineral alteration zones compared to host rocks with higher initial porosities. The host rock porewater composition may also influence the interface evolution. For example, higher ionic strength porewater is more aggressive, causing stronger concrete alteration and accelerating the clogging process due to the enhanced precipitation of secondary reaction products (Kosakowski & Berner 2013).

The alteration distances predicted by Kosakowski & Berner (2013) are significantly less than those considered by Mäder (2005), who used a conservative, mass-balance approach to show the effects of all the hydroxide released from concrete degradation diffusing into the Opalinus Clay. In this extreme case, the hydroxide would react with the kaolinite (and quartz) to form laumontite and C-S-H phases. Based on this reaction, Mäder (2005) concluded that 1 m^3 of Opalinus Clay would be able to buffer 4 m^3 of concrete with a reaction front extending 0.5 m into the host rock.

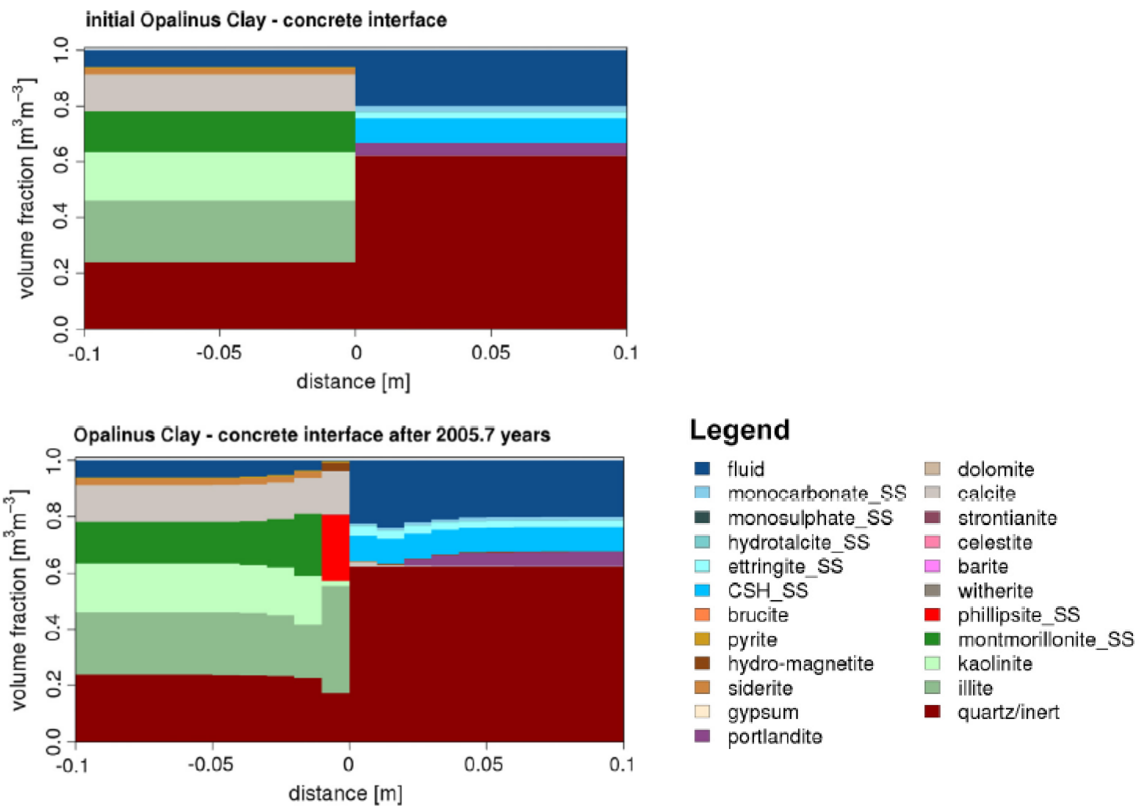

Fig. 4.5-3: Mineralogical profiles after ~ 2'000 years at the Opalinus Clay-concrete interface assuming diffusive mass transport only.

From Kosakowski & Berner (2013).

Other reaction – transport simulations of the diffusion of hydroxide ions from concrete into mudrock (e.g. Trotignon et al. 2007, De Windt et al. 2008, Marty et al. 2009, Traber & Mäder 2006) show similar alteration distances to those computed by Kosakowski & Berner (2013), i.e. distances of 0.01 – 0.15 m over a 0.1 – 25 ka time period. Evidence from the industrial analogue of concrete – mudstone interaction at Tournemire, SW France, shows a mudstone alteration thickness of up to 0.02 m after 15 years of interaction (Tinseau et al. 2006 and 2008; Fig. 4.5-4). The observed reaction rate will not remain as high as this, as gradually clogging of the interface will reduce transport across it. There is good evidence from this system to show that fluids from the mudstone have infiltrated the concrete and vice versa, whereas, in a disposal vault, fluid movement might be expected to occur principally from the host rock into the vault. In a repository, the available water inside the concrete backfill and waste compartment will be primarily consumed by degradation reactions, and will thus not be available for transport into the host rock. This could lead to the formation of a reaction zone, mainly on the concrete side, dominated by carbonation, conversion to ettringite, and Mg-substitution reactions of portlandite and C-S-H gel.

4.5.4 Impacts for a "bounding" case

In an alternative "bounding" case, transport is assumed to be advection-controlled (e.g. Fig. 4.5-2), even in the host rock where, in reality, diffusive transport is expected to dominate. Again, the results of simulations conducted by Kosakowski & Berner (2013) have been used to scope the likely scale of perturbation. In addition, the Maqarin natural analogue may be used as a case study for advection-controlled transport.

In these simulations, the backfilled emplacement caverns are treated as a porous medium with average concrete properties and composition. Advective transport in the caverns is controlled by external conditions, i.e. the local hydraulic field in the host rocks. Water, with a composition specific to the host rock, enters the emplacement caverns and interacts with the concrete. This changes the water composition and induces mineralogical changes. After passing through the cavern, the altered water re-enters the host rock formation and re-equilibrates with the down-stream host rock, which may induce mineralogical changes near the outflow interface. Here, the magnitude of water flow through the emplacement caverns as well as the inflowing host rock water composition (i.e. carbonate, sulphate), govern the concrete degradation (Kosakowski & Berner 2013).

