



TECHNICAL REPORT 24-23

Production and Fate of Gases in the
Geological Repository

September 2024

**Nagra | National Cooperative for the
Disposal of Radioactive Waste**

Hardstrasse 73 | 5430 Wettingen | Switzerland
T. +41 56 437 11 11 | info@nagra.ch | nagra.ch



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The report "Production and Fate of Gases in the Geological Repository" has been elaborated by a project team consisting of A. Papafotiou¹, T. Guillemot¹, H. Javanmard¹, N. Diomidis¹, D. Zbinden², U. Lengler², K. Luu² & P. Marschall¹

¹Nagra

²Intera

An earlier version of the report has been reviewed and commented on by Séverine Levasseur (NIRAS/ONDRAF), Eleonora Crisci (Nesol), Jose Bosch (Nesol) and Mikey Hannon (Hannon Clean Energy). The authors would like to thank them for their valuable contributions.

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Abstract

In a deep geological repository for radioactive waste, corrosion of various metals and alloys will lead to the formation of hydrogen. In addition, organic materials will slowly degrade and generate carbon dioxide, methane and other gaseous species. Depending on local conditions, gaseous species can be consumed by chemical reactions and by microbial activity. If the resulting rate of gas generation exceeds the rate of migration of gas dissolved in the porewater of the engineered barriers or the host rock, the solubility limit will be reached, and a separate gas phase will form. The accumulation and release of gases can influence the long-term evolution of the repository.

This report addresses the so-called gas synthesis that encompasses an assessment of the hydraulic evolution associated with the production and fate of gases in the combined repository at the Haberstal site. The main objectives are to:

- present a comprehensive synthesis of processes and phenomena related to the production and fate of gases in the repository;
- assess the hydraulic evolution under consideration of the transport of gases in the repository structures;
- demonstrate the functionality of the provisional repository design with respect to gas and deterministically assess associated uncertainties that affect the hydraulic evolution; and
- provide underlying argumentation for the performance assessment of the repository and the subsequent derivation of safety scenarios and analyses of radiological consequences.

The assessment of gas generation and fate in the repository builds on the previous gas synthesis report from Stage 2 of the three-stage Sectoral Plan for Deep Geological Repositories. Compared to Stage 2, the current report makes advancements in particular to:

- assess the gas-related evolution of the combined repository based on the current disposal concept and phenomenological evolution;
- implement the site-specific repository configuration in accordance with the current Swiss disposal concept;
- update the waste inventory and material inventory in support structures from the provisional design of a combined repository;
- update and comprehensively survey new data for corrosion rates of metals and degradation of organics;
- update gas generation modelling and calculate new scenarios;
- implement integrated model-based analyses of gas transport for the total system (the entire repository) as well as repository components and simulate new scenarios.

The modelling workflow from gas generation to gas transport in the repository allows for a comprehensive assessment of the fate of gas and its impact on the hydraulic evolution. The quantitative analysis is achieved through model metrics that are key inputs for the performance assessment. The analysis is undertaken by means of deterministic simulation variants, in this report termed “assessment cases”, which encompass uncertainties, evaluations of the provisional design and scenarios. The integration of assessments at repository and component scales allows for more detailed insights into the thermo-hydraulic effects in the near-field and in the repository sealing system, the implementation of a firm abstraction methodology for the model-based assessments, and the development of argumentation for the performance assessment.

This report provides an enhanced understanding of the repository system in terms of hydraulic evolution. The synthesis of results demonstrates sensitivities to the deviations considered in the assessment cases, and key processes underpinning the phenomenological evolution of the repository. The main outcome herein is a consistent hydraulic evolution of the repository that adheres to the provisional design principles and associated transport regimes for all considered cases. The key message is that gas pressures in the combined repository are moderate even for pessimistic cases of gas generation and accumulation in the repository.

Zusammenfassung

In einem geologischen Tiefenlager für radioaktive Abfälle führt die (anoxische) Korrosion verschiedener Metalle und Legierungen zur Bildung von Wasserstoff. Darüber hinaus entstehen durch den langfristigen Abbau von organischen Materialien Kohlendioxid, Methan und andere gasförmige Stoffe. Je nach den örtlichen Bedingungen können diese Gase durch chemische Reaktionen oder mikrobielle Aktivität verbraucht werden. Wenn die Gasbildungsrate die Transportrate des im umgebenden Porenwasser gelösten Gases übersteigt, wird die Löslichkeitsgrenze erreicht, bildet sich eine separate Gasphase. Akkumulation und Freisetzung von Gasen können die langfristige Entwicklung des Tiefenlagers beeinflussen.

Diese vorliegende Synthese fasst die sicherheitsbezogenen Analysen zur Entstehung, Akkumulation und Freisetzung von Gasen im Kombilager am Standort Haberstal zusammen. Die wichtigsten Ziele des Berichts sind:

- Eine umfassende Synthese der Prozesse und Phänomene im Zusammenhang mit der Entstehung und Freisetzung von Gasen im Tiefenlager,
- Die sicherheitsbezogene Beurteilung der hydraulischen Entwicklung des Tiefenlagers und des Transports von Gasen entlang der untertägigen Bauwerke,
- Der Nachweis der Funktionalität der provisorischen Lagerauslegung in Bezug auf die Gasfreisetzung, verbunden mit einer Beurteilung der sicherheitsbezogenen Ungewissheiten mittels deterministischer Methoden,
- Bereitstellung der zugrunde liegenden Argumentation für die Prüfung der Barrierenwirksamkeit des Tiefenlagers und die anschließende Ableitung von Sicherheitsszenarien und Analysen der radiologischen Folgen.

Die Beurteilung der Gasentstehung und -evolution im Tiefenlager stützt sich auf den früheren Gassynthesebericht aus Etappe 2 des dreistufigen Sachplans geologische Tiefenlager. Im Vergleich zu Etappe 2 zeigt der aktuelle Bericht vor allem Fortschritte in folgenden Bereichen auf:

- Beurteilung der gasbezogenen Entwicklung des Kombilagers auf der Grundlage des provisorischen Tiefenlagerkonzepts und der phänomenologischen Entwicklung;
- Umsetzung der standortspezifischen Tiefenlagerkonfiguration gemäss dem aktuellen Schweizer Entsorgungskonzept;
- Aktualisierung des Abfallinventars und des Materialinventars für den Tunnelausbau basierend auf der provisorischen Auslegung eines Kombilagers;
- Aktualisierung und umfassende Darstellung der neuen Daten für die Korrosionsraten von Metallen und zum Abbau von organischen Stoffen;
- Aktualisierung der Modellierung der Gasproduktion und Berechnung neuer Szenarien; und
- Durchführung integrierter modellbasierter Analysen des Gastransports für das gesamte Tiefenlagersystem sowie für einzelne Komponenten des Tiefenlagers und Simulation neuer Szenarien.

Der integrierte Modellansatz von der Gasproduktion bis zum Gastransport im Tiefenlager ermöglicht eine umfassende Beurteilung der Freisetzung der Gase sowie der Auswirkungen auf die hydraulische Entwicklung des Lagersystems. Die quantitative Beurteilung erfolgt durch Modellmetriken, die wichtige Inputs für die Prüfung der Barrierenwirksamkeit darstellen.

Die Analyse erfolgt mittels deterministischer Simulationsvarianten, in diesem Bericht als «Beurteilungsfälle» bezeichnet, die Unsicherheiten, Bewertungen des provisorischen Designs und Szenarien umfassen. Die Integration von Beurteilungen auf Tiefenlager- und Komponentenebene ermöglicht detailliertere Einblicke in die thermohydraulischen Effekte im Nahfeld und in das Verschlussystem des Tiefenlagers, die Einführung einer soliden Abstraktionsmethodik für die modellgestützte Beurteilungen und die Entwicklung von Argumenten für die Prüfung der Barrierenwirksamkeit.

Dieser Bericht ermöglicht ein besseres Verständnis des Tiefenlagersystems im Hinblick auf die hydraulische Entwicklung. Die Synthese der Ergebnisse zeigt die Sensitivitäten gegenüber den in den Bewertungsfällen berücksichtigten Abweichungen auf, sowie die Schlüsselprozesse, die der phänomenologischen Entwicklung des Tiefenlagers zugrunde liegen. Die Kernaussage ist, dass die Gasdrücke im Kombilager selbst für pessimistische Fälle von Gasbildung und -akkumulation im Tiefenlager moderat sind.

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List of Acronyms

AD or ARD	Argillaceous Dogger
AGT	Waste packages types (<i>Abfallgebindetyp</i>)
ATW	Alpha-toxic waste (<i>ATA</i>)
AV	Alternative value
BEVA	Spent fuel encapsulation plant (<i>Brennelementverpackungsanlage</i>)
BWR	Boiling water reactor
BZL	Swiss Federal Interim Storage Facility (for radioactive waste from medicine, industry and research; <i>Bundeszwischenlager</i>)
CM	Calcareous Malm
CRZ	Containment-providing rock zone
DOGG	Dogger
ELB	Disposal canister (<i>Endlagerbehälter</i>)
ENSI	Swiss Federal Nuclear Safety Inspectorate (<i>Eidgenössisches Nuklearsicherheitsinspektorat</i>)
EUU	Facilities for underground investigations (<i>erdwissenschaftliche Untersuchungen untertag</i>)
GBM	Granular bentonite material
HLW	High-level waste (<i>HAA</i>)
IER	Ion-exchange resin
IFD	Integrated finite differences
KEG	Nuclear Energy Act (<i>Kernenergiegesetz</i>)
KEV	Nuclear Energy Ordinance (<i>Kernenergieverordnung</i>)
L/ILW	Low- and intermediate-level waste (<i>SMA</i>)
LMW	Low-molecular weight (organics)
MIR	(radioactive waste from) medicine, industry and research
MIRAM	Model Inventory of Radioactive Materials
ML	Marly Lias
MM	Marly Malm
MOX	Mixed oxide (fuel)
NL	Nördlich Lägern (potential siting region for the deep geological repository)
NPP	Nuclear power plant
NZA	Auxiliary access facility (<i>Nebenzugangsanlage</i>)
OFA	Surface facility (<i>Oberflächenanlage</i>)
OFI	Surface infrastructure (<i>Oberflächeninfrastruktur</i>)

OPA	Opalinus Clay
PA	Performance assessment
PMMA	Poly(methyl) metacrylate
PVC	Poly(vinyl) chloride
PWR	Pressurised water reactor
RBG	General licence application (<i>Rahmenbewilligungsgesuch</i>)
RP-HLW	High-level waste from reprocessing
RV	Reference value
SCAD	Sandy calcareous argillaceous Dogger
S/B	Sand/bentonite (mixture)
SCD	Sandy calcareous Dogger
SEM	Scanning electron microscopy
SF	Spent fuel (assembly)
SFOE	Swiss Federal Office of Energy
SGT	Sectoral Plan for Deep Geological Repositories (<i>Sachplan geologisches Tiefenlager</i>)
SOB	Shuttle overpack canister (<i>Shuttle-Overpack-Behälter</i>)
SP	Superplasticiser
SSC	Structures, systems and components
TH	Toussaint-Heintzmann
TH ²	Two-phase thermo-hydraulic
TLB	Transport and storage cask (<i>Transport- und Lagerbehälter</i>)
VA	Encapsulation plant (<i>Verpackungsanlage</i>)
WG1/WG2	Waste Group 1 / Waste Group 2
ZWILAG	Zwischenlager Würenlingen AG (interim storage facility)

1 Introduction

1.1 Background

In Switzerland, legal regulations (Nuclear Energy Act (KEG 2003) and Nuclear Energy Ordinance (KEV 2004) and guidelines are in place for the management of radioactive waste. The Nuclear Energy Ordinance (KEV) classifies Switzerland's radioactive waste into low- and intermediate-level waste (L/ILW), alpha-toxic waste¹ (ATW) and high-level waste (HLW), the latter comprising spent fuel (SF) and vitrified HLW from reprocessing (RP-HLW). The Nuclear Energy Act (KEG) requires the disposal of all these types of radioactive waste in deep geological repositories. The feasibility of this disposal solution has been demonstrated for L/ILW in Nagra (1985) and for long-lived intermediate-level waste and HLW in Nagra (2002a).

The Sectoral Plan for Deep Geological Repositories (SGT) regulates the search for suitable siting regions for deep geological repositories in Switzerland. This site selection process is conducted in three stages (BFE 2008). Stages 1 and 2 have already been completed and Nagra is currently in Stage 3 (SGT-E3). Clarifications on the safety-related specifications for this stage are provided in ENSI 33/649 (ENSI 2018), while ENSI Guideline G03 and the corresponding explanatory report (ENSI 2020b, ENSI 2020a) specify the protection objective, protection criteria and design principles for deep geological repositories.

In SGT-E3, three siting regions located in Northern Switzerland have been considered – Jura Ost (JO), Nördlich Lägern (NL) and Zürich Nordost (ZNO) – with the objective of selecting one siting region for an HLW repository, one for an L/ILW repository, or one for a combined repository for all waste types.

Following a comparison of these siting regions, Nagra concluded that NL is the safest and most flexible siting region and is therefore applying for a general licence for a combined repository for both HLW and L/ILW at the Haberstal site.

The justification for this selection and the safety demonstration for a repository at the site are submitted as part of the general licence application (RBG²). The reports relating to post-closure safety, shown in Fig. 1-1, are structured as follows:

- The overall safety-related argumentation, including post-closure and operational safety, is summarised in an overarching safety report ("*Sicherheitsbericht*") NTB 24-01 (Nagra 2025b) shown at the top of Fig. 1-1.
- The upper left side of Fig. 1-1 shows the reports supporting Nagra's site comparison. The available options are compared with respect to safety and technical feasibility and the results are synthesised in NTB 24-03 (Nagra 2025a) ("*Bericht zur Begründung der Standortwahl*").
- The upper right side of Fig. 1-1 shows the reports documenting the post-closure safety case for the combined repository at the site, including its synthesis in the post-closure safety report NTB 24-10 (Nagra 2024g).
- The lower part of Fig. 1-1 shows a report that presents the safety and repository concept, including the provisional design, and reports providing the assessment basis.

¹ According to Nagra (2024a), ATW can coexist with L/ILW within the same emplacement caverns. As a result, for the sake of simplicity, the term L/ILW encompasses ATW without explicit mention.

² From the German *Rahmenbewilligungsgesuch*.

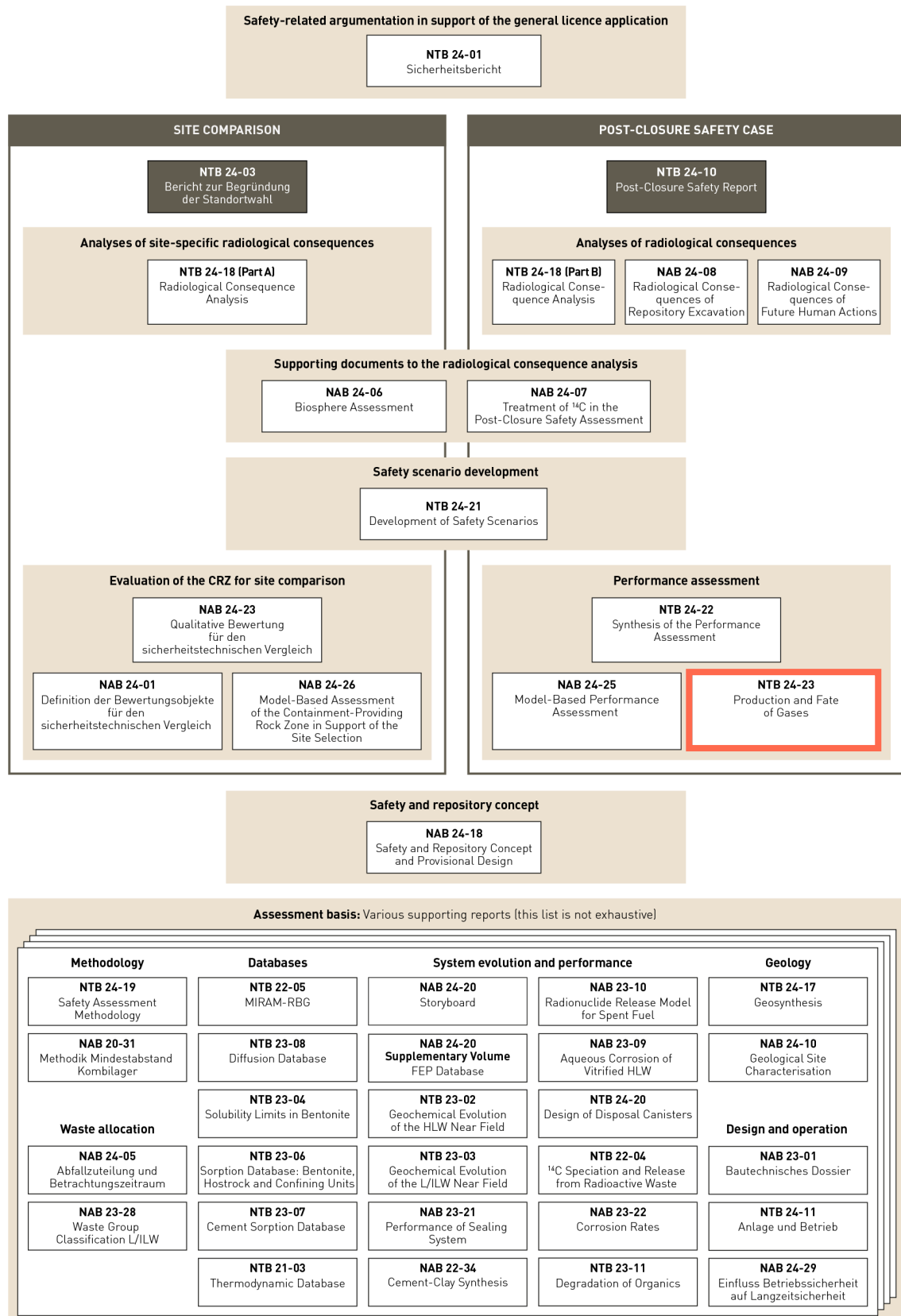


Fig. 1-1: Structure of reports covering post-closure safety aspects of the site comparison and the post-closure safety case

The post-closure protection objective for a deep geological repository is the permanent protection of humans and the environment (KEG 2003, ENSI 2020b). The protection objective, design principles, protection criteria and the safety and repository concept inform the iterative design development process. This process leads to a provisional design and implementation plan for a combined repository at the Haberstal site, to serve as the basis for the post-closure safety case and underlying safety assessment (as documented in the reports shown on the upper right side of Fig. 1-1). The safety assessment consists of four main processes:

- **performance assessment (PA)**, in which the thermal, hydraulic, mechanical, and chemical evolution of the repository system is analysed,
- **safety scenario development**, which entails the identification and description of a set of safety scenarios that capture uncertainty in initial state and subsequent evolution of the repository system over time,
- **analysis of radiological consequences**, which consists of an evaluation of radionuclide release rates to the surface environment as a function of time, and
- **demonstration of post-closure safety**, in which evidence, arguments and results from the three previous steps are brought together in the post-closure safety report (cf. Fig. 1-1).

1.2 Scope of the present report

The present report is bordered in red in Fig. 1-1. It is part of the PA and aims at a comprehensive description of the two-phase thermo-hydraulic (TH²) evolution of the repository under consideration of the production and fate of gases in the provisional repository design.