A Darcy flux of 10^{-13} m/s was assumed for the Opalinus Clay, based on information given in Nagra (2010). This flux results in a flow of 0.32 m^3 of porewater per m^2 over 100'000 years. Mineralogical alterations at inflow and outflow interfaces are restricted to zones of less than 5 cm width (Fig. 4.5-5). The outflow interface is altered as in the diffusive cases, so that mont-morillonite and kaolinite are converted to illite and phillipsite.

Fig. 4.5-4: Photograph of the interface between cement (left – light grey) and mudstone (right – dark grey banding) from the Tournemire analogue, showing the centimetric scale of mudstone alteration.

From Tinseau et al. (2008).

The most relevant analogue of the advective system is that at Maqarin, Jordan (e.g. Alexander et al. 1992, Savage 2011, Watson et al. 2016). At Maqarin, several occurrences of cement-clinker-like pyrometamorphic rocks have been hydrated to cement-like mineral assemblages. Leachates emanating from them are hyperalkaline and similar to porewater found in cement systems. Fracture-controlled groundwater flow systems carry the hyperalkaline solution into the sur-rounding bituminous clay biomicrite (clayey limestone or 'marl'). The alteration has induced locally significant changes in the porosity of fractures and the adjacent wall rock. Due to its relevance to a nuclear waste repository, the Maqarin natural analogue site has been extensively investigated through multiple field sampling campaigns. Measurements and analysis of the compositions of rock formations, the corresponding porewater and the alkaline water in the fracture system can be found in various summary reports (e.g. Smellie 1998, Linklater 1998). Although hydraulic gradients in the Maqarin system are considerably greater than those expected in a repository environment, fractures in the rocks have been sealed downstream of the hydrated cement zone by the precipitation of a complex sequence of C-(A)-S-H gels, ettringite, calcite and zeolites (e.g. Baker et al. 2002). Fracture sealing may occur extensively and over short timescales (tens to hundreds of years) at Maqarin (Smellie 1998). Computer modelling of the evolution of Maqarin has been carried out by Steefel & Lichtner (1998), and more recently by participants in the Long-Term Cement Studies (LCS) Project (e.g. Shao et al. 2013). Simulations with equal reactive surface areas and mineral rate constants in the fracture and matrix suggest that the rock matrix should seal first. In terms of the performance of a waste repository, this implies a loss of the buffering capacity of the rock matrix and, moreover, strongly diminishes the possibility for diffusion of radionuclides into the rock matrix. The loss of the buffering capacity of the rock matrix due to its cementation leads to a downstream propagation of the hyperalkaline plume. However, field observations at Maqarin indicate that the fractures eventually seal, although some initial downstream propagation of fronts is not ruled out.

Nevertheless, the small physical scale (cm) of the altered zone in the rock and accompanying physicochemical transformations mean a relatively insignificant impact upon safety-relevant parameters such as permeability and radionuclide sorption.

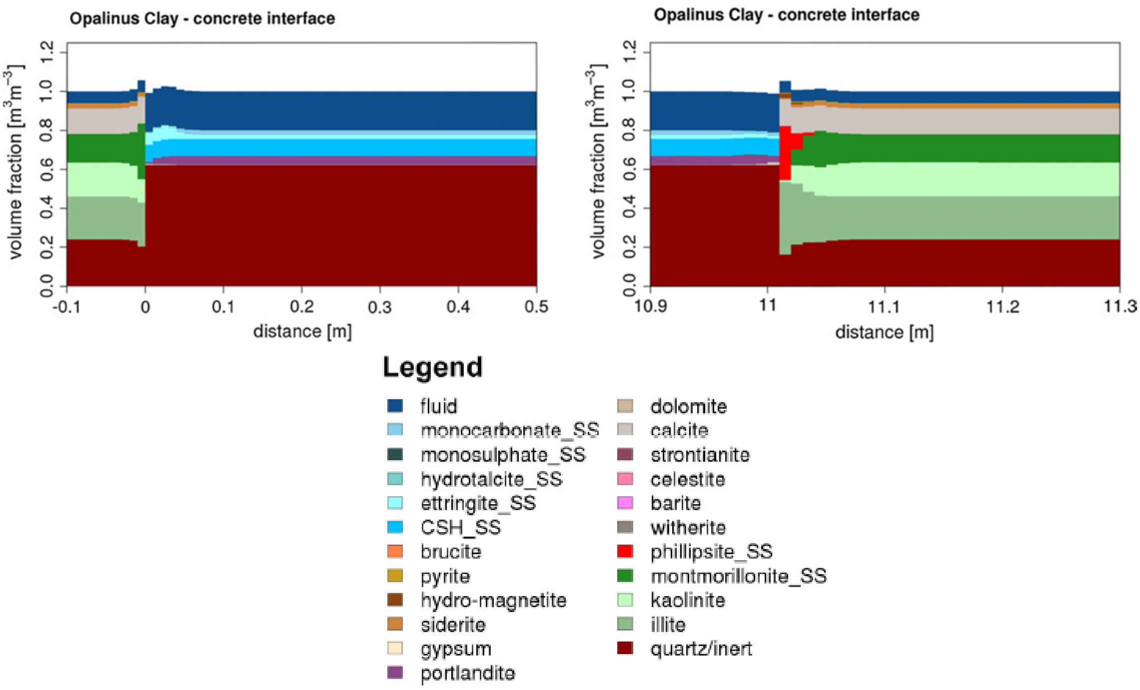

Fig. 4.5-5: Mineralogical profiles at the inflow (left-hand side) and outflow (right-hand side) concrete – rock interfaces after 100'000 years, assuming advective conditions.

Rock is on the left-hand side of the left-hand figure and on the right-hand side of the right-hand figure. See Fig. 4.5-3 for the mineral colour-coding. From Kosakowski & Berner (2013).

4.5.5 Impacts on the EGTS

In the EGTS, long-term interactions between cement and clay under fully saturated conditions may lead to localised precipitation of minerals, which could clog the pore space. A widespread occurrence of porosity clogging in the EGTS could influence the functionality of the system by decreasing mass transport properties.

1D and 2D computer simulations by Kosakowski & Berner (2013) have investigated scenarios where water flows from the access tunnel system through a transitional layer (see Fig. 2.1-4) towards the emplacement cavern[21]. Fluid flow from the tunnel through the transitional layer into the concrete is to be expected after about 1'000 years. In the transitional layer, fluid flows along the bottom of the tunnel into the emplacement cavern. The flow rates are assumed to be in the range calculated by Senger & Ewing (2009) for a repository cavern model. Although water flow is effectively restricted to the fully saturated parts of the model, the flows are slow enough that diffusive transport dominates the evolution of the system. The dominance of diffusion over advection in this scenario is confirmed by the similar mineralogical and porosity evolution in the fully saturated 2D model part and the corresponding 1D model. No strong reduction of porosity at the concrete-transitional layer interface was observed. In the partially water saturated zone, however, diffusion coefficients and hydraulic conductivities are strongly reduced. Transport-driven mineralogical and porosity changes are therefore also less developed.

Consequently, as long as the EGTS is mostly de-saturated, transport in the fluid phase (residual saturation) is very small which restricts mineral reactions causing strong porosity changes.

An issue which must be addressed in the development of the EGTS is the choice of the composition of the transitional layer which exists between the bentonite/sand and cementitious components of the repository. In the analysis presented by Kosakowski & Smith (2014), an example EGTS design is considered in which limestone gravel is used to fill the transitional layer. This choice of limestone (with calcite as the key mineral) is motivated by the fact that bentonite, cement and Opalinus Clay all contain small amounts of this mineral, and the porewaters they contain are in thermodynamic equilibrium with it. However, Kosakowski & Smith (2014) note that geochemical gradients between cementitious and other backfill materials are not completely avoided by this choice. Although this type of fill minimises the potential for the formation of porosity-filling precipitates, retardation of the high-pH front migrating from the concrete is not as effective as in the case where chemically-reactive materials are present at the interface. Examination of quartz as an alternative fill for the transitional layer by Kosakowski & Smith (2014) provides insights into the possible consequences in terms of mineralogical and porosity changes when materials in the EGTS are not in thermodynamic equilibrium. Their calculations show that only minor precipitation of C-S-H occurs, but pH decreases sharply at the interface between concrete and the transitional layer. An alternative 'reactive' material for the gravel fill would be dolomite [$CaMg(CO_3)_2$], which undergoes so-called 'dedolomitisation' reactions (e.g. Poole & Sotiropoulos 1980) in the presence of hyperalkaline fluids, producing calcite and brucite:

$$dolomite + OH^- + H_2O \rightarrow calcite + brucite + HCO_3^-$$

Not only does this reaction produce a net solids volume decrease (~ 4 %), but it also serves to retard migration of hydroxyl ions from the concrete.

Overall qualitative reasoning and quantitative illustrative analyses indicate that, for an appropriately chosen EGTS design, chemical interactions will not lead to a significant reduction in porosity and to a loss of gas permeability, and the EGTS should function as required over the 100 ka assessment time frame (Kosakowski & Smith 2014).

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[21] The simulation results for the repository cavern model of Senger & Ewing (2009) provide no indication that significant amounts of high-pH concrete porewater will flow through the seal into the sand/bentonite backfill of the access tunnels.

4.5.6 Concluding remarks on chemical interactions

Potentially safety-relevant chemical interactions in a repository for low and intermediated level wastes are mainly related to the degradation of cement. The impacts of these interactions were assessed on the basis of thermodynamic, kinetic and reactive transport models as well as mass balances. It is shown that within a million years the front of clay dissolution will be ≤ 2 m and in the EGTS the dissolution front will remain at ≤ 0.5 m.

4.6 Dose calculations for specific repository-induced effects

4.6.1 Temperature

The temperature evolution in the L/ILW repository is dominated by the heat pulse generated by cement hydration. Calculations have shown that the temperature peak for the Reference Case does not exceed 76° C and that the peak is only short-lived (Section 4.2). At this temperature, mineralogical changes occur neither in the clay rock nor in the cement matrix. As a result, no temperature effect on dose calculations is to be expected.

4.6.2 Rock mechanics

The hydraulic conductivity of the EDZ around the emplacement caverns is not expected to affect the overall radionuclide transport along the caverns, because the highly porous mortar used to backfill the caverns is likely to have a still higher hydraulic conductivity. Furthermore, the EDZ does not have any significant impact on the vertical transport through the host rock, because its limited radial extent means that the lengths of the vertical host rock transport paths are not significantly reduced. The effects of assuming that the EDZs around the access tunnels and seals are hydraulically highly conductive on water flows and calculated dose rates have been assessed in Poller et al. (2014). The total calculated dose rates are found not to be affected by water flow through the access tunnel system.

The effect of porewater squeezing due to tunnel convergence for the L/ILW repository was addressed in Nagra (2002c) and found to have a negligible effect on calculated dose rates.

4.6.3 Gas pressure build-up

The design of the repository seals and EGTS is intended to ensure that high gas pressures that could give rise to rock damage will not be reached. Nevertheless, gas pressure build-up could in principle have three effects on the long-term safety of a L/ILW repository (Nagra 2008c): i) impact on radionuclide sorption in the host rock, ii) displacement of the porewater and its dissolved radionuclides (Nagra 2008d), and iii) transport of volatile radionuclides (Nagra 2002a, Nagra 2002b, Nagra 2004). These studies have shown that the gas pressure build-up can be controlled by engineering measures such that it does not affect the long-term safety of the host rock. Gas pressure build-up has therefore no effect on the dose calculations. Site specific data will provide a better understanding of the gas pressure build-up in Stage 3 of the SGT.

4.6.4 Chemical interactions

Chemical interactions that take place in a L/ILW repository located in a host rock with diffusion-dominated transport are spatially and temporally limited. The high-pH plume from cementitious materials will take more than one million years to migrate a maximum distance of 2 m into the Opalinus Clay (Kosakowski et al. 2014). As a result, the dose calculations are not affected by the high-pH plume. In addition, any pore clogging that takes place at the cement – clay rock interface will further slow the transport of radionuclides. Owing to the large buffering capacity of the clay rock, no influence on the clay rock sorption capacity is expected. Internal cement degradation and the degradation of organics in the L/ILW are taken into account in the compilation of the cement sorption database (Wieland 2014). The influence of increased salinity (increased concentrations of Na^+, Cl^-, SO_4^{2-}, Mg^{2+}) has also been taken into account in the cement sorption database (Wieland 2014). The solubility limits in the cement matrix in the ILW repository are dependent on the porewater composition, but the latter is strongly buffered by the portlandite present in the cement. Because the diffusive water transport in the Opalinus Clay ensures slow cement degradation, the pH change in the cement is minimal.