1.2.1 Objectives

To achieve this goal, the objectives set forth in the present report can be summarised as follows:

- Obj1: a comprehensive synthesis of the repository components and processes relevant to the production and fate of gases in the deep geological repository;
- Obj2: a quantitative assessment of the hydraulic evolution of the repository under consideration of accumulation and transport of gases in the repository structures;
- Obj3: a demonstration of the functionality of the provisional design with respect to gas including a deterministic assessment of associated uncertainties affecting the hydraulic evolution of the repository;
- Obj4: underlying argumentation basis for the PA of the repository, the subsequent derivation of safety scenarios, and the analysis of radiological consequences from the release, retention and transport of volatile radionuclides through the repository barriers.

1.2.2 Methodology

The approach followed for the gas synthesis comprises two main components, namely:

- The underpinning scientific database, including a synthesis of materials and processes that determine (i) the production of gases in the repository structures, and (ii) the fate of gases in the repository and surrounding environment.
- The assessment of the hydraulic evolution, including the transient generation and transport of gas in the repository system.

Although the synthesis of the scientific database precedes the assessments of repository evolution, these two components are not decoupled, and the workflow towards the assessment is not unidirectional. The description of materials in the database corresponds to their expected characteristics at emplacement and shortly thereafter, but the changes they might undergo after closure are implicitly accounted for in the assessment of the evolution through tailored assessment cases. Similarly, the processes considered in the database are derived from the phenomenological description of the evolution of the repository (Nagra 2024f). In addition to the phenomenological description, the gas synthesis draws information from different components of the safety case. The waste inventory is provided by MIRAM-RBG, documented in Nagra (2023c). The provisional design of the current repository project is described in Nagra (2024h). The stratigraphy and lithology of the host rock and its confining geological units are summarised in the geosynthesis report (Nagra 2024d). The synthesis of the performance of the repository system, including options and bandwidths in the barriers, is given in the PA synthesis report (Nagra 2024i). The present report provides explicit description only of those sections that are essential to the gas synthesis, with references to these sources placed accordingly throughout the report.

The generation and transport of gases over the timescales considered by the PA depend on a multitude of coupled processes taking place in the wide range of porous materials present in the repository and surrounding geological environment. For that reason, assessments of the hydraulic evolution are performed with the aid of mathematical and numerical models. Depending on the purpose, different modelling tools are developed on the scale of the entire repository or on the scale of individual repository components. The implemented workflow integrates the repository- and component-scale tools and allows to elaborate a range of model-based assessments that draw a comprehensive picture of the hydraulic evolution of the repository.

1.2.3 Report outline

The report is structured as follows. Chapter 2 describes the deep geological repository and its components according to the provisional design, including the inventory of waste and materials emplaced in the repository upon its closure. Chapter 3 is dedicated to the processes and mechanisms determining the generation, consumption, and transport of gases in the repository. Chapter 4 describes the assessment methodology, including the modelling workflow and tools implemented for performing the assessment. Chapter 5 focuses on the assessment itself, with a detailed description of the assessment cases and the respective modelling results. Finally, Chapter 6 gives a synthesis of the results and main conclusions of the report.

The objectives stated in Section 1.1.1 are addressed as follows. Objective *Obj1* is addressed in Chapters 2 to 4. Objectives *Obj2*, *Obj3*, *Obj4* are addressed in Chapters 4, 5, and 6.

2 The combined repository

2.1 Overview

The following paragraphs describe the provisional Nagra project for a deep geological repository for combined disposal as documented in Nagra (2025b). This exemplified project is the basis for the analyses documented in the present report. New findings made before the construction work begins (e.g., underground geological investigations, advances in technology and materials science, experience in other programmes, etc.), will lead to the project being adapted for the purposes of optimisation and industrialisation.

The provisional Nagra project for the combined repository envisages two repository sections, one for HLW (consisting of SF and RP-HLW) and one for L/ILW (including ATW) co-located at the same site as illustrated in Fig. 2-1. The underground facilities of the repository in the provisional layout described here are located roughly in the middle of the Opalinus Clay layer, at a depth between 800 and 900 m below ground level (b.g.l.).

The repository will include a series of dead-end emplacement drifts for HLW and dead-end emplacement caverns for L/ILW. The drifts and caverns are accessed by interconnected underground openings, including operations, ventilation, and access tunnels, facilities for underground geological investigations (EUU) and the shafts that connect the repository to the surface. However, the HLW emplacement drifts will be spatially separated from the L/ILW emplacement caverns such that interactions between the two parts are minimised. The waste emplacement rooms will be backfilled in parallel with the emplacement of the waste, and a sealing system will be installed to close the repository.

Sections 2.2 and 2.3 provide a general overview of the L/ILW and HLW emplacement rooms, respectively. A general description of the sealing and backfill system implemented in the repository is given in Section 2.4. More detailed schematic illustrations, including the dimensions of the waste emplacement rooms, waste packages, and elements of the seals, are given in App. A.

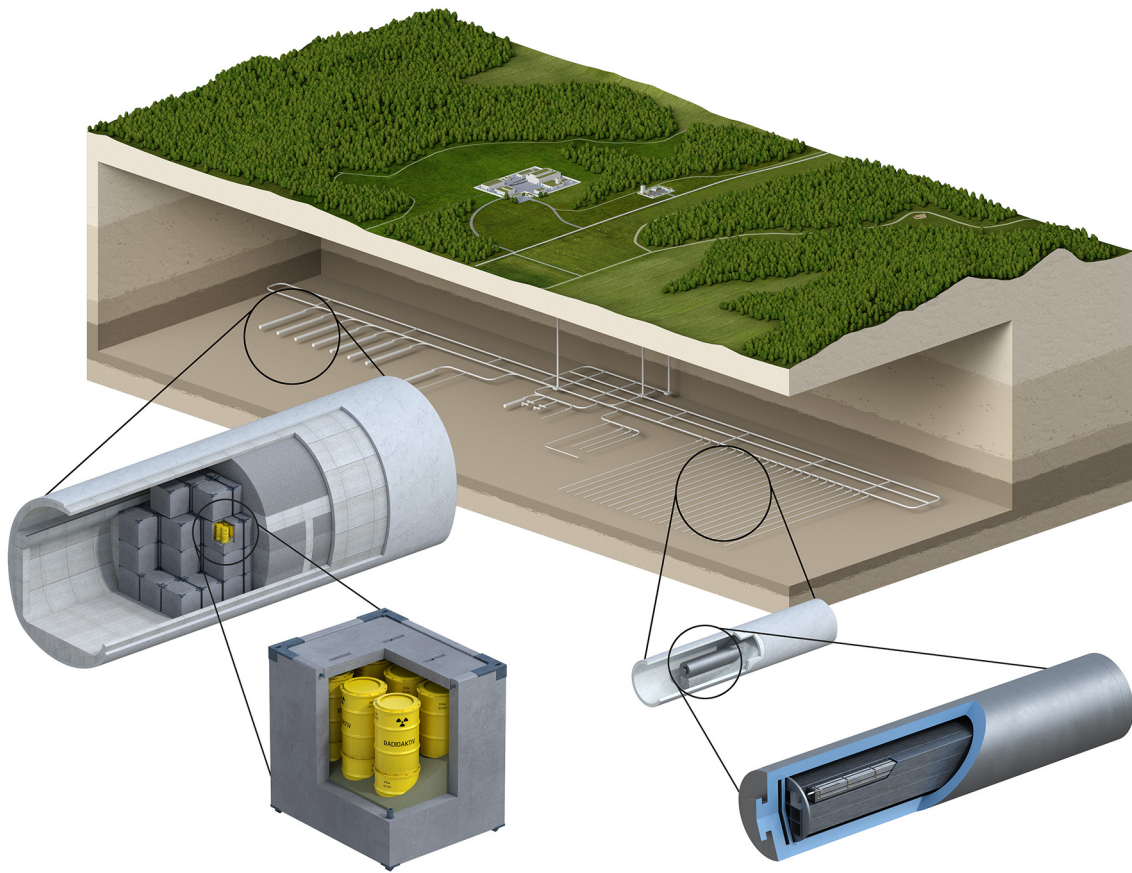


Fig. 2-1: Schematic view of the provisional repository design with the L/ILW emplacement caverns (left) and the HLW emplacement drifts (right)

2.2 L/ILW repository

A schematic view of an L/ILW emplacement cavern is shown in Fig. 2-1. The ~ 240 m long caverns will have a cross-section of approximately 12.5 m × 13.5 m (see App. A), supported by rock bolts and a two-shell lining made of sprayed reinforced shotcrete and unreinforced concrete. The disposal containers will be stacked in arrays and the void spaces between the cavern walls and the containers as well as gaps between containers will be filled with a porous cementitious mortar. In the model-based assessments presented in this report, it is assumed that disposal containers correspond to type LC-86H (Nagra 2023c, see also App. A). The emplacement caverns are accessed from the operations tunnel through branching tunnels with an area for unloading and receiving disposal containers at the mouth of the cavern (see App. A).

2.3 HLW repository

A schematic view of an HLW emplacement drift is shown in Fig. 2-1. The ~ 800 m long drifts will have a diameter of about 3.2 to 3.9 m (see App. A), including prefabricated concrete liner segments (tubing) to provide support. The gap between the tubing and the rock will be filled with mortar material. The disposal canisters (cf. Section 2.5) will be emplaced every 3 m on pedestals made of compacted bentonite blocks. The remaining space between the disposal canisters and the tubing will be backfilled with granular bentonite material.

The emplacement drifts will be accessed from the operations tunnel through branching tunnels with an area for transferring the waste into the drifts.

2.4 Sealing and backfill system

The design of the sealing and backfill system is key to the fate of gases and the repository performance with regard to gas-induced effects. An overview of the provisional design is given in Section 2.4.1, followed by a more detailed description of individual components in Section 2.4.2. In addition to App. A, further information on the provisional engineering design and functions of the sealing system are given in Martin et al. (2023).

2.4.1 Overview

The sealing and backfill system will include multiple individual seals as well as the backfilling of all underground openings (Fig. 2-2). The current repository concept foresees the following types of seals:

- V1 seals, which will be placed at the entrances to the HLW emplacement drifts and L/ILW emplacement caverns. As explained later in this section, the notations V1-HLW and V1-L/ILW have been adopted due to different requirements and, accordingly, design options put in place for these seals.
- V2 seals, which will close off the disposal areas for HLW and L/ILW, as well as the pilot repositories, after the waste has been emplaced. Similar to the V1 seals, the notations V2-HLW and V2-L/ILW have been adopted.
- V3 seals, which will be placed in the access, ventilation and operation shafts to seal the repository from the surface environment and protect it from external impacts.

Backfill material will be emplaced in the underground openings between these seals. Backfill material VF1 will be emplaced between the V1 and V2 seals and backfill material VF2 will be emplaced between the V2 and V3 seals.

The operations tunnel will be closed with a V3 seal immediately after emplacement of all V2 seals. The access and ventilation shafts will be closed later, again with V3 seals, after the end of the final monitoring phase.

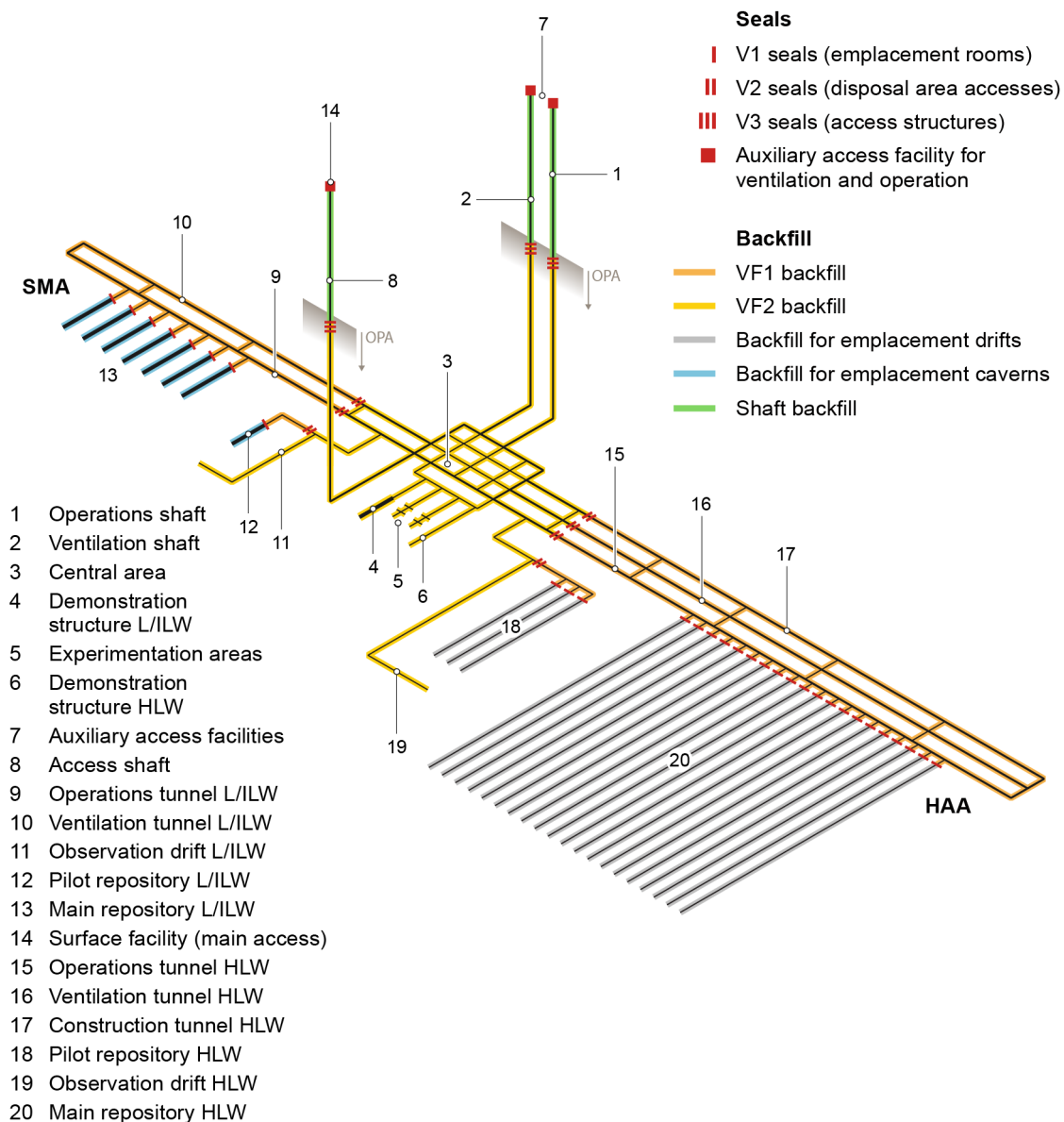


Fig. 2-2: Location of the closure structures in the combined repository

From Nagra (2022).

2.4.2 Description of seals

The V1-L/ILW seal consists of the following elements (listed in the direction of cavern to tunnel):

- A section containing backfill mortar is followed by a transition layer, which serves to physically separate the sand-bentonite sealing element (see below) from the cement to limit chemical interactions. The transition layer may consist of calcareous aggregates and calcareous sand and is supported by partitioning walls.
- A sealing element consisting of a mixture of 70 – 80% sand and bentonite (S/B). The sealing section is currently designed to allow the release of gas generated within the repository, but also to limit water flow across the seal.

- After the sealing element, a second transition layer is installed, similar to the first one.
- At the end of the seal, a concrete abutment is emplaced in situ, which is keyed into the tunnel liner and surrounding Opalinus Clay. Its primary function is to act as the main load-bearing element.

The V1-HLW seal is similar but is currently designed with lower hydraulic conductivity of the sealing element (i.e., bentonite material) and a second concrete abutment with adjacent transition layers on both sides. The concrete abutments in the V1-HLW seal can be shorter than in the V1-L/ILW seal due to the smaller tunnel diameter.

The V2-L/ILW seal is very similar to the V1-L/ILW seal. Instead of the interface to the backfill mortar, the V2-L/ILW seal has a second concrete abutment with adjacent transition layers on both sides.

The V2-HLW seal differs from the V2-L/ILW seal in the sealing element, where a lower hydraulic permeability (i.e., bentonite material) is employed to further limit water flows.

The V3 seal consists of the following elements (listed in the direction of the repository to the ground surface):

- A lower abutment made of hard rock ballast (i.e., limestone rubble) filling the entire shaft sump and vertically upwards to over three times the height of the tunnel at the base of the shaft.
- A transition layer used to separate the lowermost sealing element (see bullet below) from the lower abutment.
- Sealing elements consisting of bentonite material in the form of granules, pellets, shaped blocks or a combination of these, with low hydraulic conductivity. Every ten metres, the sealing elements are interrupted by filter layers of fine sand contributing to the even saturation and swelling of the bentonite material.
- A second transition layer used to separate the uppermost sealing element from the upper abutment (see below).
- An upper abutment composed of non-reinforced, high-quality structural concrete able to absorb swelling pressure from the sealing element below and hydrostatic pressure of the overburden water above.

2.5 Waste inventory

The inventory of all of Switzerland's radioactive waste that exists today and prognoses for the waste to be produced in the future is compiled in the database called "Model Inventory of Radioactive Materials" (MIRAM). A dedicated release of MIRAM was prepared in support of the RBG, called MIRAM-RBG (Nagra 2023c). Within MIRAM-RBG, the individual waste packages are classified into L/ILW, ATW and HLW (including SF) in accordance with the Nuclear Energy Ordinance (KEV 2004). They are also grouped by waste package types (AGTs from the German term "Abfallgebindetyp") having similar radiochemical characteristics and waste category (i.e., operational, decommissioning, reprocessing and reactor waste). MIRAM-RBG also includes information about the type (i.e., inorganics, metals and organics) and geometry of materials present in the waste form, infill and containers for each AGT.

This section provides an overview of the materials that generate gas, based on the waste inventory. Section 2.5.1 especially describes the gas-producing L/ILW, while the gas-producing HLW is listed in Section 2.5.2.

2.5.1 L/ILW

L/ILW arises during the operation and decommissioning of nuclear power plants (NPPs) and also as a result of medical, industrial and research activities (MIR waste). It includes inorganics, metals and organic materials, respectively representing ~ 62%, ~ 36% and ~ 2% of the total L/ILW mass, including the waste form, containers and backfill (Nagra 2023c). L/ILW AGTs are classified into two groups, Waste Group 1 (WG1) and Waste Group 2 (WG2) (German term: Abfallgruppen AG1 and AG2), respectively referring to waste that either does or does not contain substances in concentrations relevant enough to reduce radionuclide retention and impair cement (Nagra 2023b).

2.5.1.1 Inorganic materials

A total of 113 inorganic materials are listed in MIRAM-RBG, with almost all of them being present in L/ILW (Nagra 2023c). They are generally assumed to not contribute to gas generation during the course of degradation.

However, Cloet et al. (2014) and Nagra (2023b) mention that one of these inorganic materials, the Prussian blue or $\text{Fe}_4[\text{Fe}(\text{CN})_6]_3$, can degrade and generate CO_2 and CH_4 (cf. Section 3.3; Tab. C-2). A total of $\sim 1.3 \times 10^3$ kg of $\text{Fe}_4[\text{Fe}(\text{CN})_6]_3$ is inventoried only in L/ILW (Nagra 2023c).