Additionally, Poller et al. (2014) show that, for realistic parameter values, radionuclide release along the access structures of a deep geological repository is extremely low. Thus they confirm the reference assumption that radionuclide release occurs predominantly through the host rock.

4.7 Evolution of the repository

The THM-C evolution of the L/ILW repository near field after closure is strongly controlled by the saturation conditions and the pore pressure evolution in the backfilled underground structures and the surrounding host rock. Senger & Papafotiou (*in prep.*) simulated the evolution of the hydraulic state conditions after repository closure for a variety of geological settings. The subsequent discussion of repository evolution refers to the base case simulations in Senger & Papafotiou (*in prep.*). Fig. 4.6-1 displays the gas saturation and the gas pressure distribution in the repository near field from early post-closure times to the late times (after 100'000 years).

Gas saturation after 1'000 years shows that waste-generated gas flows through the backfilled repository structures, accumulates in the emplacement tunnels as well as in the operations, ventilation, perimeter and access tunnels and the facility for underground geological investigations (Fig. 4.6-1 left). Fig. 4.6-1 (right) shows the corresponding pressure distribution after 1'000 years with a rather uniform increase within the different repository structures, with slightly elevated values in the emplacement cavern above hydrostatic conditions.

It is indicated that the gas phase flows through the operations and the access tunnel, driven by the pressure gradient from the emplacement tunnels to the boundary conditions prescribed at the repository ramp, thus reaching the repository seal. At the same time, gas migrates from the tunnels into the surrounding host rock. The gas front reaches the top boundary of the model after 4'000 years, and continues to expand in the model domain, reaching the lateral boundaries between 50'000 and 100'000 years. This indicates that the model no-flow boundaries are located too close to the repository, and limit gas migration farther into the host rock. This, however, provides a conservative approach with respect to the pressure build-up associated with gas accumulation in the repository tunnels and surrounding host rock. Gas saturation in the host rock surrounding the repository continues to increase continuously, reaching a maximum value of approximately 0.015 between the emplacement caverns and after 100'000 years.

Pressures in the repository structures continue to increase after 5'000 years with a more pronounced increase within the emplacement caverns, reaching a peak pressure of 9.32 MPa in the second cavern from the left end of the operations and ventilation tunnels. Consequently, pressures begin to dissipate uniformly and very slowly, with the maximum value decreasing to 9.17 MPa after 100'000 years.

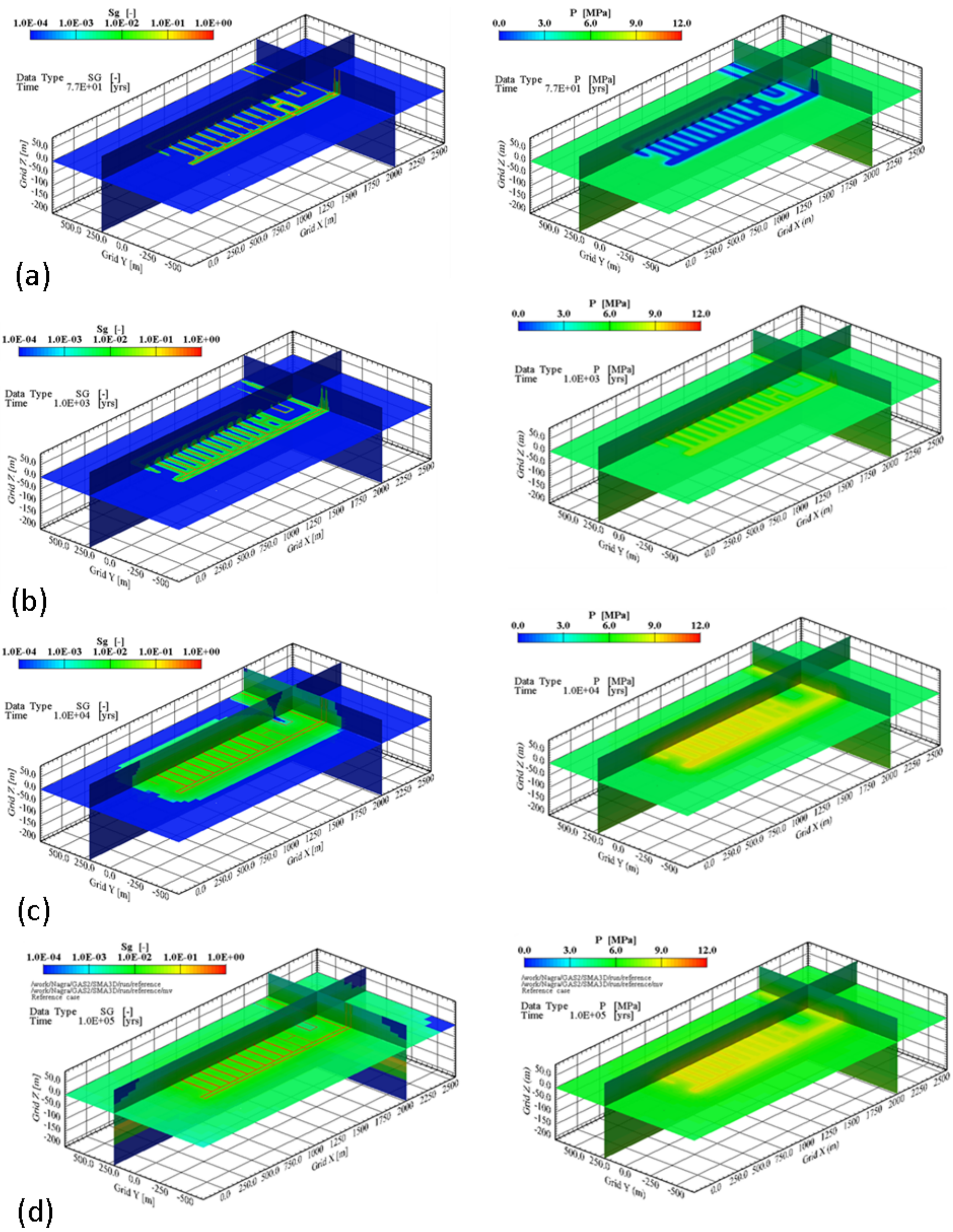

Fig. 4.6-1: Distribution of gas saturation (left) and gas pressure (right) at different time steps: (a) the end of the monitoring phase, (b) after 1'000 years, (c) after 10'000 years and (d) after 100'000 years (base case simulation from Senger & Papafotiou *in prep.*).