In the previous study of Cloet et al. (2014) about waste group classification using chemical criteria, ashes resulting from incineration were assumed to contain 5 wt.% of residual organic substances, as complete incineration could not be confirmed. These residual organics could therefore be subject to degradation, generating CO_2 and CH_4 . In the context of this report, this assumption is no longer taken into consideration as any organic substances remaining after incineration at extreme temperatures are expected to be refractory and therefore not degradable in conditions relevant for a cementitious L/ILW repository.

2.5.1.2 Metals

The metals and alloys present in L/ILW (including waste form and containers), correspond to the large majority (~ 94%) of the L/ILW materials generating gas.

A total of 51 metals and alloys are inventoried in MIRAM-RBG (Nagra 2023c). These metallic materials can be grouped according to their corrosion properties (Tab. 2-1). Iron and carbon steel form the largest corrosion group of L/ILW metals and represent ~ 77% of their total mass (Fig. 2-3; Tab. 2-1). They are followed by stainless steel and Ni alloys, that reach ~ 13% of the total mass of metallic materials disposed of in L/ILW caverns. Aluminium, lead, copper and Zircaloy contribute ~ 4%, ~ 4%, ~ 1% and ~ 1%, respectively. The other groups (i.e., zinc, unclassified metals³ and magnesium) cumulatively represent less than ~ 0.1% (Fig. 2-3; Tab. 2-1).

³ Unclassified metals comprise materials that are not relevant in terms of mass and/or are not expected to corrode under the expected repository conditions.

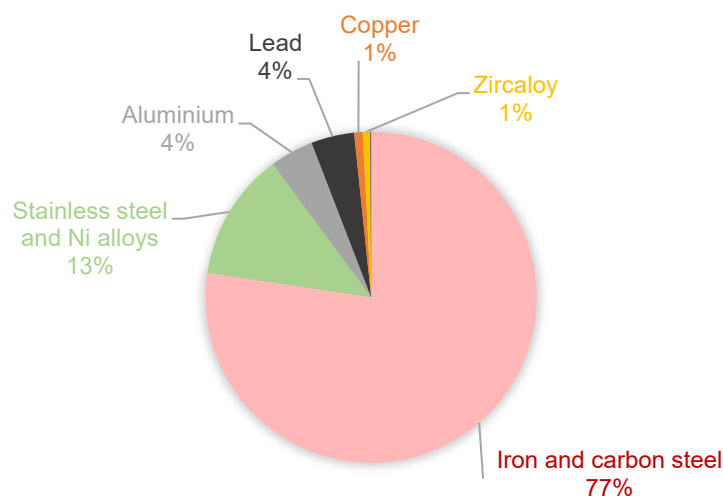


Fig. 2-3: Mass distribution of the corrosion groups disposed of in L/ILW caverns
Including metals from waste form and containers. Based on Nagra (2023c).

Tab. 2-1: Grouping and amounts of metallic L/ILW materials
Based on Nagra (2023c).

Metals present in L/ILW	Mass (kg)
Iron and carbon steel	3.3E7
Stainless steel and Ni alloys	5.3E6
Aluminium	1.8E6
Lead	1.8E6
Copper	3.5E5
Zircaloy	3.0E5
Zinc	2.6E4
Unclassified	1.5E4
Magnesium	8.5E2
Total	4.2E7

The complete list of metals and alloys disposed of in the L/ILW repository, their respective amounts and the corresponding corrosion group are provided in App. B.1.

2.5.1.3 Organic materials

A total of 48 organic substances are listed in MIRAM-RBG (Nagra 2023c) and were regrouped into 43 main classes (Guillemot et al. 2023). Organics are almost exclusively part of the waste form (i.e., ~ 95%), whereas only a very small portion is present in the conditioning materials and in tunnel support, such as cement additives.

Ion-exchange resins (IERs; including polystyrene and styrene), polyvinyl chloride (PVC), bitumen, plastics (including polyethylene, polypropylene, polyester and polycarbonates), cellulose, poly(methyl) metacrylate (PMMA, or commonly known under the trademark name Plexiglas®) and superplasticisers (SPs, mainly polycarboxylates) are the principle organic materials in terms of mass (Nagra 2023c). They respectively contribute ~ 45%, ~ 23%, ~ 14%, ~ 6%, ~ 3%, ~ 1% and ~ 1% of the total mass of organics (including the waste form and filling materials) as shown in Fig. 2-4. The remaining 7% are distributed among all the other organic materials found in MIRAM-RBG (Nagra 2023c).

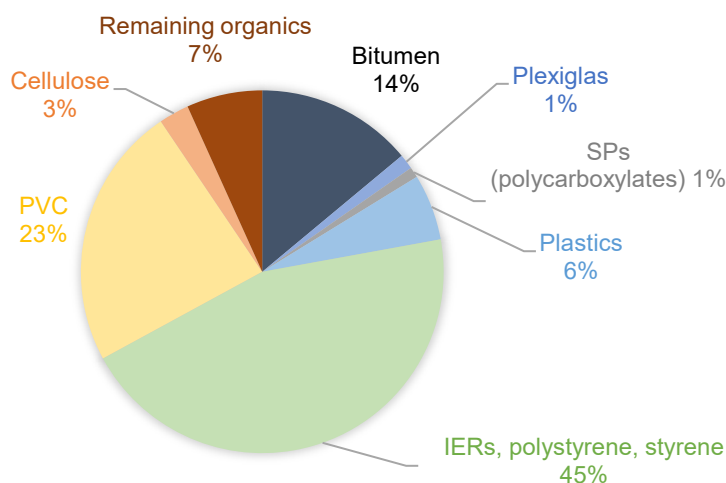


Fig. 2-4: Mass distribution of organic materials

Based on the waste package type inventory published in Nagra (2023c).

Based on their chemical structure and associated degradation rates, two categories of organic materials were defined (Cloet et al. 2014). O1 organics represent easily degradable organic compounds such as non-polymeric and short-chained molecules (i.e., cellulose), while O2 organics are less degradable substances like long HC-chained and aromatic polymers (i.e., IERs, polystyrene, PVC, bitumen, plastics and Plexiglas®). In MIRAM-RBG, the O2 group corresponds to ~ 92% of the total mass of organics present (Nagra 2023c). Based on new experimental data on the degradation of cellulose (Small et al. 2017), the O1 group has been recently subdivided into two subclasses: O1a including cellulose, polyester and polycarbonates and O1b with low-molecular-weight (LMW) organics (Guillemot et al. 2023). This classification, however, represents a simplification of the complexity of the degradation processes that organic waste undergoes in an L/ILW repository (cf. Section 3.2.1). The general lack of experimental data for the degradation of organics in conditions relevant for a cementitious L/ILW repository does not allow the definition of a rate for each organic material.

A complete list of organics, including their chemical formulae, group and associated mass is available in App. C.

2.5.2 HLW

In HLW, metals are the materials that predominantly contribute to gas generation. Inorganics are not expected to generate gas during their course of degradation and only 34 kg of organics are inventoried, corresponding to $8 \times 10^{-5}\%$ of the total mass of HLW materials that are expected to produce gas.

A total of 11 metals and alloys are inventoried in HLW (Nagra 2023c). As for L/ILW metals, they can be grouped based on their corrosion properties (Tab. 2-2). Iron and carbon steel form the largest corrosion group of HLW metals and represent $\sim 97\%$ of their total mass (including waste form, backfill and canisters). They are followed by Zircaloy and stainless steel, which only reach $\sim 3\%$ and $\sim 1\%$ of the total mass of HLW, respectively (Fig. 2-5; Tab. 2-2). The other groups (i.e., aluminium, lead, copper, and zinc) cumulatively represent $\sim 7 \times 10^{-3}\%$.

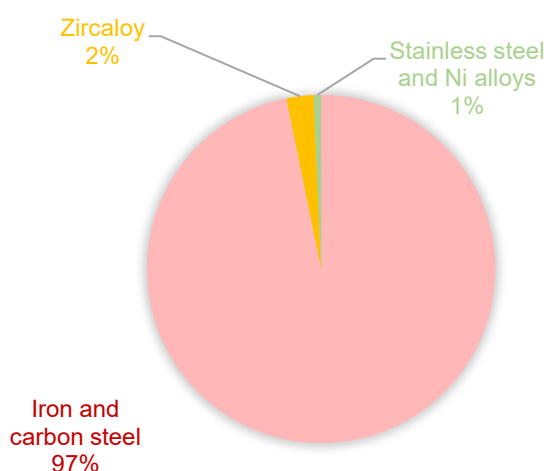


Fig. 2-5: Mass distribution of the corrosion groups disposed of in HLW emplacement drifts Including metals from waste matrices and containers. Based on Nagra (2023c).

Tab. 2-2: Grouping and amounts of metallic HLW materials
Based on Nagra (2023c).

Metals present in HLW	Mass (kg)
Iron and carbon steel	4.1E7
Zircaloy	1.1E6
Stainless steel and Ni alloys	2.9E5
Aluminium	2.8E3
Lead	1.4E2
Copper	2.1E1
Zinc	2.1E1
Total	4.3E7

The complete list of metals and alloys disposed of in the HLW repository, their respective amounts and the corresponding corrosion groups are provided in App. B.2.

2.6 Construction materials

In the current concept for the Swiss deep geological repository, metals will also be used as building materials for tunnel support, concrete reinforcement and shaft lining. A total mass of $\sim 7.6 \times 10^7$ kg is foreseen to be used based on the provisional design. This is the average value of a so-called *optimistic* and a so-called *pessimistic* scenario of 7.5×10^7 kg and 7.7×10^7 kg, respectively (App. B.3). Based on this, metals used for the construction correspond to $\sim 47\%$ of the total metal mass foreseen in the repository (including L/ILW and HLW matrices, backfilling, containers and canisters). Steel fibres, anchors, ribs and reinforced steel for cast-in-place concrete are expected to be made of carbon steel and can be classified in the corrosion group of iron and carbon steel. On the other hand, the steel lining of the shaft is foreseen to be stainless steel. However, the steel lining of the shafts where the V3 seals will be installed is planned to be removed prior to repository closure. Therefore, the amount of steel corresponding to the lining of the shafts is not relevant to gas-induced effects or safety and is excluded from the calculations of gas generation rates.

3 Gas generation, consumption and transport processes

Modelling the hydraulic evolution of the deep geological repository relies on the phenomenological description of coupled processes associated with the production, consumption, and transport of gases in the repository structures and surrounding rock. The mechanisms, reactions, and resulting corrosion rates for metallic materials are described in Section 3.1. The degradation of organic and inorganic materials is addressed in Sections 3.2 and 3.3, respectively. Finally, processes responsible for the consumption of gas are discussed in Section 3.4, and the fundamentals of gas transport in porous media, with a focus on clay materials relevant to the planned repository, are described in Section 3.5.

3.1 Corrosion of metallic materials

3.1.1 Mechanisms

Metallic corrosion in an aqueous environment is an electrochemical process involving two separate, but coupled, half-reactions proceeding simultaneously. The oxidation reaction of the metal produces metal ions and liberates electrons, resulting in material loss. The produced electrons are subsequently consumed by the reduction reaction, thus preserving electrical neutrality. During the operational phase and during the early stages after repository closure, the corrosion of metallic materials will proceed by the reduction of O_2 until all available O_2 in the repository has been consumed. In the absence of O_2 or other oxidising agents, the consumption of electrons will occur by the reduction of water, which results in the production of H_2 and is thus a source of gas. In the present study, the oxidation of metallic materials due to the presence of O_2 or other oxidants, before and shortly after repository closure, is conservatively disregarded. Consequently, all the available metallic materials contribute to H_2 generation and the associated gas pressure buildup.

For the majority of the engineering metals and alloys, general corrosion results in low-solubility corrosion products that tend to precipitate and form layers on the surfaces of the metals. Such layers form the interface between the metal and the environment and thus play a critical role in determining the nature and rate of the interfacial electrochemical reactions involved in further corrosion. The composition and properties of such surface layers depend on the metal, the environment and local conditions. In some cases, the presence of surface layers, which can be more or less uniformly distributed over the metal surface, can shield the metal from the environment and hence considerably decrease its corrosion rate.

In the context of corrosion, the main difference between the L/ILW and HLW repository sections is the chemical environment of the near-field (cf. Chapter 2). In the L/ILW repository section, cement grout is used as backfill material and the porewater that will be in contact with it will be strongly alkaline. In contrast, bentonite is used as a buffer around the disposal canisters in the HLW repository section, and the pH of the porewater in contact with it will be near neutral. In the approach used in the present report, the difference in the pH of the environment influences the corrosion rates of some materials but is not assumed to influence the corrosion mechanisms.

3.1.2 Reactions

For the estimation of gas pressure in the deep geological repository over time, it is necessary to define the stoichiometry of the corrosion reactions under anoxic conditions, generating only H_2 as gaseous species.

The following stoichiometric reactions are assumed for the different corrosion groups defined in Section 2.5. Even though metals foreseen for disposal in the deep geological repository are mainly alloys containing a principal alloying element plus various additional ones, each group is represented by a single element and a single stoichiometric reaction for the calculation of the number of H₂ moles produced for one mole of corroded metal. The defined stoichiometry generally results in a conservative assessment of the volume of generated H₂.

Iron and carbon steel

The product of the corrosion of iron and carbon steel under anoxic conditions is defined as magnetite Fe₃O₄ and formed via:



An alternative corrosion product under anoxic conditions is ferrous hydroxide Fe(OH)₂, which results in only 1 mole of H₂ per mole of corroded Fe. The assumption that Fe₃O₄ is the stable corrosion product is hence conservative in terms of gas generation.

Stainless steel and Ni alloys

Stainless steels and Ni alloys contain various elements, including Fe, Ni, and Cr, with Fe as the main constituent of stainless steel and Ni as the main constituent of Ni alloys. It is assumed that the corrosion product of the corrosion of both stainless steels and Ni alloys is Fe₃O₄ with the same stoichiometry as Reaction 3-1.

This assumption results in a conservative assessment of H₂ production from the corrosion of the Ni and Fe constituents, if Ni(OH)₂ and Fe(OH)₂ are the respective stable corrosion products. While this leads to an underestimation of the amount of H₂ produced by the corrosion of Cr and by forming Cr(OH)₃, it is expected to be balanced by the overestimation of the amount of H₂ produced by the corrosion of Fe and Ni. Overall, it is considered that the assumption of the formation of Fe₃O₄ results in a realistic or slightly conservative assessment.

Aluminium

Based on the Pourbaix diagram for the Al-H₂O system (Pourbaix 1974), the predominant oxidation state for corroded aluminium for the entire range of pH and redox potential expected in the context of a deep geological repository is +3. Therefore, the stoichiometry can be represented by:



Lead

Similarly, the predominant oxidation state for corroded lead over the pH and redox potential range of interest is +2 (Pourbaix 1974). The corrosion reaction can be expressed as:



Zircaloy

The predominant oxidation state for zirconium for the pH and redox potential range expected in the near-field of a deep geological repository is +4 (Pourbaix 1974). The corrosion reaction could hence be represented by:



It is conservatively assumed that 100% of the H₂ produced contributes to gas generation and that no H₂ remains, i.e. it is neither absorbed in the metal nor present in the form of zirconium hydride.

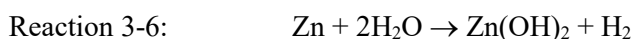
Copper

Copper is not expected to corrode under anoxic conditions (Diomidis & King 2022). However, a finite upper bound corrosion rate was defined (cf. Section 3.1.3), for the purposes of which the corrosion product is assumed to be Cu₂O:



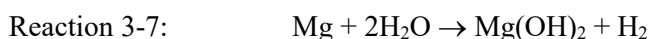
Zinc

Zinc corrodes in the +2 oxidation state over the entire pH and redox potential range of interest (Pourbaix 1974). The corrosion reaction stoichiometry is given by:



Magnesium

Finally, magnesium dissolves in the +2 oxidation state for the pH and redox potentials in the conditions relevant for a deep geological repository (Pourbaix 1974). The corrosion reaction can be represented by:



3.1.3 Rates

The corrosion rates of metals are usually not constant with time. They are initially high and tend to decrease as the surface layers (made of corrosion products) thicken and their protective character increases. After some time, which can be up to a period of several years, a steady state is reached in which the rate of layer growth is equal to the rate of its dissolution, and thus the thickness of the surface layer and the corrosion rate of the metal remain stable. Since the time required to reach the steady state is small compared with the time period under consideration for safety assessment (i.e., 10⁵ years for the L/ILW repository and 10⁶ years for the HLW repository), the corrosion rates of metals are assumed to be constant at their steady state values for the whole assessment period.

The corrosion rates given in Tab. 3-1 include a best estimate, as well as lower and upper bounding rates. The best estimates represent the average of selected corrosion rates available in the literature and from Nagra's own experiments. The lower and upper bound corrosion rates reflect the evolution of the near-field conditions and local inhomogeneities. They usually correspond to the lowest and highest reported values from relevant corrosion studies found in the literature. The corrosion rates were selected based on duration and environmental conditions, reflecting the different environments metallic materials may be exposed to during disposal in a deep geological repository. As an example, pH-dependent corrosion rates are used, reflecting the effect of pH differences due to variability in the disposal environment (i.e., L/ILW and HLW repository sections) or due to the carbonation of cement. The scientific basis for the definition of the corrosion rates, including the full list of selection criteria, are discussed in detail in Diomidis et al. (2023).

Tab. 3-1: Reference corrosion rates for metallic materials predominantly present in MIRAM-RBG

From Diomidis et al. (2023).

Materials	Environment	Lower bound	Best estimate	Upper bound
		(nm/a)		
Iron and carbon steel	pH $\geq$ 10.5	0.03	6	20
	pH < 10.5	0.3	1E3	7.5E3
	In compacted bentonite	26	3E2	7E2
Stainless steel and Ni alloys	pH $\geq$ 10.5	2E-2	0.6	1.4
	pH < 10.5	0.2	0.4	1
Aluminium	pH $\geq$ 10.5	10	6.4E4	3E5
	pH < 10.5	7E3	7E3	7E3
Lead	pH $\geq$ 10.5	0	0	0.5
	pH < 10.5			
Zircaloy	pH $\geq$ 10.5	0.4	3	9
	pH < 10.5	1.5	2.3	3
Copper	pH $\geq$ 10.5	0	0	5E-2
	pH < 10.5	0	0	0
Zinc	pH $\geq$ 10.5	90	1.5E2	2E2
	pH < 10.5			
Magnesium	pH $\geq$ 10.5	8E2	1.1E4	2.8E4
	pH < 10.5			

It should be noted that, based on data from MIRAM-RBG (Nagra 2023c), the amount of graphite in the emplaced waste is insignificant and, consequently, the impact on the corrosion rates is deemed to be negligible.

The milieu of the compacted bentonite environment is specifically assigned to the outer surface of the HLW canisters, assigning specific corrosion rates with lower uncertainty in such an environment.

3.2 Degradation of organic materials

3.2.1 Mechanisms

In order to estimate the impact of organic materials on gas generation, a comprehensive literature review on the abiotic and biotic degradation of organic materials under conditions relevant to an L/ILW repository was conducted in Guillemot et al. (2023). A short summary of the main degradation processes expected to occur are provided below.

Almost exclusively present in L/ILW, organics are subjected to three possible abiotic degradations in addition to biotic degradation: (i) irradiation (radiation-induced degradation); (ii) hydrolysis in alkaline conditions (chemical degradation); and (iii) thermal degradation.