100's of years

At the end of the operational phase the backfilled underground structures are largely unsaturated and the pore pressure in the immediate vicinity of the repository is close to atmospheric (Fig. 4.6-1a). At the same time a steep pore pressure gradient is observed in the host rock around the backfilled cavities. Porewater is flowing into the tunnel from the host rock as well as from the repository ramp. After 500 years the pressure build-up due to gas generation in the emplacement caverns becomes discernible, even though the pressure level in the backfilled cavities is yet significantly below hydrostatic conditions. Porewater flow in the host rock is still directed towards the repository. Gas flow predominantly takes place along the EGTS from the emplacement and pilot caverns towards the repository seals.

During this period, the most important processes affecting the near-field evolution are saturation of the concrete and cementitious grouts with groundwater migrating inwards from the host rock. This process initiates dissolution of solids such as portlandite and C-S-H gel within the cement components, together with potential precipitation of ettringite, through reaction of dissolved sulphate and aluminium ions within the rock porewater. Although dissolution of primary cement solids would increase the porosity, the molar volume of ettringite (710 cm^3) compared with portlandite (33.06 cm^3) is such that a net porosity decrease is likely in cement grouts and concrete during this phase of repository evolution.

Cracking of cement grouts and mortars would occur during the early post-closure period, predominantly through the hydration of cements and also as a result of mechanical stresses from the thermal expansion of EBS materials and mineral transformations.

Although the engineered barriers will degrade slowly as a result of the interaction with the groundwater and with each other, they will remain sufficiently intact that they are able to perform their intended safety functions fully. Throughout this period, the near-field porewater would be conditioned to high pH by the dissolution of components of the near-field cementitious materials. Cracking of grouts and mortars is not expected to have a significant impact on the overall performance of the cementitious barriers.

Redox processes will be dominated initially by the consumption of oxygen in entrapped air through the corrosion of steel waste packages and engineered structures such as rock bolts. Goethite is the most likely product of aerobic steel corrosion.

With time, all oxygen will be consumed and steel will corrode anaerobically, leading to the production of hydrogen through the dissociation of water.

Overall therefore, this period of evolution is characterised by initial consumption of dissolved oxygen followed by gas (hydrogen) generation through anaerobic corrosion of steel. There may be small increases in the volume of cement grouts and concretes, with a more substantial expansion of steel corrosion products, potentially leading to cracking of grouts/mortars.

Organic materials within the waste packages will begin to degrade by chemical, microbiological and radiolytic processes before the repository is closed and sealed. Degradation is expected to continue at a slow rate for many years after closure and would lead to the production of gases and radionuclide-complexing agents.

Nevertheless, because of slow steel corrosion rates, there would be a high degree of physical containment of radionuclides resulting from disposal containers maintaining their mechanical integrity over many hundreds of years. The barriers would remain sufficiently intact that they are able to perform their intended safety functions fully. The majority of the degradation reactions that affect the engineered barriers are water-mediated, so limiting the water influx limits both the rate of barrier degradation and the rate at which dissolved contaminants can be transported away from the waste packages.

1'000's of years

After 1'000 years (Fig. 4.6-1b) gas saturation in the backfilled tunnels is yet high and an unsaturated fringe of significant extent starts to develop in the host rock around the repository. Gas pressure in the repository system is expected to increase above hydrostatic, indicating that porewater is being expelled into the host rock and along the EGTS. The maximum gas pressure is observed in the emplacement caverns between 1'000 and 10'000 years after repository closure. Pressure decreased gradually, when the gas front in the host rock has reached the upper confining units (Fig. 4.6-1c).

During this period of evolution, the near field would be characterised by equilibration of the porewater to high pH (pH = 12.5) due to dissolution of portlandite and C-S-H gel from cement, together with chemically-reducing conditions (Eh = -450 mV at pH = 12.5), the latter due to continuing anaerobic corrosion of steel waste packages and engineered structures.

During this phase, $H_2(aq)$ is generated and accumulated in aqueous solution until it reaches the pressure threshold of the system. Once achieved, $H_2(g)$ escapes from the system and redox conditions stabilise. There is a 110 % increase in solid molar volume for the conversion of steel (Fe) to magnetite such that continued expansion of corrosion products would further decrease porosity, potentially inducing cracking of grouts and mortars. Despite these changes in total material volumes the gas storage volume in the pore space is not significantly reduced.

Other near-field materials may take part in redox buffering reactions (e.g. blast furnace slag in cementitious grouts; degradation of organic materials in waste packages) and reactions with these materials also tend to buffer low porewater redox potentials. Microbially-mediated reactions may also influence redox conditions and, again, these reactions tend to drive the system towards chemically-reducing conditions.

Significant volumes of gas (mostly hydrogen, but also some methane and carbon dioxide) may be generated in the near field from the corrosion of the various steel components and the degradation of organic materials in the waste. However, the gas generation rate may be limited by the availability of water. Carbon dioxide is expected to either dissolve or react with the cementitious grouts and mortars. Other gases are likely to accumulate in the near field, within pore spaces in the grout, initially dissolved in porewater, then as a free gas phase as the concentration increases above the solubility limit. Gas migration through the host rock via diffusion is relatively slow, so it is expected that some pressurisation in the near field will occur as a free gas phase develops, but the high-porosity backfill is designed to mitigate the localised build-up of excessive gas pressures and seals will allow the passage of gas whilst restricting the flow of water. In operational tunnels, backfilled with a sand bentonite mixture or crushed Opalinus Clay, microorganisms might find a suitable environment to utilise H_2 gas by reducing sulphate or carbonate in the porewater and so reduce the gas pressure build-up.

Organic material such as cellulose, halogenated and non-halogenated plastics, ion exchange resins and rubber would be present in the wastes. These materials would degrade over time to produce a range of degradation products, some of which might form aqueous complexes with radionuclides in the waste. The formation of such complexes could stabilise the radionuclide in solution, causing an increase in solubility and a reduction in sorption. Cellulose contained in the waste will degrade to a range of water-soluble cellulose degradation products, the most important of which is isosaccharinic acid (ISA). Although ISA can increase actinide solubility many orders of magnitude relative to the situation where ISA is absent, over time concentrations of organic complexants in the waste would be reduced by chemical, radiolytic or microbial degradation as well as by processes such as dilution or sorption.