The resistance of the different types of polymers to radiation is largely determined by their chemical structure. In general, polymers with aromatic groups in their molecular structure have a significantly higher radiation resistance than aliphatic polymers, regardless of the position of the aromatic groups in the chain. In the case of the less degradable O2 organics, the consequence of the radiation-induced degradation is expected to be mainly cross-linking, further improving their chemical stability by forming a three-dimensional network of polymer chains. In the case of the easily degradable O1 organics, scission or fragmentation of the polymers into LMW compounds is likely more important. Radiation-induced degradation of organics is expected to be predominant only during interim storage and at early stages after repository closure, due to the initial dose rate in the waste form, which also contains residual O₂ and water. After repository closure and when conditions are anoxic, the chemical stability of the carbon backbone of the main O2 organics may have improved over time due to predominance of the radiation-induced cross-linking mechanism. As O2 represent ~ 92% of the total mass of organics present (Nagra 2023c) (cf. Section 2.5.1.3), a significant proportion of the organic waste is therefore expected to be unsusceptible to subsequent degradation.

Hydrolysis is considered as the most important abiotic degradation process, taking place since interim storage, especially in the waste packages backfilled with cementitious materials where highly alkaline conditions prevail. However, only few organic compounds such as cellulose, polyester, and PC, not being the most abundant in the L/ILW inventory (Nagra 2023c), are susceptible to degradation by alkaline hydrolysis.

In the current concept, with the repository located at ca. 900 m below ground level, “pure” thermal degradation of organic wastes, occurring only at strongly enhanced temperature (i.e., above 200 °C for pyrolysis), is considered of no importance. In the temperature range expected in the L/ILW repository section following repository closure (i.e., between ~ 25 °C and ~ 60 °C; Papafotiou & Senger 2016), the radiation-induced and alkaline degradation rates are only slightly influenced by the temperature and increase by a factor of below ~ 2.

The biotic degradation of organics by microbial activities is expected to be initially limited after L/ILW repository closure due to (i) the highly alkaline conditions present in the cemented waste forms and surrounding cementitious backfill (pH ~ 12.5); (ii) the low water availability (only in the waste form); (iii) the limited nutrient accessibility; and (iv) the strong radiation field. Unfortunately, the impact of microbial activity on the degradation of organics cannot be accurately assessed. In general, it can be assumed that the more extreme conditions coexist (the highly alkaline conditions, low water availability and nutrient accessibility, and strong radiation field), the less likely microbial activity should be. However, it should be noted that methanogenesis is possible from a thermodynamic point of view up to pH 12.5, and low water availability per se does not completely inhibit microbial life. Due to the heterogeneity of the waste and conditioning processes, small-scale niches may exist where conditions for microbial activity are favourable. This could be the case at the bottom of the emplacement caverns, where resaturation occurs more

quickly, or in waste packages solidified by bitumen or styrene, where near-neutral to slightly alkaline conditions prevail. Due to limited water availability and pore space, a slow spread of microbes from these niches is to be expected. Over time, microbial activity may increase due to: (i) the presence of LMW molecules which could be used as substrates, produced by hydrolysis and from the radiation-induced scission and fragmentation processes; (ii) the weakened radiation field; (iii) the slow resaturation of the caverns from the bottom, thereby increasing water availability, and (iv) the increase in the number of small-scale environments with lower pH due to ongoing internal degradation and carbonation of the solidifying cementitious matrix.

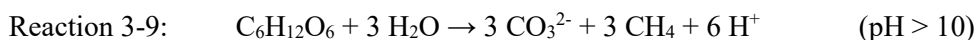
It should be noted that water availability is considered to be the most important limiting factor for all the abiotic and biotic processes of degradation described above.

In general, only limited relevant empirical data regarding the stability and degradation mechanisms of organic compounds are currently available from experiments, since the majority of the organics degrade very slowly and because experimental conditions are often not comparable with those expected in the repository. Moreover, the conditions in the waste packages might not be entirely homogeneous, and different degradation paths may occur.

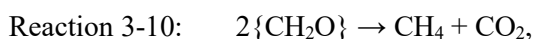
3.2.2 Reactions

Initially, Wiborgh et al. (1986) assumed that the degradation of organics in an L/ILW repository will most likely take place by a combination of hydrolysis and microbial degradation. Hydrolysis reduces the molecular size of complex polymers before microorganisms degrade them mainly via methanogenesis, producing equimolar amounts of CH₄ and CO₂ as final products.

Methanogenesis can be illustrated by the following reactions, using the glucose molecule as substrate:



which could be simplified as follows:



where {CH₂O} represents an average composition of organic materials.

Depending on the redox potential of the environment and the presence of electron acceptors, several microbial degradation reactions can take place before methanogenesis. For example, if NO₃⁻ and SO₄²⁻ are present in the repository system, other degradation reactions, i.e., denitrification and SO₄²⁻ reduction, would occur in place of methanogenesis, reducing the amount of CH₄ and CO₂ produced (Hooker 2007). Only a small portion of the organic matter is expected to decompose by microbial degradation using NO₃⁻, Fe(III), SO₄²⁻ and Mn(IV) as terminal electron acceptors, as the estimated amounts in the waste materials and cement paste are always lower than required for the microbially mediated oxidation of the organic materials (Kosakowski et al. 2014).

Consequently, the decomposition of organic matter is expected to occur predominantly via methanogenesis in the long term. This approach is further consistent with the notion that at complete thermodynamic equilibrium, CO₂ (or its aqueous species HCO₃⁻ and CO₃²⁻) and CH₄ are the thermodynamically stable carbon species in anoxic alkaline conditions (Wieland & Hummel 2015). The disproportionation of organic matter into CO₂ and CH₄ was further used to estimate the amount of gas produced during the degradation of organics (Cloet et al. 2014). This process was assumed to depend on the carbon content and the average oxidation state of carbon in the organics, while no dependence on pH was considered.

The degradation equations of the organic materials inventoried in MIRAM-RBG defining the numbers of CO₂ and CH₄ moles produced per mole of organic are available in Tab. C-2. As CO₂ is expected to react with cement-based engineering elements of the L/ILW repository, CH₄ is expected to contribute more significantly to the gas pressure.

It should also be noted that hydrolysis such as methanogenesis requires water. The amount of water available is therefore crucial for estimating the kinetics of organic matter degradation and the rate of gas generation (Wieland et al. 2018, Wieland & Kosakowski 2020).

3.2.3 Rates

After an extensive literature review on the possible degradation processes of organic materials occurring in the near-field of a cementitious L/ILW repository (Guillemot et al. 2023), no information about the kinetics of degradation have been found, except for cellulose for which only two studies are available and show controversial results (i.e., five orders of magnitude difference) (Van Loon & Glaus 1998, Pavasars et al. 2003).

Furthermore, only a limited number of degradation experiments have reported gas generation rates from the degradation of organics and of these few studies, to date, none have been conducted under highly alkaline conditions relevant to an L/ILW repository near-field. Most of the rates available concern gas generation from cellulose degradation, while only few studies provide gas generation rates measured during the degradation of IERs, PVC and bitumen. Due to the lack of data, assigning gas generation rates to single materials, except cellulose, is not pursued. Hence, the simplified classification into easily degradable (O1) and slowly degradable (O2) organics was retained (Guillemot et al. 2023). The only difference compared to the approach in SGT-E2 concerns the classification of two plastics polyester and polycarboxylates, recently classified with the easily degradable O1 organics as they are prone to hydrolysis, in contrast to the other plastics and O2 organics in general (Guillemot et al. 2023).

The gas generation rates for less degradable (O2) and easily degradable (O1) organics are listed in Tab. 3-2 and justified in detail in Guillemot et al. (2023). Since SGT-E2, the upper bounds were set to the highest generation rates measured for the group of organics considered, equal to 0.05 mol gas/kg a⁻¹ for O2 (asphalt) and 0.7 mol gas/kg a⁻¹ for O1 (cellulose). For the best estimate rates, the reference rate of 0.005 mol gas/kg a⁻¹ was retained for O2 due to the lack of new experimental data. The O1 group was subdivided into two subclasses (Guillemot et al. 2023): O1a regrouping cellulose, polyester and polycarboxylates, and O1b with low-molecular-weight organics, each having best estimate rates of 0.07 mol gas/kg a⁻¹ and 0.02 mol gas/kg a⁻¹, respectively. The lower bounds correspond to the lowest generation rates measured for the group of organics considered as, in contrast to SGT-E2, it was assumed that degradation can occur (to a more or less important extent) for all considered organics in the near-field of a cementitious L/ILW repository over the period for assessment (Guillemot et al. 2023). In the case of the O2 organics, the lower bound was set to 1×10⁻⁶ mol gas/kg a⁻¹, while it was fixed at 3×10⁻⁴ mol gas/kg a⁻¹ for both O1a and O1b organics.

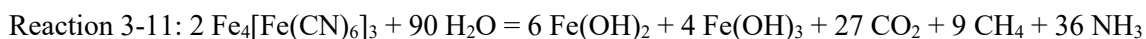
Tab. 3-2: Gas generation rates for less (O2) and easily (O1) degradable organics
From Guillemot et al. (2023).

Organic groups	Upper bound	Best estimate	Lower bound
	(mol gas/kg a ⁻¹)		
O2	0.05	0.005	1E-6
O1a	0.7	0.07	3E-4
O1b	0.7	0.02	3E-4

Based on gas generation rates, a simplified kinetic model of the degradation of O1 and O2 organics was developed by Wieland et al. (2018), using the same stoichiometric approach as Cloet et al. (2014). The gas generation rates could be accordingly converted into degradation rates of the organics.

3.3 Degradation of inorganic materials

As cyanide is highly soluble in alkaline solutions and can be degraded by gamma irradiation, and as microbial decomposition of hexacyanoferrate cannot be ruled out, it is assumed that $\text{Fe}_4[\text{Fe}(\text{CN})_6]_3$ might generate CO_2 and CH_4 via Reaction 3-11 (Cloet et al. 2014).



No degradation experiment and associated quantification of gaseous species have been performed to date. According to its chemical structure, it can be grouped together with O1a compounds (Tab. C-2).

3.4 Gas consumption processes

Depending on local conditions, distinct processes can lead to the chemical and biological consumption of repository-produced gases, representing gas sinks. Gas sinks can reduce the buildup of gas pressure in the deep geological repository if the microbial, chemical and physical *in-situ* conditions are favourable. Fig. 3-1 shows a simplified view of the potential biotic and abiotic reactions resulting in gas generation or consumption in the context of a deep geological repository.

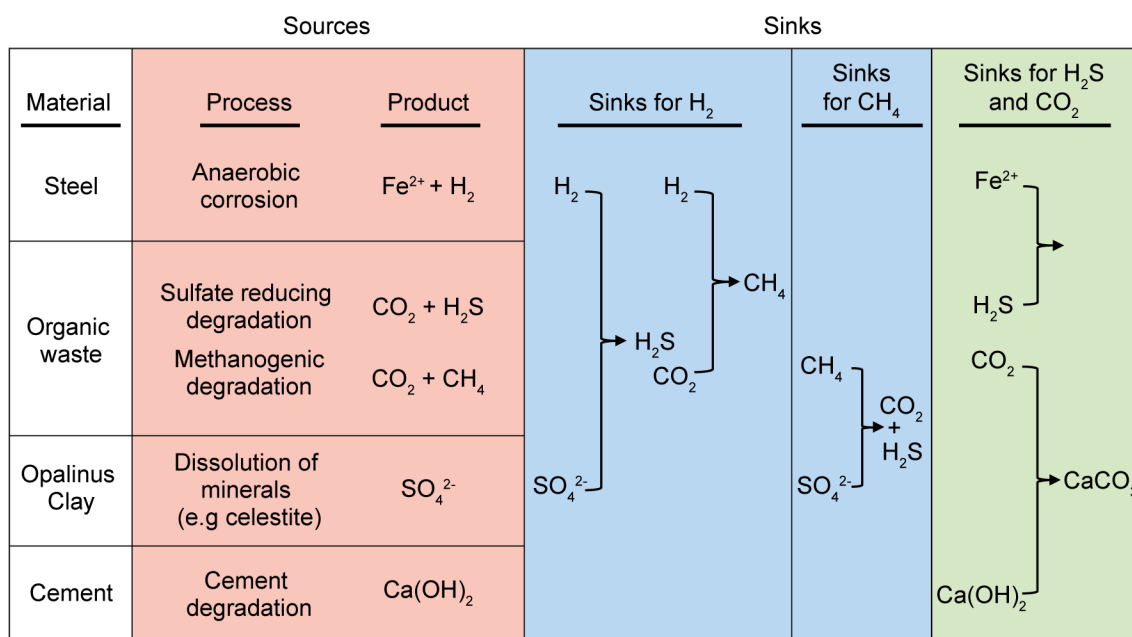


Fig. 3-1: Schematic representation of potential sources and sinks of species related to the production and consumption of gases

Taken from Leupin et al. (2016). Gas sources are shown in red, microbial sinks are shown in blue, while abiotic sinks are illustrated in green.

Such gas sources and sinks are distributed in both the L/ILW emplacement caverns and the operations tunnels (Fig. 3-2), as the V1-L/ILW seals and backfill materials of the L/ILW caverns are currently designed to promote gas release (Nagra 2024i, Martin et al. 2023). The amount of gas that can be consumed or fixed by mineral formation or biological activity depends on the abundance of the reactants and on the geochemical conditions (e.g., water content). The conditions in the backfilled operations tunnels (especially in terms of near-neutral pH and availability of substrates) are expected to promote microbial activity, as opposed to the L/ILW emplacement caverns (Guillemot et al. 2023).

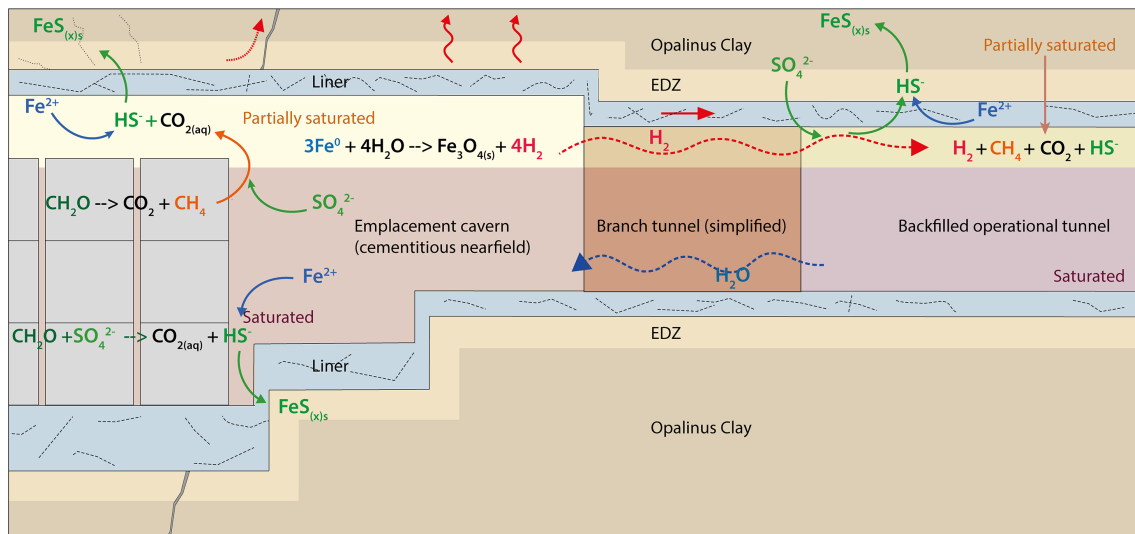


Fig. 3-2: Conceptual schematic illustration of the possible gas-related reactions in an L/ILW repository, depending on local physical and geochemical conditions of the different repository compartments

From Leupin et al. (2016). Adapted from Nagra (2008).

CO_2 , NH_3 and H_2S are highly soluble gas species, and can be readily consumed by micro-organisms, or react with minerals. Other gases such as CH_4 and H_2 are less soluble and are therefore considered to mainly contribute to gas pressure buildup. Nonetheless, in their dissolved form, they can also be substrates for microbial activity.

More details about quantitative assessments of abiotic and biotic gas consumption can be found in Diomidis et al. (2016), Leupin et al. (2016) and Miron (2024).

3.5 Gas transport

Gas transport in clay-rich geomaterials is governed by different transport mechanisms, explained in Section 3.5.1. Additional considerations specific to clay materials, namely S/B mixtures, pure bentonite, and Opalinus Clay, are given in Section 3.5.2. A comprehensive compilation of Nagra's gas related data bases, addressing both engineered barriers and the geological barriers is given in Nagra (2024c).

3.5.1 Overview of transport and storage processes

Gas transport in geological and engineered clay barriers has been the subject of numerous international research programmes in various geoscientific disciplines during the last three decades. Early studies of gas transport in the context of radioactive waste disposal were reported in Volckaert et al. (1993) and Horseman et al. (1996). In the Swiss radioactive waste disposal programme, gas-related studies were initiated in the Wellenberg project (Nagra 1997), followed by comprehensive studies on gas transport in the Opalinus Clay (Marschall et al. 2005, Nagra 2002b). Laboratory and field investigations on gas release through clay-based engineered barrier materials (granular bentonite, S/B mixtures) have been conducted within the framework of several international research platforms, encompassing large-scale, in-situ experiments at the Grimsel Test Site (Nagra 2024c), laboratory experiments and modelling activities within the EURATOM research programmes FORGE (Jacops et al. 2014, Norris et al. 2013) and EURAD-GAS

(Levasseur et al. 2024) and a dedicated laboratory programme on gas transport in granular bentonite material within the framework of SKB's EBS Task Force (Nagra 2024c).

Broad consensus has been established in the scientific community concerning the gas transport mechanisms in clay-based geomaterials (Levasseur et al. 2024, Levasseur et al. 2020). Gases generated in the repository near-field will initially be fully dissolved in the porewater, but eventually, when the solubility limit is exceeded, a separate gas phase will form. At elevated gas pressures, the porous media in which the gas is present (host rock, buffer, backfill and sealing materials) could undergo mechanical deformation. Gas transport is thus controlled by the hydraulic and mechanical properties of the porous media (e.g., their intrinsic permeability, porosity, water retention and mechanical parameters) as well as by the hydromechanical state (i.e., water saturation, gas and porewater pressure, stress state). Phenomenological considerations suggest the following subdivision of the basic transport mechanisms, as illustrated for the Opalinus Clay in Fig. 3-3a (see also Marschall et al. 2005; Nagra 2008):

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

The transport mechanisms include complex hydromechanical processes that can be understood in terms of the coupling between the transport of immiscible fluids (Fig. 3-3b) and geomechanics (Fig. 3-3c). An overview of gas transport mechanisms is given in Sections 3.5.1.1 to 3.5.1.4; the mathematical formulations used to represent these in the modelling performed in the present report are provided in App. D.

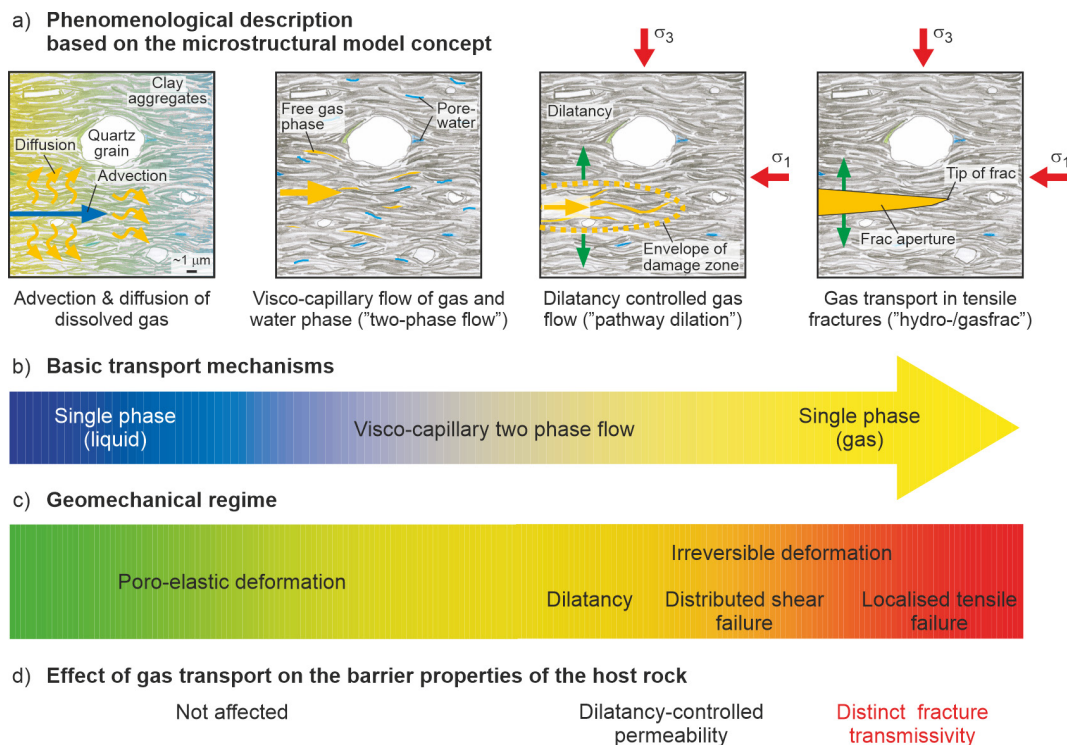


Fig. 3-3: Classification and analysis of gas transport processes in the Opalinus Clay
From Marschall et al. (2005).

3.5.1.1 Transport of gas dissolved in porewater

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

- Darcy's law, which describes advective groundwater flow under the influence of pressure and gravitational forces.
- Fick's law, which represents the diffusion of dissolved gas (and other solutes) due to the concentration gradients in the porewater.
- Henry's law, which describes the solubility of gas in porewater.

3.5.1.2 Visco-capillary two-phase flow

In visco-capillary (two-phase) flow, gas transport is controlled by the interaction between the visco-capillary forces, gravity/buoyancy, solubility and diffusion (Section 3.5.1.1), and the connectivity and spatial variability of the pore network. Lenormand et al. (1988) identified three major flow regimes, namely viscous fingering, capillary fingering and stable displacement. The capillary number Ca , defined as the ratio of viscous and capillary forces, and the viscous ratio M , defined as the ratio of the viscosities of the defending and invading fluids, determine the transition between these flow regimes (Lenormand et al. 1988). Additional two-phase flow phenomena, such as migration (buoyancy-controlled transport), fragmentation (competition between capillary and buoyancy effects), and coalescence (interaction with trapped gas) are described by a third dimensionless number, K , which is defined as the ratio between viscous and gravity forces.

In a geomechanical sense, and for the purposes of modelling gas transport and storage, consolidated clay rocks such as the Opalinus Clay can be assumed to behave as elastic porous media, characterised by a porosity and compressibility (additional considerations regarding phenomena occurring in bentonite and S/B mixture are given in Section 3.5.2). A controlling factor for two-phase flow in a porous medium is the gas entry pressure, also known as capillary threshold pressure and hereafter referred to as capillary strength, which represents the difference between gas pressure and water pressure needed to displace porewater from the medium when it is initially fully saturated. Considering the medium on a pore scale, the capillary strength corresponds to the capillary pressure of the largest-radius pores that the gas pressure needs to overcome so that gas entry occurs in these pores. Once the capillary strength has been exceeded, gas flow is mostly controlled by the intrinsic permeability (k) of the medium, the permeability-saturation relationship (commonly known as relative permeability), and the relationship between the capillary pressure and water saturation (also known as suction or water retention curve). The functional dependency between pore space saturation and the relative permeability or the capillary pressure is commonly described with parametric models, such as in the van Genuchten approach (see App. D).

3.5.1.3 Dilatancy-controlled gas flow

Dilatancy-controlled flow (or “pathway dilation” after Horseman et al. 1996) is a transport mechanism of special importance in clay media with low tensile strength. In general, clay-rich media may undergo structure changes at gas pressures that exceed the magnitude of the minimum principal strength acting on the material (Valkó & Economides 1996). Due to the expected microscale variability of the geomechanical material properties, it is plausible that microfractures will form before yielding (ductile fracturing, subcritical fracture growth). The process of gas-driven microfracturing leads to an increase in the void space, which is accompanied by a detectable increase in intrinsic permeability and a change in the capillary pressure-saturation relationship.

Porosity, permeability and capillary strength are linked to rock deformation through empirical relationships. In the terminology of multiphase flow concepts, gas flow is still controlled by visco-capillary forces (see Section 3.5.1.2). The extension compared with the conventional two-phase flow described in Section 3.5.1.2 is that the transport properties of the solid phase are no longer viewed as invariants, since they depend on the state of deformation of the material. Exemplary formulations of enhanced effective permeability are given in App. D.3. A more comprehensive literature review is given in Nagra (2024c).

3.5.1.4 Gas transport along macroscopic tensile fractures

In general, a macroscopic tensile fracture (hydraulic or gas fractures) develops when the gas pressure exceeds the sum of the minimal principal stress and the tensile strength of the rock (e.g., Valkó 2014). Fracturing is initiated quasi-instantaneously without precursory plastic deformation, and the fracture propagates at about the velocity of a shear wave (e.g., Gross & Seelig 2007). Gas flow in such a macroscopic tensile fracture can be seen as a single-phase process. The propagation comes to a halt when the gas pressure in the fracture drops below the value of the minimum principal stress (shut-in pressure). In a rock with low tensile strength, a macroscopic fracture develops only when the gas pressure buildup is rapid, i.e., when the combined effect of porewater displacement and formation of small-scale fractures (dilatancy) no longer counter-balances the gas generation rate.

3.5.2 Gas transport in clay materials

A comprehensive synthesis and literature review on gas transport in clay materials is given in (Nagra 2024c). In the following, short overviews are given for sand/bentonite mixtures (Section 3.5.2.1), pure bentonite (Section 3.5.2.2), and the Opalinus Clay (Section 3.5.2.3).

3.5.2.1 Sand/bentonite mixtures

Comprehensive research studies have been conducted in the past decades to characterise gas transport in S/B mixtures (e.g. Graham et al. 1997, Japan Nuclear Cycle Development Institute 1999, Tashiro et al. 1998, Nagra 2008). A mature understanding of the microstructure of such mixtures has been developed, and the importance of this microstructure for gas transport behaviour has been investigated. It has been shown that S/B mixtures with a moderate bentonite content of 20–30% are characterised by a multi-modal pore-size distribution. The form of the pore-size distribution depends on a variety of factors, such as the degree of compaction and the water content of the S/B mixture (Fig. 3-4), enabling these materials to be tailored in such a way that they exhibit the desired properties. In particular, through the application of appropriate techniques for their emplacement (compaction), their gas transport properties can be tailored to the performance and provisional design requirements.

In S/B mixtures with relatively low bentonite content that are intended for use in the sealing system (Romero 2013), the sand grains form a “shielding skeleton” that carries the external stresses, while the bentonite (once saturated) can swell to effectively fill the pore space within this skeleton. Romero (2013) suggests filling fractions of $\sim 98\%$ for 80/20 S/B provided the swelling of the bentonite is not inhibited (the swelling pressure developed by the bentonite is a function of effective dry density and fluid chemistry).

As part of the Gas Migration Test (GMT) at the Grimsel Test Site, investigations of relatively low S/B mixtures were performed to characterise the dependency of the pore-size distribution on the (i) emplacement density and (ii) degree of saturation (Romero & Castellanos 2004). Manca (2015) provides an analysis of the hydro-chemo-mechanical (HCM) behaviour of an 80/20 S/B mixture, including the main mechanisms of liquid and gas transport under both saturated and unsaturated conditions.

Fig. 3-4a shows that, with increasing mixture density, the macroporosity, and hence the pore space available for water flow and solute transport, decreases significantly. If the material is saturated with water, the bentonite swells and fills the pore space of the sand matrix, thus resulting in a very pronounced decrease in the macropores, as shown in Fig. 3-4b;c;d. However, laboratory tests on as-compacted S/B material (e.g., within the GMT Project) show that permeabilities to gas under fully desaturated conditions are significantly higher than the permeabilities to water in fully saturated conditions. Furthermore, a small desaturation of the material can be sufficient to create a connected pore space available for gas flow and can result in a high gas permeability. The relevant gas flow mechanism is two-phase flow through the macroporosity of the S/B associated with a very low capillary strength (Nagra 2008, Nagra 2024c, see also App. D).

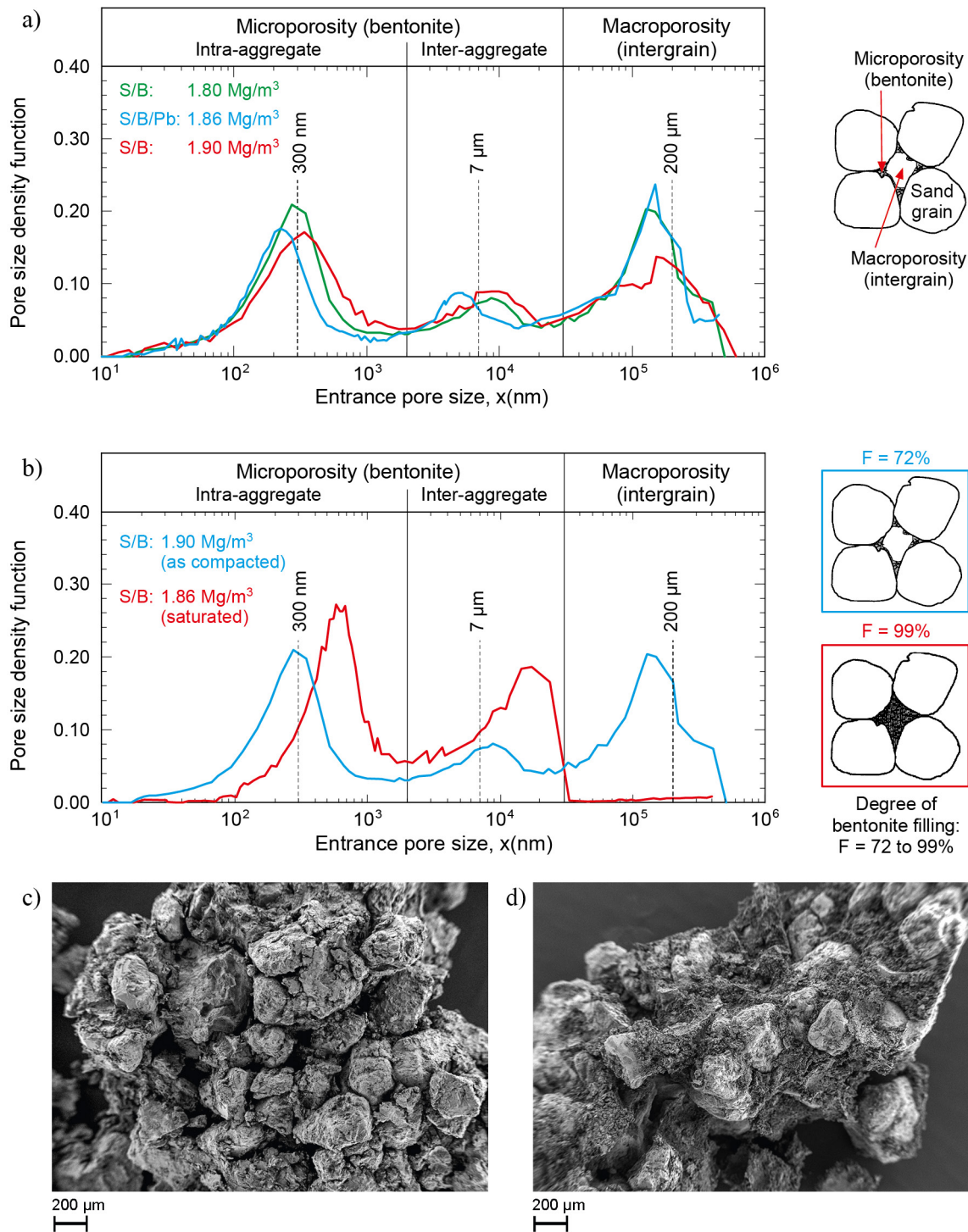


Fig. 3-4: Evolution of microstructure of S/B during wetting at nearly constant volume

(a) pore-size distribution of S/B mixtures (80/20) with various densities (Nagra 2008);

(b) pore-size distribution of an S/B mixture (80/20) with different degrees of saturation (Nagra 2008); SEM image of compacted 80/20 S/B (Manca 2015); SEM image of 80/20 S/B after saturation with distilled water (Manca et al. 2016).

3.5.2.2 Pure (compacted) bentonite

Gas transport through pure (compacted) bentonite is relevant to the buffer around the HLW canisters and to the sealing elements of the V1-HLW, V2-HLW and V3 seals, which are composed of compacted bentonite. Pure bentonite also exhibits a multi-modal pore-size distribution (Madaschi & Laloui 2018, Guo & Fall 2021). This is particularly true if it has been compacted from an initially granular form. During saturation of compacted bentonites, the macroporosity is slightly or even strongly reduced, depending on the saturation history. At the same time, micro- and mesoporosities increase slightly during hydration at the expense of the macropores (Romero & González-Blanco 2019). Important influencing factors are the duration of the saturation process and the stresses to which the material is subjected during saturation.

In a fully saturated and highly compacted bentonite, the porosity within the aggregates (micro- and mesopores) may comprise 70 to 90% of the total porosity. This porosity is, however, characterised by a very high capillary strength. When the confining pressure (total pressure acting on the bentonite) is lower than the capillary strength, the porosity within the aggregates is not at all accessible to gas. As shown with oedometric tests on MX-80 granular bentonite samples reported in Romero & González-Blanco (2017), Romero & González-Blanco (2018), and Romero & González-Blanco (2019), gas entry and the associated water uptake by the micropores results in expansion of the bentonite sample, whereas the subsequent gas pressure decrease results in the collapse of the macropores, disconnection of the gas pathways and compression of the sample. These experimental investigations have been additionally interpreted by numerical analyses using a double porosity approach to model the gas-accessible pathways through the macroporosity (Senger et al. 2018).

The comprehensive experimental characterisation of the behaviour of granular bentonite (MX-80) accounting for thermo-hydronechanical processes, together with microstructural evolution, is described in detail in Seiphoori (2015), Romero & González-Blanco (2017) and in Romero & González-Blanco (2019). For repository modelling, work from the PEBS (Long-term Performance of Engineered Barrier Systems) project (Gaus et al. 2014a, Gaus et al. 2014b) provides thermal, hydraulic and two-phase properties of the different bentonite materials.

Macroscopic fracture flow in pure bentonite and sand-bentonite elements of a repository is not expected, since the current repository concept is designed to avoid scenarios of rapid gas pressure buildup (Diomidis et al. 2016, see also Chapter 5).

3.5.2.3 Opalinus Clay

The Opalinus Clay is a moderately overconsolidated claystone that has been selected as the host rock for the disposal of radioactive waste in Switzerland (Nagra 2021). The potential gas pathways through the Opalinus Clay include the microscopic pore space of the intact rock matrix and possible discrete tectonic structures (cracks, fractures, faults), as well as excavation-induced fractures in the vicinity of the backfilled underground structures. From the long-term safety perspective, gas release through the microscopic pore space is of particular significance, because this release pathway always has the potential to exist, even when other pathways, such as tectonic faults and the excavation-damaged zone (EDZ), can be considered to be gas-impermeable (due to resealing), or when there are none at all. Within the framework of gas-related studies for Nagra's Project "Entsorgungsnachweis" (Nagra 2002a, Nagra 2004), comprehensive databases were compiled to phenomenologically, conceptually and quantitatively describe gas transfer through the Opalinus Clay. Further studies on gas transport through the Opalinus Clay were also later initiated as part of Nagra's RD&D programme. Important focal points of these investigations are the effect of spatial variability on gas propagation in the surroundings of a repository (scale dependency of the gas-related parameters) and an improved process understanding of the dependency of the transport capacity of the Opalinus Clay on overburden depth (in-situ stress).

Gas transport in low-permeability formations is largely controlled by the microstructure of the rock. A balanced assessment of gas transport processes in the Opalinus Clay therefore requires careful consideration of both structure and texture. The mineralogical and structural features of the Opalinus Clay have been extensively investigated on various scales (Nagra 2008, Nagra 2002a). Petrophysical logs and analysis of cores retrieved from investigation boreholes indicate moderate variability of clay content. Extensive analyses have been performed to characterise the pore space of the Opalinus Clay, e.g., in Keller et al. (2011), Keller et al. (2013a), Keller et al. (2013b) and Romero et al. (2012). The anisotropy due to bedding is largely a result of microscopic heterogeneity, as seen in thin sections, where diagenetic cementation of the pore space has been observed in the silty and sandy layers. The pore space of the rock is thus formed by a network of micro-, meso- and macropores, which dominate the flow and transport properties of the rock. A comprehensive synthesis is provided in Nagra (2024c) and Levasseur et al. (2024).

Water retention curves for the characterisation of viscous-capillary flow in the Opalinus Clay were determined through the desaturation and resaturation of core samples under controlled humidity (Zhang & Rothfuchs 2007, Muñoz et al. 2003; Ferrari et al. 2014; Favero et al. 2013; Nagra 2002b). In addition, the mobility of gas in the intact Opalinus Clay has been determined by water and gas testing in the laboratory and by in-situ gas injection tests in boreholes (Nagra 2002b; Marschall et al. 2005; Romero et al. 2012; Romero & Gómez 2013; Romero & González-Blanco 2015; Senger et al. 2013). Characteristic features of the Opalinus Clay based on these studies are its high capillary pressures, even at high water saturations, and low intrinsic permeability (Senger et al. 2014). A detailed description of the water retention behaviour is given in Nagra (2024c) and Levasseur et al. (2024).

Pressure-dependent permeability approaches have been adopted to describe dilatant gas transport through the Opalinus Clay when gas pressure exceeds the threshold pressure for pathway dilation (see also Section 3.5.1.3, App. D). This has been successfully applied for the interpretation of gas injection tests in the HG-D experiment at Mont Terri (Marschall et al. 2013).

In the early post-closure period of the repository, the initial gas storage capacity has been shown to be sufficient to dampen the pressure buildup when high gas generation rates are expected (Diomidis et al. 2016). At later times, the gas generation rates decrease and the gas transport capacity of the host rock and sealing system is sufficient to accommodate the generated gas (Diomidis et al. 2016; see also Chapter 5). Therefore, neither hydraulic nor gas fractures are expected under the conditions relevant for the repository. Gas flow along macroscopic tensile fractures is expected to occur only within the EDZ of the deep geological repository.