Continued steel corrosion will eventually lead to the penetration of disposal containers, but radioactive decay (including ingrowth) will contribute to a decreasing inventory of radio-nuclides in waste packages. There may be crystallisation of some amorphous solids in cement grouts and mortars.

100'000's of years

During this period of evolution, the near field would be characterised by long-term chemical conditioning (pH and redox) of porewater, slow mineralisation (ageing) reactions in the cement grouts and mortars that would effectively prevent the migration of the radionuclides through solubility limitation, precipitation, co-precipitation and sorption.

The pH value would slowly decrease from 12.5 to 10 through incongruent (non-stoichiometric) dissolution of C-S-H gel of cement grouts and mortars. Other (mineralisation) reactions occurring would include:

- carbonation through reaction with dissolved bicarbonate ions in groundwater and through the generation of carbon dioxide gas arising from the microbial degradation of organic wastes to form calcite ($CaCO_3$)
- reaction of magnesium in groundwater with calcium-rich minerals to form magnesium hydroxide (brucite, $Mg(OH)_2$)
- reaction of aluminium with calcium and sulphate in groundwater to form sulphate minerals such as ettringite

These reactions may influence both the evolution of the mineralogical composition of the cements and the composition of the cement-equilibrated porewater. The potential significance of such reactions would depend on the composition of the groundwater, the concentrations of the solutes, and volume changes associated with mineralogical changes. The spatial distribution of such precipitates also may influence the evolution of heterogeneity of the near field.

Over this very long timescale, the EBS is not expected to provide complete containment. However, the degraded EBS barriers are likely to continue to retard the release of contaminants to some degree by chemical interactions, although by this time the vast majority of the inventory would have decayed.

The reducing capacity of the L/ILW disposal systems is very large, because of the presence of large amounts of steel (structural supports and disposal containers). In the long-term, steel corrosion would continue to lead to the formation of magnetite, which is the thermodynamically stable iron phase under expected near-field conditions. The redox conditions influence the solubility and sorption of a small number of radioelements. Typically, the solubility of most of these redox-sensitive radioelements tends to be lower, and the sorption stronger, under reducing conditions where lower oxidation states of the elements are thermodynamically more stable, e.g. Tc and Np.

Gas would continue to be produced from the corrosion of metals, but the production rate would be expected to have significantly declined by this time. The pressure curves from the different locations indicate a uniform pressure gradient with increasing distance between the gas source (emplacement caverns) and the outlet of the pathway through the tunnels (repository ramp). Gas saturations at the corresponding locations increase steadily from 50 % (emplacement saturation) to approximately 67 % after 100'000 years (Fig. 4.6-1d).

4.8 Synthesis of the system behavior under site conditions

Deep geological repositories are designed to avoid, minimise or mitigate the impact of potentially detrimental repository-induced effects on long-term safety. In the case of clay rock with a thickness of about 100 m, detrimental effects are limited because chemical and mechanical impacts are largely confined to the rock adjacent to the excavation, thermal impacts are minimal and gas effects can be mitigated by an appropriate design of the L/ILW repository ensuring gas transport in the facility and measures to reduce gas production. Specific measures that are part of the current reference design are discussed in Chapter 5 in relation to their significance with respect to repository-induced effects.

The disposal system described in this report is founded on a system of passive barriers that provide multiple safety functions. The disposal system has been designed to allow for a range of siting conditions. The barriers include the host rock, its surrounding geological setting, the waste forms, drums and the backfill. They have a range of attributes that intrinsically favour safety and that avoid or minimise detrimental phenomena and uncertainties or mitigate their effects. Nevertheless, there are potentially detrimental repository-induced effects that, in the present report, have been investigated and discussed considering a broad spectrum of parameters, reflecting, among other things, the range of potential siting conditions.

In some variant cases of the gas pressure build-up in the L/ILW repository, gas pressure can reach critical values that could potentially harm the integrity of the host rock. These values are more likely to be reached if the EGTS porosity is being partially clogged by mineral precipitation or by the varying parameters associated with the geological conditions, the configuration of the EGTS, and the assumptions regarding gas generation rates. In the case with upper bounding gas generation rates, gas pressures in the L/ILW caverns exceed lithostatic pressures. The results indicate that the depths of 500 and 700 m bgl are less sensitive with respect to gas pressure build-up. Furthermore, the simulations indicate the important role of the EGTS especially in the case of enhanced gas generation rates.

It is shown that pressure build-up directly relates with the capacity of the pathways for gas transport between the main repository and the repository ramp. Results obtained with the sensitivity cases for a repository depth at 500 m bgl indicate that pressure build-up can be modified through the hydraulic properties of the EGTS.

When designing and assessing the performance of a L/ILW repository, the relevant chemical interactions are taken into account. With the current reference design, it is expected that degradation of the cementitious backfill, the concrete tunnel liner and the corrosion of the steel drums and other supporting structures will lead to some alteration of the near field and Opalinus Clay. These detrimental effects are taken into account in dose calculations and have been found not to have a significant impact on the calculated dose rates.

5 Engineering options for mitigating repository-induced effects on long-term safety

The disposal system described in this report is founded on a system of passive barriers that provide multiple safety functions which are well understood and ultimately result in robustness. The barriers include the Opalinus Clay host rock, its surrounding geological setting and also the waste forms, canisters and backfill. The attributes of these barriers intrinsically favour safety, and also avoid or mitigate the impact of potentially detrimental repository-induced effects and their associated uncertainties.

Repository-induced effects and their associated uncertainties have been investigated and discussed in detail in this report. It is concluded that, although not all such effects can be avoided, sufficient safety can nonetheless be achieved. The main arguments to support this conclusion are as follows:

1. For the chosen disposal system, many repository-induced effects can be ruled out because they are shown to be irrelevant for safety through a preliminary assessment of their impact. In particular, qualitative reasoning and quantitative considerations based on prior calculations have shown that, for the chosen disposal system, their domain of influence and/or their effects on radionuclide release are very limited (Chapter 3).
2. Where significant effects on those natural or engineered barriers could not be excluded, a wide range of additional detailed and rigorous analyses have been carried out to quantify their impact. Most of the analyses indicate that the repository barriers would continue to provide their designated safety functions, in spite of a number of conservative or pessimistic assumptions, demonstrating the robustness of the disposal system with respect to the detrimental phenomena and uncertainties considered (Chapter 4).
3. Dose calculations taking into account the potentially detrimental impact of the most significant repository-induced effects have illustrated their limited impact on repository performance (Section 4.6).