4 Assessment methodology

4.1 Background

The “storyboard” report (Nagra 2024f) provides a general phenomenological description of the expected evolution of the deep geological repository over the entire assessment period. This includes coupled processes that may be relevant to safety and take place during construction and ventilation of the repository as well as after emplacement of the waste, the backfill and the sealing materials. A brief overview is given here to help outline requirements for the assessment.

The excavation of the repository structures introduces pore pressure changes in the rock and creates an EDZ where hydraulic properties of the Opalinus Clay are altered. The subsequent ventilation of the underground structures at prescribed temperature and relative humidity causes depressurisation and partial desaturation of the EDZ and surrounding rock. After emplacement and backfilling of the repository, the EDZ will start to resaturate, and pressure in the host rock will gradually recover. At the same time, gas will be generated in the repository (see Chapter 3) and can increase the gas pressure. Porewater will migrate between the host rock and the backfill materials depending on the interplay of capillary, viscous and gravity forces at different times and sections of the repository. In general, transport in the low-permeable host rock is diffusion-dominated, whereas transport in some parts of the repository, comprising materials with higher porosity and permeability, can be driven by advection. The two-phase hydraulic evolution in the combined repository is thus determined, on the one hand, by properties of the rock, the waste and backfill materials (which impact the distribution of water and gas in the near-field) and, on the other hand, by the repository configuration as an overall system (i.e., volumes accessible to gas migrating through the repository). In the HLW repository section, the hydraulic evolution is further coupled with thermal effects from heat generated by the waste. More detailed appraisals are provided in Section 5.3.

This chapter describes the modelling workflow developed and implemented to achieve objectives *Obj2* to *Obj4* outlined in Chapter 1. Objective *Obj2* calls for a comprehensive assessment of the hydraulic evolution of a combined repository with separate HLW and L/ILW repository sections, taking into consideration gas accumulation and transport in the repository and surrounding geological environment. Based on the expected processes summarised above for the assessment of the hydraulic evolution (see also Nagra 2024f), the workflow needs to account for:

- Geometric representations of the repository and its components within the geological environment (the latter according to the geological dataset, see Nagra 2024d).
- The presence of porous media with different hydraulic and transport properties, including materials emplaced in the repository, the EDZ, host rock, and (where necessary) other geological formations; and interfaces between these materials to model saturation contrasts across the interface.
- Hydraulic effects in the rock surrounding the repository structures while they are ventilated.
- Generation of gas from the corrosion and degradation of materials after their emplacement in the repository.
- Coupled two-phase flow and transport of generated gas and porewater in the backfilled structures and surrounding rock.
- Thermal-hydraulic coupling, at least for the HLW repository section.

Furthermore, objective *Obj3* calls for assessments to address the functionality of the provisional repository design with respect to gas (i.e., for specified material properties), sensitivities and uncertainties (i.e., for the expected bandwidths around the specified material properties) or scenarios (i.e., when properties differ significantly from their design values). In general, it is possible to formulate assessment cases so they simultaneously serve multiple purposes (i.e., a case with an extreme property value can provide insight into sensitivity as well as into the impact of a hypothetical malfunction of that material). To condense the number of assessment cases and simulations, the assessments in this report leverage this approach and are formulated generically as part of a deterministic sensitivity analysis. In that sense, the workflow comprises a base case that corresponds to the expected evolution of the repository, and cases that represent deviations thereof. The complete list of assessment cases is provided and discussed in Chapter 5.

Finally, objective *Obj4* calls for the quantitative underpinning of the phenomenology associated with gas transport in the combined deep geological repository. To achieve this, the workflow must allow a balanced appraisal of effects taking place locally within sections of the repository system (i.e., within emplacement rooms and seals) as well as the total system evolution (i.e., across the entire repository).

4.2 Description of modelling workflow

The modelling workflow developed and implemented for the assessments is outlined schematically in Fig. 4-1. This section describes the main steps of the workflow. More detailed information on the modelling tools is given in Section 4.3.

4.2.1 Specifications of assessment cases

The first part of the workflow is to define specifications of the cases to be assessed. As mentioned earlier, an assessment case can address design functionality, uncertainties, or scenarios related to the repository and its evolution. The description of what needs to be assessed in each case can be qualitative (i.e., overall functions of a seal) or quantitative (i.e., performance of the seal for a specified design and with regard to a specific function). The description is then used to conceptualise the problem in the model representation and formulate it in terms of a quantitative configuration and input. In practical terms, this can include relatively simple operations such as defining an input parameter in a transport model (i.e., permeability of a seal) or defining an input used for estimating gas source terms in the repository (i.e., corrosion rate of a material under specified conditions).

4.2.2 Model-based assessments

Estimating the quantities of various gases generated in the repository is an essential step towards assessing the potential effects induced by their accumulation and transport in the underground structures and surrounding rock. Given the range of materials, mechanisms and timescales associated with gas generation in the environment of the deep geological repository, such estimates are achieved through modelling a conceptualised and mathematically formulated representation of the expected physical processes. This is undertaken with the so-called *gas generation tool* that provides the range of potential gas generation rates in the repository with time, based on the inventory of materials and the corrosion rates and degradation rates of organics (Fig. 4-1). Modelling of gas generation has been part of several earlier studies that investigated potential gas-induced effects in L/ILW and HLW repositories (e.g., Diomidis et al. 2016; Poller et al. 2016). The current modelling approach largely follows that of Poller et al. (2016), with two main changes, namely (i) rewriting the gas generation tool, previously developed in macro-

enabled Excel sheets, into the JavaScript programming language to facilitate more robust integration with subsequent gas transport modelling, and (ii) updating all input data and assumptions to the current state of the scientific database. Further details are given in Section 4.3.1.

Estimates on the fate of gases in the repository and surrounding geological environment are achieved by means of numerical modelling. The current approach is similar to that of earlier studies (i.e., Diomidis et al. 2016) but uses an updated and extended model portfolio for gas transport (Fig. 4-1). Part of the configuration done in this stage is to identify which model(s) are appropriate for the assessment. The computational demand associated with coupled two-phase flow and transport problems in materials with (sometimes high) contrasts in their properties limits the model size that can efficiently and robustly implement model-based assessments. To achieve comprehensive analyses at the total system and component levels, the modelling workflow integrates separate transport models that are implemented on the scale of the entire repository and on the scale of individual components of the repository (Section 4.3.2). For this approach to work, the modelling tools used in the workflow need to be designed for the purpose within the workflow and implemented such that they are consistent with and complementary to each other (Fig. 4-1).

The total system analyses are based on a so-called *repository model* that represents the entire combined repository with two separate HLW and L/ILW repository sections. The geometric representation of the repository structures in the repository model is not exact but approximated through appropriate volumetric scaling. Accordingly, materials within the repository structures are represented as homogenised units with effective properties. More details on the repository model are provided in Section 4.3.2.5.

Analyses at the repository component level are carried out by means of so-called *component models* that represent selected parts of the repository that are significant to gas transport, namely the emplacement rooms for HLW and L/ILW and the V1, V2, and V3 sealing sections. This renders the geometric representations more accurate on this scale, and materials explicitly represented in the models mostly match materials seen in the provisional design. More details on the component models are provided in Sections 4.3.2.1 through 4.3.2.4.

The repository and component models exchange information as follows:

The component models rely on the repository model for inputs that originate outside the component represented in each case. These are typically boundary conditions and transient flows reaching the component. For example, a component model representing a shaft with the V3 seal does not explicitly model the emplacement caverns and the gas generated in them but uses the transients of gas arriving at the base of the shaft as input, i.e., as computed by the repository model. On the other hand, the component models allow for a more detailed appraisal of the hydraulic evolution, and thereby help to evaluate and improve the abstracted, homogenised representation adopted in the repository model. If multiple models are used in an assessment case, the results are integrated and compared for consistency and validation (Fig. 4-1).

4.2.3 Synthesis

The synthesis of results provides the outcome of the assessment (Fig. 4-1). The synthesis is based on direct comparison between the assessment cases in terms of selected model metrics. The comparison highlights sensitivities and responses in the hydraulic evolution to the deviations considered in the assessment cases. The envelope of responses shows the key characteristics and transport regimes underpinning the phenomenological evolution of the repository.

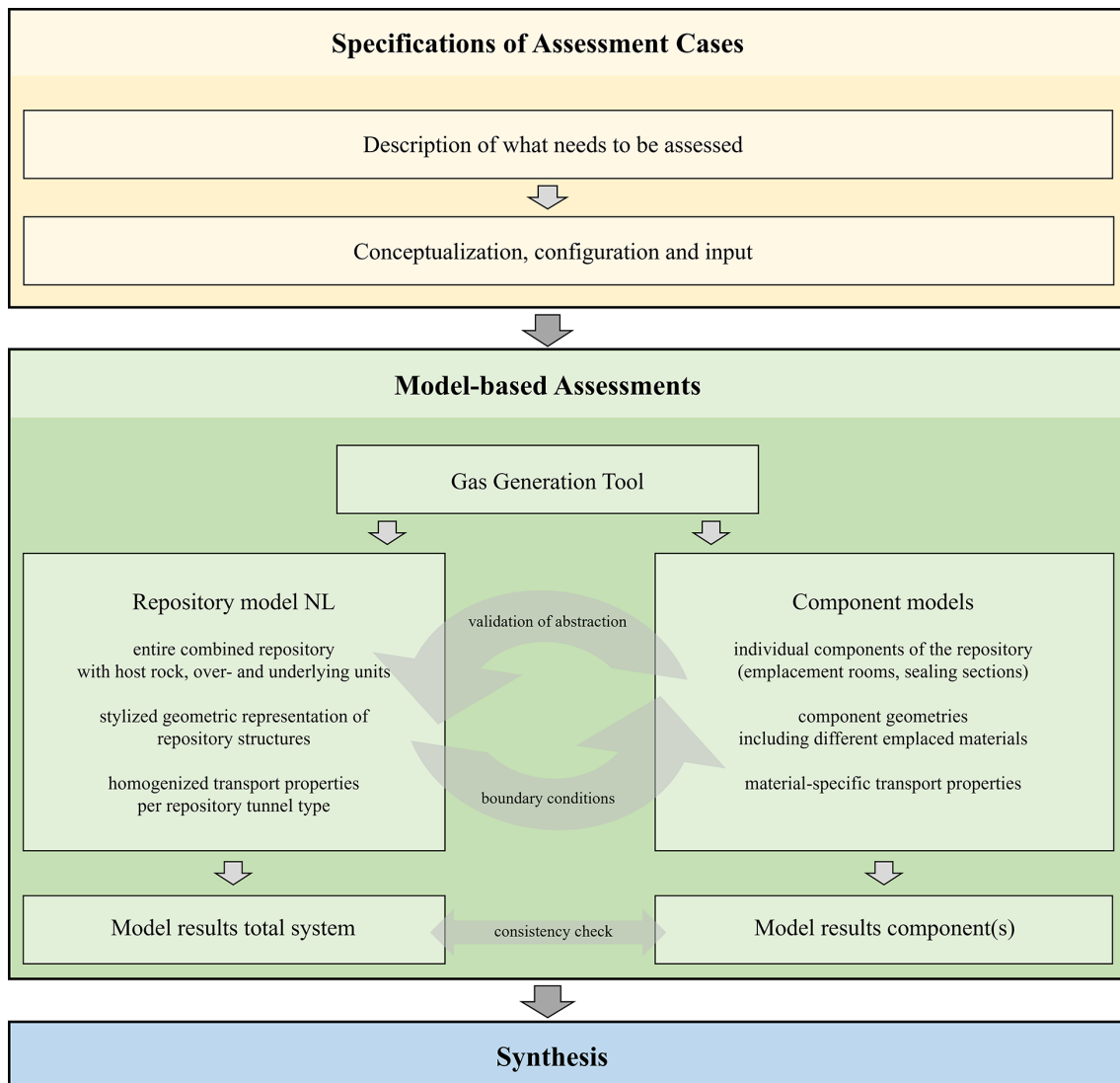


Fig. 4-1: Schematic outline of modelling workflow with its key components: specification of assessment cases (top), model-based assessments (middle), and synthesis of results (bottom)

4.3 Model portfolio

The model portfolio comprises two separate types of tools used in the calculations: for source and sink terms, and for transport. The tool used for calculating source and sink terms in the repository is described in Section 4.3.1. The models used for gas transport simulations are described in Section 4.3.2.

4.3.1 Gas generation modelling

The gas generation tool calculates transients of gas generation and water consumption rates over the timeframes relevant to the performance assessment and safety analyses of the geological repository. The start time for gas generation is assumed to correspond with the simultaneous emplacement and backfilling of the respective section of the repository.

Any substance or material in the repository that potentially contributes to gas generation after its emplacement is considered a component of the gas generation tool. There are two main sources of gas in the repository: the emplaced waste, including the disposal containers (see also Section 2.5), and the construction materials used to support the underground structures (see also Section 2.6). Gas generation is calculated separately for these two sources.

Waste materials are separated into components of a waste package type, namely:

- C: waste product, including raw waste and additives;
- D: waste containment, including the hulls of the fuel assemblies and the disposal containers for L/ILW;
- E: filler material;
- F: fittings and inserts;
- CAN: disposal canisters for SF and RP-HLW.

The gas generation tool calculates the amount of gas generated from each of these components as well as the total amount of generated gas. The tool also allows to filter the gas generation rates based on the following groupings of the emplaced waste:

- specific name(s) of AGT(s), e.g., “J-B-000007A”;
- specific name(s) of waste sorts, e.g., “BA-B-S-F2-SMA”;
- “SMA” (L/ILW), “ATA” (ATW), or “HAA” (HLW), according to the KEV;
- “AG1” or “AG2”, for L/ILW only;
- “all SMA” and/or “all HAA” (all L/ILW and/or all HLW);
- “M” (metals), “O1a”, “O1b” or “O2” (organics).

In a similar fashion, the gas generation tool separates the construction materials into different components (e.g., anchors, ribs, etc.) and calculates gas generation rates for each within the different tunnel types planned for the combined repository (see also App. B).

Each material, whether from waste or construction, is assigned a shape model. The shape models are described in Poller et al. (2016) and serve to calculate the corroding or degrading surface area over time as well as the corresponding amount of remaining material and associated time when the material corrodes or degrades completely. The detailed assignment of shapes to the individual materials within each waste package type is described in MIRAM-RBG (Nagra 2023c).

Each material, whether from waste or construction, corresponds to a metallic or organic material, which is in turn assigned to a corrosion or degradation group, respectively (see Sections 2.5 and 2.6 and App. B, App. C). Similarly, each material is assigned a chemical milieu, namely for a cement environment at $\text{pH} \geq 10.5$ and $\text{pH} \leq 10.5$, a clay environment and a compacted bentonite environment at $\text{pH} \leq 10.5$. Based on the corrosion and degradation mechanisms and reactions, corrosion and degradation rates are assigned to each metal and organic group under the corresponding environment (see Sections 3.1 and 3.2).

The milieu of the compacted bentonite environment is specifically assigned to the outer surface of the HLW disposal canisters. This feature is newly added to the gas generation tool since the availability of high-quality data made it possible to assign specific corrosion rates with lower uncertainty for carbon steel within such environments as reported in Tab. 3-1.

The gas generation tool allows the user to vary all these inputs at execution (shape parameters, milieus, corrosion and degradation rates). Gas generation (and water consumption) rates are essentially calculated based on the shape and corrosion/degradation rate of each material or component found in the waste, containers/canisters and tunnel support.

4.3.2 Gas transport modelling

The workflow outlined in Section 4.1 requires the modelling of two-phase flow through the repository structures and surrounding rock. This is performed using the EOS5 Equation-of-State module of TOUGH3 for simulating the isothermal or non-isothermal, fully coupled flow and transport of hydrogen and water in porous media (Jung et al. 2018).

The rocks represented in the modelling performed in this report, including the EDZ, are assumed to be homogeneous from a macroscale consideration as described in Nagra (2024e). All gas transport modelling is performed for the combined repository with the respective geological dataset of properties of the Opalinus Clay (Nagra 2024d). The Opalinus Clay hydraulic and two-phase flow properties are summarised in Tab. 4-1. The intrinsic permeability of the EDZ surrounding the repository tunnels is assumed one order of magnitude higher than that of the Opalinus Clay in all directions. The capillary strength of the EDZ is derived accordingly using Leverett scaling (see also Tab. 4-1). In addition, thermal and mechanical properties used for simulations accounting for thermal effects are shown in Tab. 4-2. The properties listed in these tables are used consistently across all models in the workflow (where applicable).

In addition, the thermo-hydraulic and two-phase properties of the confining geological units are given in Nagra (2024e). Note that the geological dataset also provides uncertainty ranges for each geological unit, including the Opalinus Clay (best estimates, upper and lower bound values). The propagation of uncertainty from these ranges is not addressed in this report as it is treated in a probabilistic framework in Nagra (2024e). Similarly, heterogeneity and associated variability in hydraulic properties is addressed in Nagra (2024e).

Model-specific input parameters relevant to the models used in this report, i.e., those related to materials emplaced in the repository, are provided in the following sections for each model.

Tab. 4-1: Hydraulic and two-phase flow parameters of the Opalinus Clay

Parameter	RV	AV	Remarks
Intrinsic permeability normal to bedding $k_{\perp}$ [m ²]	1×10^{-21}	1×10^{-20}	RV: Best estimate value from Nagra (2024d); AV: Upper bound value from Nagra (2024d).
Capillary pressure - saturation relationship			van Genuchten parametric model
Capillary strength P_o [MPa]	$P_{o,i} [MPa] = 34 \sqrt{\frac{k_{ref}}{k_i}}$		Leverett scaling, based on previous capillary pressure measurements: $k_{ref} = 2E-21$ m ² ; Default value $T_0 = 20$ °C for temperature scaling; Residual water saturation $S_{wr} = 0.01$.
Shape parameter n (van Genuchten)	1.67	1.54	RV: derived from capillary pressure measurements (drying path); AV: derived from capillary pressure measurements (wetting path).
Relative permeability – saturation relationship			van Genuchten/Mualem parametric model using the shape parameter n from the P_c - S curve
Residual water saturation S_{wr} [-]	0.5	0.1	RV: according to the results of adsorption / desorption measurements, suggesting that 50% of the total pore space can be classified as micro- and mesopores; AV: assuming that most of the porewater is mobile (not supported by experimental data).
Residual gas saturation S_{gr} [-]	0.00	0.003	RV: effective gas entry pressure of the rock is infinitesimal; AV: the residual gas saturation determines the effective gas entry value. Effective gas entry values were determined by gas permeability testing at Mont Terri and Benken.
Total porosity [%]	12%	10%	RV: corresponds to the reference value for the porosity in northern Switzerland; AV: Previous porosity values in ZNO; also used in Curti et al. (2023) for diffusion models.

RV: reference value; AV: alternative value.

Relationship between intrinsic permeability and hydraulic conductivity:

$$k \left[m^2 \right] = \frac{\eta_w}{\rho_w \cdot g} \cdot K \approx 1 \times 10^{-7} \cdot K \left[m/s \right] \text{ for } T = 20 \text{ °C}$$

η_w - dynamic viscosity of water, [Pa·s]

ρ_w - density of water, [kg m⁻³]

g - gravitational acceleration, [m s⁻²]

Linear permeability enhancement assumed, when gas pressure exceeds threshold pressure for pathway dilation (see Senger et al. 2013)

Tab. 4-2: Thermal and mechanical parameters used for the Opalinus Clay and EDZ

	Unit	Opalinus Clay	EDZ	Comment
Thermal parameters				
- Density - Bulk - Grain	ρ [kg/m ³]	2,450 ¹ 2,700 ²	2,450 2,700 ²	¹ Curti et al. (2023): 2,380 kg/m ³ ² Input parameter for TOUGH3 simulations
Rock grain specific heat	C_r [J/(kgK)]	995.0	995.0	Values used in this study
Thermal conduct. - Parallel¹ - Perpendicular¹ - Dry² - Saturated²	T_c [W/m K]	2.8 1.6 1.36 2.1	2.4 1.2 1.36 1.7	Note: the EDZ values are derived from Seiphoori (2022) – “Thermal conductivity of shallow Opalinus Clay (BCI-21B)” ¹ Seiphoori (2022) – Vomvoris et al. (1992) ² harmonic mean
- Therm. expansion grain - Rock framework - Water	T_x [1/ K]	1.5E-6 1.7E-5 ¹ 3.4E-4	1.5E-6 1.7E-5 ¹ 3.4E-4	Wileveau & Rothfuchs (2007) ¹ Input parameter for TOUGH3 simulations: rock framework
Rock compressibility				
- Young's Modulus - Poisson ratio - Porosity	E [MPa] ν [-] ϕ [-]	6,500 ¹ 0.23 ¹ 0.12	3,900 ² 0.115 ² 0.14	¹ Nagra (2024e): derived from bulk modulus – best estimate (drained) ² Nagra (2024e): derived from bulk modulus – minimum (drained) ^{1,2} Nagra (2024e): average perpendicular and parallel to bedding
Compressibility: $\alpha = 3(1-2 \nu)/E$	α [1/ Pa]	2.5E-10	5.9E-10	Computed from E-modulus
Pore compressibility: $C_p = \alpha/\phi$	C_p [1/ Pa]	2.1E-09	4.2E-09	Input parameter for TOUGH3 simulations

4.3.2.1 L/ILW near-field & V1-L/ILW model

The L/ILW near-field & V1-L/ILW model is implemented with a nested rectangular integrated finite difference (IFD) mesh in 3D and represents half (width-wise) of a L/ILW emplacement cavern with the adjacent waste transfer area, unloading area, V1-L/ILW seal, branching tunnel and part of the operations tunnel. Selected views of the model are shown in Fig. 4-2.

The operations tunnel is assigned a length of 1,616.5 m representing the total length (scaled for half cavern and cut in half width-wise) up to the V2-HLW seal that restricts gas flow. Alternatively, the length is reduced to 245.1 m, corresponding to the total length up to the V2-L/ILW seal. The storage volume of the operations tunnel is scaled down accordingly to account for 7 caverns contributing gas and water flux through their branching tunnels. The branching tunnel has a length of 113.5 m, including the V1 seal. The unloading and transfer areas have a length of 9 m and 11 m, respectively. The modelled half-cavern has a length of 229 m. The

model extends an additional 36 m beyond the cavern into the host rock. Perpendicular to the main cavern axis, this half-cavern model assumes symmetry between adjacent caverns and therefore extends 40 m into the surrounding host rock. In the vertical direction, the model assumes a thickness of the host rock of 109 m with the cavern placed horizontally in the middle of the Opalinus Clay (see also repository model in Section 4.3.2.5). The resulting dimensions of the model are thus $2015 \times 40 \times 111$ m (L×W×H) for the variant with the operations tunnel reaching up to the V2-HLW and thus $643.6 \times 40 \times 111$ m for the variant with the operations tunnel reaching up to the V2-L/ILW, respectively. The two variants of the model with regard to the operations tunnel are evaluated in selected assessment cases (see Chapter 5).

The V1 seal is discretised into its main components with their respective dimensions, namely the sealing element, the abutment, and the transition layers (Fig. 4-2, see also App. A). For the sake of modelling, it is assumed that the entire L/ILW emplacement cavern is filled with LC-86H containers, stacked in an array of 3×3 with 2 additional containers placed on the top row (Fig. 4-2). The L/ILW cavern features two levels of discretisation:

- The first 7.5 m (starting from the mouth of the cavern) are discretised with finer detail to resolve the walls and lids of the LC-86H containers as well as waste packages and filling material contained within. To balance computational effort and level of detail, the waste packages are not all explicitly represented but lumped into 4 subdomains per container with filling material between and on top of them. Similarly, the two-shell lining of the cavern is represented with a single liner material, and other concrete materials (e.g., support structures, sole) are outlined in a simplified manner. The resulting volume fractions are consistent with the provisional cavern design for the $3 \times 3 + 2$ array (ca. 35% M1 mortar; 14% LC-86H; 25% waste and filling; 26% liner and concrete).
- To reduce computational effort, the rest of the cavern (7.5 to 222.5 m) is discretised with a coarser mesh that still allows each of the LC-86H containers to be represented with the mortar-filled gaps between them (Fig. 4-2b).

Emplaced near-field materials explicitly discretised in the model include the M1 mortar, LC-86H container, waste package, container filling (Dorodur), liner, support concrete and cavern sole. The corresponding hydraulic and two-phase flow parameters used in the base case (prior to any volumetric scaling) are given in Tab. 4-3.

The Opalinus Clay is assumed to be initially fully water-saturated, and hydrostatic pressures are assigned to the model nodes prior to repository construction. The top and bottom of the 3D grid correspond to constant pressure boundaries. All sides of the model correspond to no-flow boundary conditions. This implies that, in a general sense, the model version with the operations tunnel reaching the V2-L/ILW is consistent with an impermeable seal of the L/ILW repository. On the other hand, the model version reaching the V2-HLW is consistent with permeable repository structures throughout the L/ILW repository and the facilities for the EUU up to an impermeable seal in the HLW repository. The initial pressure distribution and hydrostatic values at the top and bottom boundaries correspond to a cavern depth of 803 m b.g.l.. The numerical simulations with this model are run isothermally (i.e., with constant temperature), and fluid properties such as viscosity and density depend on temperature, which is depth-dependent assuming a temperature gradient of 0.043 °C/m and a surface temperature of 10 °C. Internal boundary conditions are assigned to open tunnels during ventilation through prescribed atmospheric pressure and a capillary suction corresponding to relative humidity of 60% and temperature of 28 °C (see also Tab. 4-7). However, all materials are emplaced at ambient temperature at repository depth with the initial saturation values listed in Tab. 4-3.

Gas source terms (and water sink terms, where applicable) are assigned to the model nodes representing the waste packages. Source (and sink) terms are distributed equally across all waste packages in the L/ILW cavern.

Tab. 4-3: Hydraulic and two-phase flow parameters for the materials in the L/ILW near-field

	Symbol, unit	Mortar M1	LC-86H container	Waste package, Dorodur	Liner, concrete
Hydraulic parameters					
Porosity	ϕ [-]	0.20	0.10	0.35	0.10
Intr. permeability	k [m ²]	1.E-10	3.E-16	1.E-15	3.E-16
Pore compressibility	C _p [1/Pa]	3.0E-10	5.0E-10	5.0E-10	7.0E-10
Initial water content	w _r [%]	12.	5.	25.	7.
Initial saturation	S _w [-]	0.50	0.33	0.70	0.70
Two-phase flow parameters					
van Genuchten capillary strength ¹	P ₀ [Pa]	5.E02	2.E06	1.E06	2.E06
Shape param.: vG-n (k _r) vG-n (P _c) vG-n (P _c)	vG-n (k _r) vG-n (P _c) vG-n (P _c)	2.0 2.0 2.0	2.0 2.0 2.0	2.0 2.0 2.0	2.0 2.0 2.0
Residual water sat.	S _{lr} (k _r)	0.05	0.05	0.05	0.05
	S _{lr} (P _c)	0.01	0.01	0.01	0.01
Residual gas saturation	S _{gr} (k _r)	0.0	0.0	0.0	0.0

¹ default value T₀ = 20 °C for temperature scaling

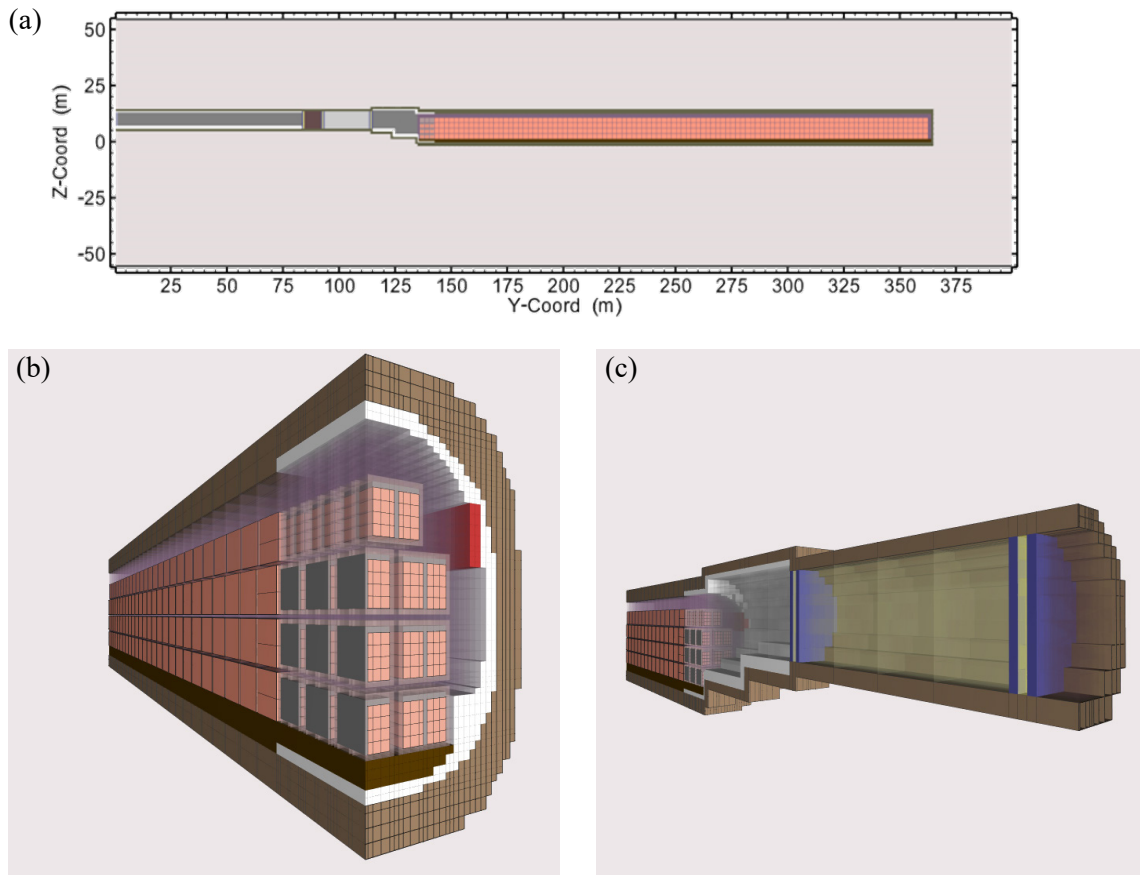


Fig. 4-2: Geometry of L/ILW near-field & V1-L/ILW model

(a) half-cavern cross-section through the entire model; (b) half-cavern close-up with vertical cross-section through waste packages; (c) half-cavern close-up with vertical cross-section through transition layer of V1 seal.

It should be noted that the geometry of the L/ILW near-field & V1-L/ILW model is based on a provisional design may be refined and modified in future stages of the project.

4.3.2.2 HLW near-field & V1-HLW model

The HLW near-field & V1-HLW model is implemented with a hybrid radial-rectangular mesh in 3D and represents half (width-wise) of a HLW emplacement drift including the V1-HLW seal. Selected views of the model are shown in Fig. 4-3.

In the HLW disposal area, transport of gas and water occurs predominantly radially as opposed to along the underground structures (see also Section 5.3). The branching and operations tunnels are therefore not included in the HLW near-field model. The modelled half-drift has a length of 887 m, including 23 m of V1-HLW. The model extends a further 150 m beyond the drift into the host rock. Perpendicular to the main tunnel axis, this half-model assumes symmetry between neighbouring emplacement drifts with uniform spacing of 40 m and therefore extends 20 m into the surrounding host rock. In the vertical direction, the model assumes a thickness of the host rock of 106 m, with the entire drift placed at the middle of the Opalinus Clay (see also repository model in Section 4.3.2.5). In addition, 3 m of the overlying DOGG (Dogger) and underlying ML (marly Lias) units are included in the model mesh at the top and bottom, respectively. The resulting dimensions of the model are thus 1037×20×112 m (L×W×H).

The V1-HLW seal is discretised into its main components (sealing element, the abutments, and the transition layers) with their respective dimensions (Fig. 4-3, see also App. A).

It is assumed that the entire HLW drift is filled with HLW disposal canisters, with a constant spacing of 3 m between them (Fig. 4-3). The HLW drift features two levels of discretisation:

- The first 32 m (from the edge of the V1 seal to the half-distance between canisters 3 and 4) are discretised in greater detail to resolve the lids of the HLW disposal canisters. To balance computational effort and level of detail, the bentonite pedestal is approximated with a wedge of the radial mesh rather than a rectangular shape. Similarly, the tubbing and filling mortar between tubbing and rock are represented with a single liner material. The resulting volume fractions are consistent with the provisional emplaced tunnel design (for one canister plus half pitch ~ 42.9% bentonite buffer; ~ 6% pedestal; ~ 5.7% canister incl. contents; ~ 45.3% liner).
- To reduce computational effort, the rest of the drift (32 to 887 m) is discretised with a coarser mesh that omits the lids of the canisters but still allows representation of all canisters with the 3-m pitch between them (Fig. 4-3).

Note that only the canister hull is considered in the model (dimensions provided in App. A), with elements representing the contents of the canister removed from the model and source terms assigned to the hull. Emplaced near-field materials explicitly discretized in the model therefore include the bentonite buffer, bentonite pedestal, steel canister and liner. The corresponding hydraulic and two-phase flow parameters used in the base case are given in Tab. 4-4, with additional values for the V1 seal materials provided in Tab. 4-5.

The modelled rock formations are assumed to be initially fully water-saturated, and hydrostatic pressures are assigned to the model nodes prior to repository construction. The top and bottom of the 3D grid (or Opalinus Clay, respectively) are connected to 1D elements extending the model to corresponding ground surface and Permo-Carboniferous. For this, it is assumed that the HLW emplacement drift is located approximately in the middle of the HLW disposal area at 925 m b.g.l (in accordance with the repository model, see also Section 4.3.2.5). The numerical simulations are run under non-isothermal conditions with initial, ambient temperatures corresponding to 10 °C surface temperature and a basal heat flow of 120 mW/m² assigned at the bottom of the model (see also Section 4.3.2.5). Prior to emplacement, the tunnel is ventilated for 2 years (see also Tab. 4-7). All materials are emplaced at 28 °C with the initial saturation values listed in Tab. 4-4.

Gas and heat source terms are assigned to the model nodes representing the HLW disposal canisters. Source terms are distributed equally across all canisters in the HLW emplacement drift.

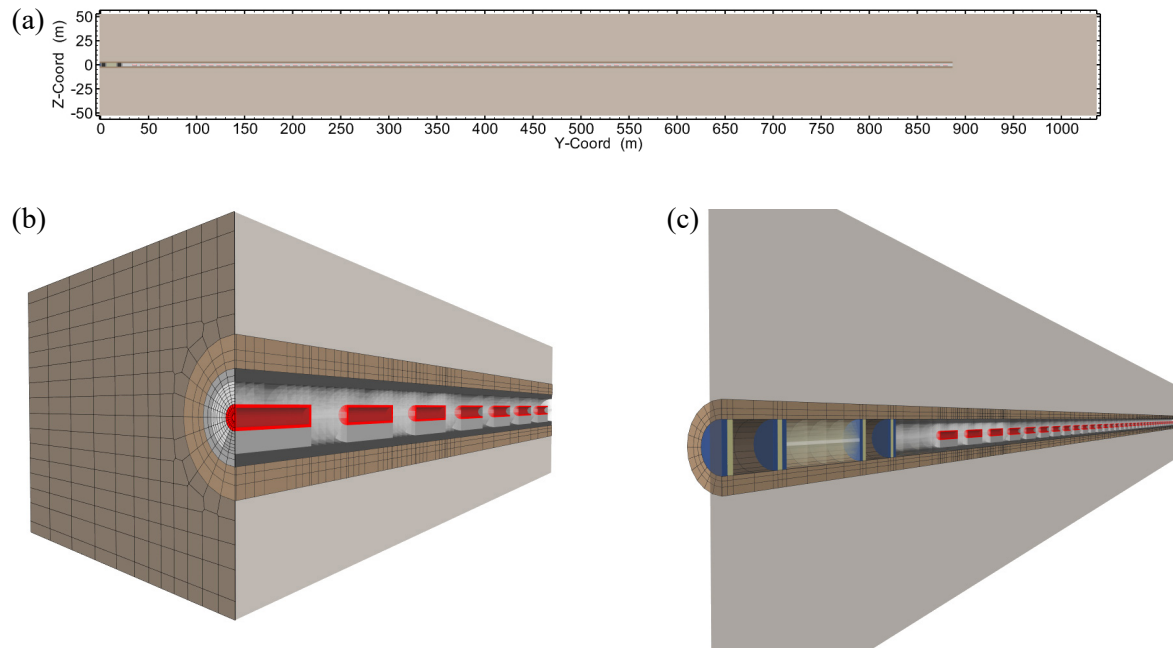


Fig. 4-3: Geometry of HLW near-field & V1-HLW model

(a) half-tunnel cross-section through entire model; (b) half-tunnel close-up with vertical cross-section through canister; (c) half-tunnel close-up with vertical cross-section through transition layer of V1 seal.

It should be noted that the geometry of the HLW near-field & V1-HLW model is based on a provisional design may be refined and modified in future stages of the project.

Tab. 4-4: Hydraulic, thermal and two-phase flow parameters for the materials in the HLW near-field

	Symbol, unit	Bentonite blocks	Granular bentonite	Canister	Tubbing
Thermal parameters					
Density • dry • bulk • grain	ρ [kg/m ³]	1,806 1,874/1,993 2,700	1,492/1,457 1,581/1,543 2,700	7,850	2,650
Rock grain specific heat	C_r [J/(kg K)]	1,058	893	440	905.5
at T = 20 °C		800	856	775	
at T = 110 °C		1,315	1,020	902	
Therm Cond. • Dry • Wet	T_c [W/mK]	0.35 1.30	0.35 1.30	52.5	1.4 2.3
Thermal exp.	T_x [1/ K]	2.5E-5	2.5E-5	1.5E-5	1.5E-5
Hydraulic parameters					
Intr. permeability	k [m ²]	2.5E-21	3.5E-20	1.0E-50	1.0E-18
Porosity	ϕ [-]	0.33	0.33	0.001	0.10
Compressibility $C_p = \alpha/\phi$	α [1/Pa] C_p [1/Pa]	1.0E-9 3.0E-9	1.0E-9 3.0E-9	0	7.0E-10
Initial water content	w_r [%]	16.5	6.6	0	7.0
Initial saturation	S_w [-]	0.5	0.2	0	0.70
Two-phase flow parameters					
Van Genuchten cap. strength ¹	P_0 [MPa]	21.9 ²	10	--	2.0
Shape param.: vG-n (k_r) vG-n (P_c)	vG-n (k_r) vG-n (P_c)	1.42 1.42	1.67 1.67	--	2.0 2.0
Residual water sat.	S_{lr} (k_r) S_{lr} (P_c)	0.00 0.01	0.00 0.01	--	0.05 0.01
Residual gas saturation	S_{gr} (k_r)	0.	0.	--	0.