Furthermore, the disposal system design incorporates flexibility to allow for different siting conditions, and a range of engineering options exist to further mitigate repository-induced effects, such as measures to reduce gas pressure build-up in the L/ILW repository and avoid critical values that could potentially harm the integrity of the host rock. These measures are described further in the following paragraphs.

Engineering options to mitigate effects related to rock mechanics

The L/ILW emplacement caverns are designed to have sufficient geomechanical stability for safe construction, operation (including backfilling) and closure[22]. This also ensures that only restricted deformation will occur during construction, operation and after closure, thus avoiding large-scale loosening of the host rock. Caverns with smaller diameters would limit the formation of an EDZ but would require more and/or longer caverns for the disposal of the waste and would thus be less efficient for handling and operation.

[22] The optimisation of repository depth is discussed separately (see below).

Engineering options to mitigate effects related to gas pressure build-up

Various engineering measures have been assessed that have the potential to avoid or reduce excessive gas overpressures in the emplacement caverns. As noted in Section 4.4, measures can be taken if needed to reduce the gas production rate (e.g. melting of the metallic waste). In addition, the gas-forming materials can be significantly reduced in the L/ILW caverns (e.g. pyrolysis of organics). Also, the use of steel, e.g. in supporting structures, could potentially be reduced, although there are probably only a few existing materials that could be used as alternatives.

There are also options to increase the gas storage volume and increase the gas transport capacity of the backfilled underground structures. The concept of an engineered gas transport system (EGTS) has been developed, aimed at providing 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 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 relatively high. With the EGTS concept, the gas transport capacity of the backfilled underground structures can be increased significantly without a significant negative impact on their radionuclide retention function.

Engineering options to mitigate chemical impacts

Chemical conditions in the repository, as well as their temporal changes, are driven by the interactions between hydrated cement, steel, aggregates and clays. Considering the chemical nature of the major materials involved, two processes dominate: reactions of cement minerals with aggregate/clays and the corrosion of iron.

By using aggregates with a low SiO_2 content (e.g. carbonate gravel) the detrimental interactions with cement resulting in precipitates, e.g. at the interface to the sand/bentonite in the EGTS, could be effectively mitigated.

The cement recipe can be adjusted to some degree to reduce the amount of alkali leached into the clay and thus reduce the pH in the porewater. It can also be adjusted to resist sulphate attack by increasing the amount of silica, preventing the formation of ettringite minerals.

Engineering options to mitigate the mutual influence between the sections of a combined repository

In Appendix A of Leupin et al. (2016), it is shown that the main conclusions regarding the repository-induced effects in a combined L/ILW and HLW repository are basically the same as for separate L/ILW and HLW repositories. The mutual influence between the L/ILW and HLW sections of the repository can be limited by ensuring an adequate spatial separation between the two sections, although this increases the space required for the combined repository. In the current stage of planning, the reference minimum horizontal distance between the emplacement caverns of the two sections is taken to be 200 m.

Optimisation of repository depth

Feasibility and safety can – in principal – be ensured also at greater depth. By following a precautionary approach, however, the repository depth should be limited to avoid damage to the host rock. With increasing depth a larger EDZ might result from stress redistribution during excavation leading to an additional pore volume around the near field and expressed in terms of an enhanced EDZ porosity.

Repository-induced effects might influence the overall performance of the L/ILW repository with increasing depth: the higher degree of rock compaction makes the rock less permeable to gas (Section 4.4) that may result in higher gas overpressures. But these processes might be counterbalanced by increased rock strength at greater repository depths. Increasing mean effective stresses at greater repository depths will also result in a need for substantial engineered structures for supporting the emplacement tunnels which will as well positively affect the gas pressure build up.

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Appendix A: Pore volume change in a L/ILW repository due to corrosion

Corrosion in a L/ILW repository

Metallic waste in the L/ILW repository includes decommissioning waste, reactor fittings, operational waste etc. Based on the MIRAM 2014 inventory (Nagra 2014d), the L/ILW repository contains 6.68×10^7 kg metallic and 3.01×10^6 kg organic waste. Under repository conditions (anoxic and alkaline environment), the metals corrode slowly at a well-documented corrosion rate (Diomidis 2014). For reasons of simplification and because steel is the largest metallic component in the L/ILW caverns (80 vol. %), iron is taken as a model element to calculate the volume increase due to corrosion. According to the reaction below, anaerobic iron corrosion will lead to the formation of magnetite (Fe_3O_4), which has according to a Pilling-Bedworth ratio a larger molar volume than metallic iron of ca. 2.1.

$$3\ Fe(s) + 4\ H_2O \rightarrow Fe_3O_4(s) + 4\ H_2(g)$$

The amount of Fe_3O_4 produced can be estimated using the H_2 gas production rates. These H_2 gas production rates can be derived from the corrosion rates (Diomidis 2014) and the conversion factors described in Diomidis (2014). The amount of Fe_3O_4 can be estimated based on the stoichiometric reaction and the volume of $H_2(g)$ produced.

Initial pore space in a L/ILW repository

The following mass balance approach allows the estimation of volume changes considering a K09 cavern design (Fig. A-1) with an average container density of 50 m^3/TM (tunnel meter). The cavern contains different types of concrete (mortar, filling concrete, shotcrete etc.) that are characterised by different porosities (Nagra 2008a). Tab. A-1 gives an overview of the porosities for the different concretes used in the cavern and the resulting pore volume per tunnel meter (TM).

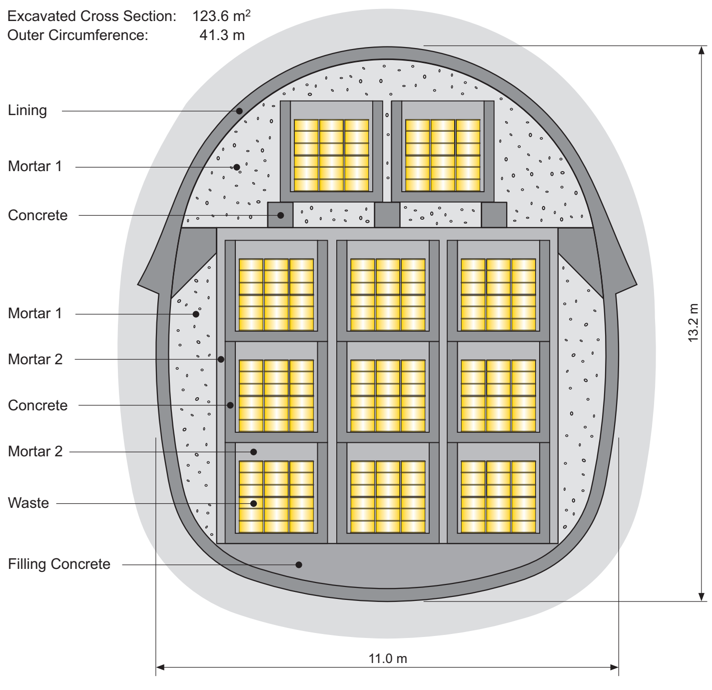

Fig. A-1: Cavern K09 with 11 LC1 containers.

Tab. A-1: Overview of materials in cavern K09 with various concrete materials and their porosities.

From Nagra (2008a).

Material	**Volume** [m^3/TM]	**Porosity** [%]	**Pore space** [m^3/TM]
Mortar for backfill	29.4	30	8.82
Mortar in crane columns void space	15	30	4.6
Mortar in LC	8.8	30	2.6
Shotcrete	12.3	25	3.07
Filling concrete	9	20	1.8
Bulkhead	2.3	20	0.46
Concrete bedding	1.1	20	0.22
Disposal container	7.8	20	1.56
Waste matrix	37.5	20	7.5
Total volume	123.6	23.8	30.695
Total volume of a K09 cavern excluding shotcrete and filling concrete	102.3	24.3	25.82

A total initial pore space of 25.82 m^3/TM is used in the following calculations, together with the input data shown in Tab. A-2.

Tab. A-2: Material properties of iron and magnetite: input data to calculate the volume of Fe_3O_4 per TM and year.

	Molecular weight [g/mol]	**Density** [kg/m^3]
Fe	55.85	7580
Fe_3O_4	231.55	5175

Results

The cumulative Fe_3O_4 volume increase as a function of time is given in Fig. A-2. The figure also shows that, after approximately 160'000 years, all iron has corroded and the Fe_3O_4 increase comes to a halt. The corresponding cumulative volume of Fe_3O_4 formed after 160'000 years is 3.11 m^3/TM. This means that, with an average initial pore space of 25.82 m^3/TM, there will be 22.71 m^3/TM pore space left after 160'000 years. Based on these mass balances, a complete clogging of the pore space in the cementitious environment does not seem likely and enough pore space remains present for the storage of gases. However, it is possible that locally the pore space is filled with precipitates and is no longer accessible to gases as discussed in detail in Sections 3.4 and 4.5.

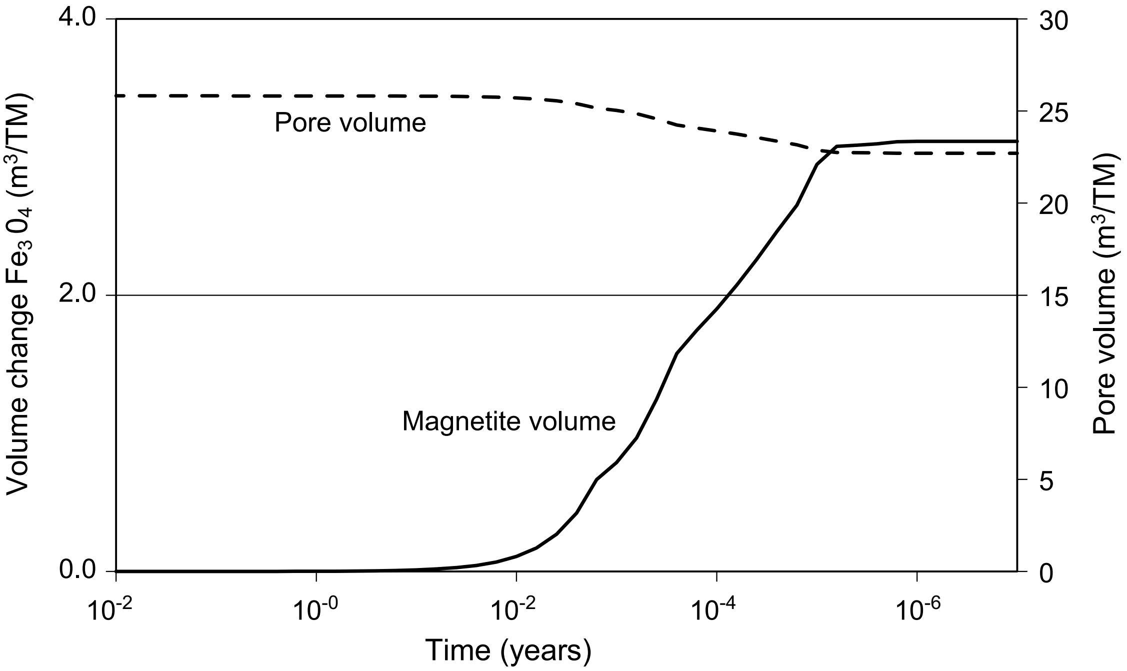

Fig. A-2: Evolution of pore space and magnetite volume in a L/ILW repository as a function of time.

Concluding remarks

The gas production rate that was used in these calculations is an average rate that takes into account the corrosion rate of different metals and the degradation of organic substances (Papafotiou & Senger 2014). These rates therefore slightly overestimate the gas production rate due to iron corrosion, since they also include, in particular, the production of methane from organic compounds. However, the latter makes up only 5 vol. % of the total gas volume, therefore these gas production rates are considered as a good approximation for the total process.

In these calculations, any other porosity reducing or increasing effects such as degradation of cement or organics are neglected.

Clogging of pores resulting from the corroding steel may decrease the overall porosity by around 12 %. Enough pore volume remains though for the storage of gases at all times.