¹ default value $T_0 = 20$ °C for temperature scaling

4.3.2.3 V2-L/ILW model

The V2-L/ILW seal model is implemented with a hybrid radial-rectangular mesh in 3D and represents part of the operations tunnel in the L/ILW repository with the V2-L/ILW seal. The radial part of the mesh is used for the tunnel and seal, and the rectangular portion is used for the Opalinus Clay and confining geological units. Selected views of the model are shown in Fig. 4-4.

The V2-L/ILW seal itself has a length of 40 m. On each side of the seal, 30 m of operations tunnel are accounted for in the direction of the L/ILW emplacement caverns on the left and the access tunnel/facilities for EUU on the right (as shown in Fig. 4-4a). Perpendicular to the main tunnel axis, the model extends 27 m into the surrounding host rock on each side of the tunnel. In the vertical direction, the model extends from the bottom of the argillaceous Lias (AL) unit to the top of the marly Malm (MM2) (see Nagra 2024e for complete list of stratigraphic units or formations and their respective representation in performance assessment modelling). The geological units in this interval are grouped in 5 layers in the V2 model, namely (from bottom to top): AL, ML, Opalinus Clay, DOGG including the sandy calcareous argillaceous unit (SCAD), the sandy calcareous one (SCD) and the argillaceous one (ARD), Herrenwis, argillaceous Dogger (AD), and MM including the two MM units (MM1+MM2) and the calcareous one (CM). The formation thicknesses correspond to those at the V2-L/ILW location (extracted from the repository model, see Section 4.3.2.5). The thickness of the host rock is 110 m with the V2 seal and operations tunnel placed horizontally in the middle (see also Section 4.3.2.5). The resulting dimensions of the model are thus 100×54×310 m (L×W×H).

The V2-L/ILW seal is discretised into its main components with their respective dimensions, namely the S/B sealing element, the abutments and the transition layers (Fig. 4-4, see also App. A). The tunnel liner is included only in the tunnel sections outside the V2-L/ILW seal and consists of two layers. The corresponding hydraulic and two-phase flow parameters used in the base case are given in Tab. 4-5. Values for the backfill materials in the operations tunnel are provided in Tab. 4-6 (L/ILW operations tunnel, excluding V2).

The modelled rock formations are assumed to be initially fully water-saturated, and hydrostatic pressures are assigned to the model nodes prior to repository construction. The top and bottom boundaries of the 3D grid have imposed constant pressure conditions. The initial pressure distribution and hydrostatic values at the top and bottom boundaries correspond to a tunnel depth of 857 m b.g.l, which is consistent with the repository model (Section 4.3.2.5). The numerical simulations with this model are run isothermally, and fluid properties such as viscosity and density depend on temperature, which is depth-dependent assuming a temperature gradient of 0.043 °C/m and a 10 °C surface temperature. Internal boundary conditions are assigned to open tunnels during ventilation through prescribed atmospheric pressure and a capillary suction corresponding to a relative humidity of 60% and temperature of 28 °C (see also Tab. 4-7). However, all materials are emplaced at ambient temperature at repository depth with the initial saturation values listed in Tab. 4-5. After backfilling, a pressure boundary condition is assigned to the model nodes, representing the backfill material at the right boundary of the model, in other words, the operations tunnel connecting to the access tunnel and the facilities for EUU. The pressure prescribed at this boundary is equal to the pressure computed at the corresponding location in simulations using the repository model (see Section 4.3.2.5).

Similarly, a gas source term is assigned to the model nodes, representing the backfill material at the left boundary of the model, in other words, the operations tunnel connecting to the L/ILW emplacement caverns. The source term is equal to the transient of gas flux arriving at the V2-L/ILW seal as computed with simulations using the repository model (see Section 4.3.2.5).

The extraction of pressure transients and gas fluxes from the repository model as input for the V2-L/ILW model is always done within the same assessment case, so that a simulation with V2-L/ILW model always corresponds to a “parent” simulation of the repository model.

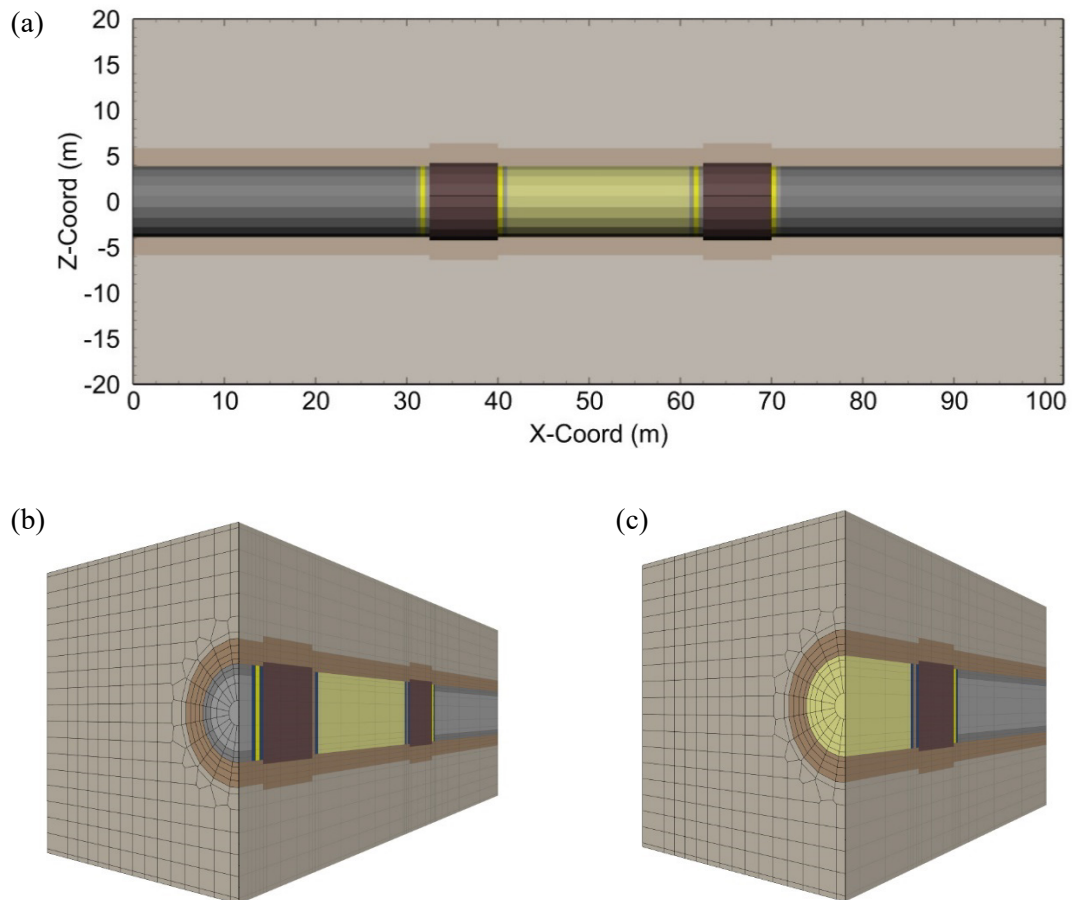


Fig. 4-4: Geometry of the V2-L/ILW model

(a) 3D view of operations tunnel with seal; (b) half-tunnel close-up with vertical cross-section through the operations tunnel; (c) half-tunnel close-up with vertical cross-section through sealing element.

It should be noted that the geometry of the V2-L/ILW model is based on a provisional design may be refined and modified in future stages of the project.

Tab. 4-5: Hydraulic and two-phase flow parameters for the materials in the sealing sections

	Symbol, unit	S/B ¹	Compacted bentonite ²	Transition layers	Abutments	Liner
Hydraulic parameters						
Porosity	ϕ [-]	0.35	0.45	0.30	0.20 ⁴	0.10
Intr. permeability	k [m ²]	5.0E-18	1.0E-20 ²	1.0E-14	1.0E-17	3.0E-16
Pore compressibility	C_p [1/Pa]	1.0E-09	3.0E-09	1.0E-09	7.0E-10	7.0E-10
Initial water content	w_r [%]	18.0	18.0 ²	15.0	10.0	7.0
Initial saturation	S_w [-]	0.50	0.40 ²	0.50	0.50	0.70
Two-phase flow parameters						
van Genuchten capillary strength ³	P_0 [Pa]	4.0E03	2.2E07 ²	4.0E03	4.0E03	2.0E06
Shape param.: vG-n (k_r) vG-n (P_c) vG-n (P_c)	vG-n (k_r) vG-n (P_c) vG-n (P_c)	2.5 ¹	1.5	2.0	2.0	2.0
Residual water saturation	$S_{lr}(k_r)$	0.30 ¹	0.00	0.05	0.05	0.05
	$S_{lr}(P_c)$	0.01	0.01	0.01	0.01	0.01
Residual gas saturation	$S_{gr}(k_r)$	0.0	0.0	0.0	0.0	0.0

¹ Sealing element assumed to be S/B in V1-L/ILW and V2-L/ILW; alternative values $n = 1.5$ and $S_{lr}(k_r) = 0.05$.

² Sealing element assumed to be compacted bentonite in V3, V1-HLW, V2-HLW.

³ Default value $T_0 = 20$ °C for temperature scaling.

⁴ Capillary porosity 15%.

4.3.2.4 V3 model

The V3 model is implemented with a hybrid radial-rectangular mesh in 3D and represents part of the central area connecting to the access shaft, along with the access shaft itself. The radial part of the mesh is used for the shaft, whereas the rectangular part is used for the Opalinus Clay and confining geological units surrounding the shaft. The access tunnel to the shaft (here referred to as “access tunnel”) is approximated with a rectangular cross-section. Selected views of the model are shown in Fig. 4-5.

The shaft section included in the model extends from the shaft sump in the Opalinus Clay to the bottom of the Malm formation, which also corresponds to the top boundary of the model. Below the repository, or below the shaft, the model extends to the bottom of the AL unit (see Nagra 2024e for complete list of stratigraphic units and formations as well as their respective representation in performance assessment modelling). The geological units in this interval are grouped in 5 layers in the V3 model, namely (from bottom to top): Lias (ML+AL), Opalinus Clay, SCAD, Herrenwis, AD, and Malm (MM1+CM+MM2). The formation thicknesses correspond to those at the shaft location (extracted from the repository model, see Section 4.3.2.5). In the horizontal direction, the model extends 200 m into the rock away from the axis of the shaft. The

access tunnel has a T-shape with two sides representing the connection to the rest of the repository and a 26-m-long dead-end part connecting to the shaft. The resulting dimensions of the model are thus 400×226×317 m (L×W×H).

The V3 seal is discretised into its main components (the compacted bentonite sealing element, the filter layers within the sealing element, the abutments and the transition layers) with their respective dimensions (Fig. 4-5, see also Appendix A). The hydraulic and two-phase flow parameters used in the base case are given in Tab. 4-5.

The modelled rock formations are assumed to be initially fully water-saturated, and hydrostatic pressures are assigned to the model nodes prior to repository construction. The top and bottom boundaries of the 3D grid have imposed constant pressure conditions. The initial pressure distribution and hydrostatic values at the top and bottom boundaries correspond to a depth of 859 m b.g.l at the centre of the access tunnel. The numerical simulations with this model are run under non-isothermal conditions, and fluid properties such as viscosity and density depend on temperature. This is depth-dependent, assuming a temperature gradient of 0.043 °C/m and a surface temperature of 10 °C. Internal boundary conditions are assigned to open tunnels during ventilation through prescribed atmospheric pressure and a capillary suction corresponding to a relative humidity of 60% and temperature of 28 °C (see also Tab. 4-7). However, all materials are emplaced at ambient temperature at repository depth with the initial saturation values listed in Tab. 4-5. After backfilling, a pressure boundary condition is assigned to the model nodes representing the backfill material at the right boundary of the model, where the access tunnel at the side of the HLW repository is located. The pressure prescribed at this boundary is equal to the pressure computed at the corresponding location in simulations using the repository model (see Section 4.3.2.5).

A gas source term is assigned to the model nodes representing the backfill material of the access tunnel at the left boundary of the model where the access tunnel at the side of the L/ILW repository is located. The source term is equal to the transient of gas flux arriving at the access tunnel connecting to the access shaft as computed with simulations using the repository model (see Section 4.3.2.5).

The extraction of pressure transients and gas fluxes from the repository model as input for the V3 model is always done within the same assessment case so that a simulation with the V3 model is always bound to its corresponding “parent” simulation of the repository model.

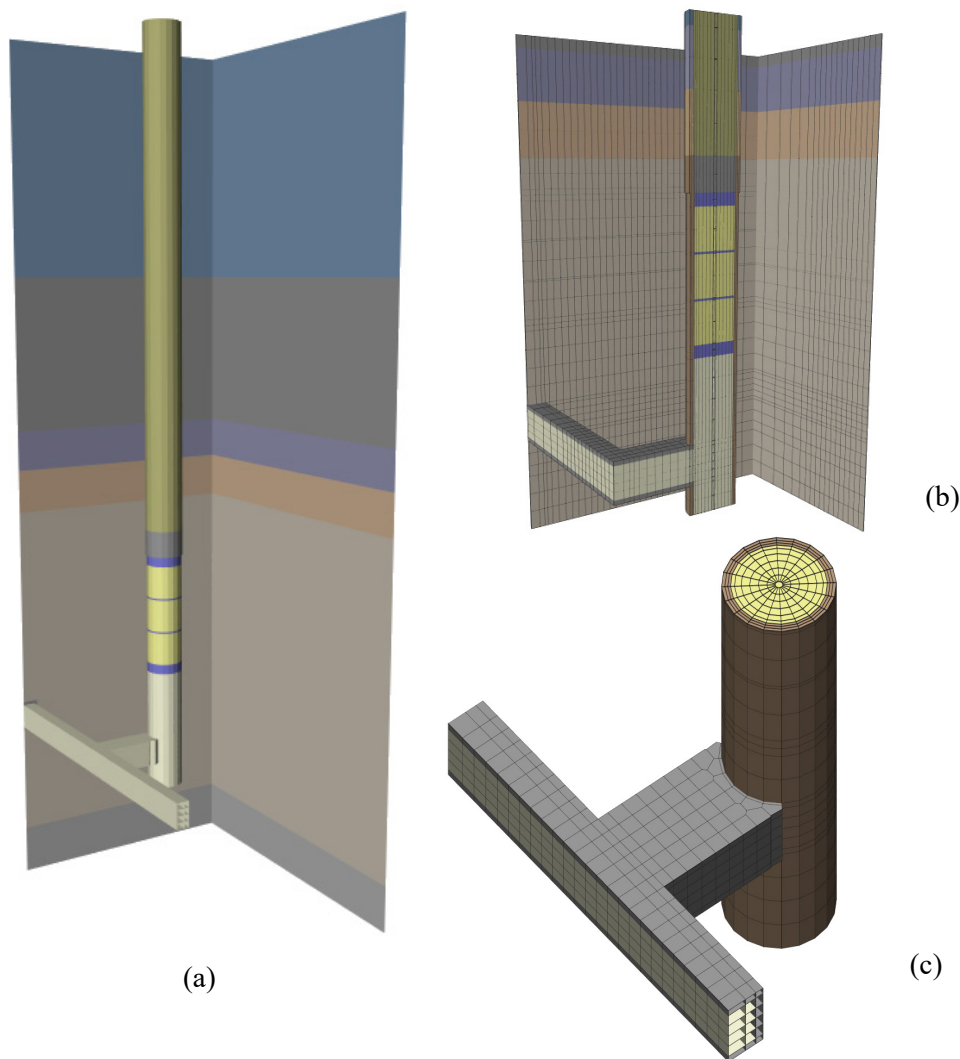


Fig. 4-5: Geometry of the V3 model

(a) 3D view of entire length of modelled shaft; (b) close-up with vertical cross-section through the middle of the shaft, incl. EDZ; (c) close-up with horizontal cross-section through the shaft below the sealing element, including EDZ.

It should be noted that the geometry of the V3 model is based on a provisional design may be refined and modified in future stages of the project.

4.3.2.5 Repository model

The repository model is implemented with a nested rectangular IFD mesh in 3D based on a stylised representation of the entire combined repository with the surrounding host rock and confining geological units. Selected views of the model are shown in Fig. 4-6.

In the vertical direction, the model spans approximately 2.3 km from top to bottom with thickness varying by location, depending on the formation thicknesses, or seismic surfaces. Geological groups represented explicitly in the model include the upper part of the Permo-Carboniferous (ca. 1,000 m thickness), the Muschelkalk, the Keuper (subdivided into 5 subunits), the Lias (subdivided into 2 subunits), the Opalinus Clay, the Upper Dogger (subdivided into 3 subunits),

the Malm (subdivided into 4 subunits) and the Tertiary. Nagra (2024e) describes the subdivisions within the geological abstraction of the stratigraphy for performance assessment modelling as well as the parameters assigned to the modelled geologic units.

In the horizontal direction, the X-axis of the model is oriented along the operations tunnels, which corresponds to $\sim 10^\circ$ counterclockwise rotation from the NS axis (Fig. 4-6). The model covers an area of $6.7 \times 3.24 \text{ km}^2$ spanning from (675460, 264370) in SW to (681520, 268690) in NE. Repository structures represented explicitly in the model include the emplacement rooms (7 L/ILW emplacement caverns and 20 HLW emplacement drifts), branching tunnels, operations/ventilation/construction tunnels, access tunnels, pilot repositories (separate for L/ILW and HLW, including emplacement rooms, branching/operations and observation drifts), tunnels to the central area and the facilities for the EUU, and operations/ventilation/construction shafts. The model discretisation is finer within the repository structures and coarsens in the direction of the model boundaries. The L/ILW emplacement caverns are discretised in 4 layers and 2 rows of elements in the model, each measuring $5 \times 10 \times 2.5 \text{ m}$ (Fig. 4-6b); the HLW drifts are discretised with a single layer and single row of elements with the same size (Fig. 4-6c). The adjacent branching and operations tunnels as well as tunnels in the central area and EUU are similarly discretised in 2 layers and 2 rows. The EDZ is modelled on all sides of the L/ILW emplacement caverns and only at the top and bottom of the remaining repository tunnels. Each tunnel in the repository, including the emplacement rooms, is represented as a homogenised material with the effective properties listed in Tab. 4-6. The porosities of homogenised materials are subsequently subject to volumetric scaling to adjust for geometric differences between modelled and designed cross-sections.

The modelled rock formations are assumed to be initially fully water-saturated. Pressures and temperatures prior to repository construction are calculated with a steady-state run. The top boundary corresponds to the ground surface and is assigned constant atmospheric pressure and a temperature of 10°C . The numerical simulations are run under non-isothermal conditions. The initial, ambient temperature assigned to the model corresponds to a surface temperature of 10°C and a basal heat flow of 120 mW/m^2 assigned to the bottom of the Permo-Carboniferous. All materials within the repository are emplaced at 28°C with 50% initial saturation. The operational and ventilation phases are summarised in Tab. 4-7.

Gas source terms (and water sink terms, when applicable) are assigned to the model nodes representing the L/ILW emplacement caverns and HLW emplacement drifts, respectively, as well as to all remaining tunnels except the shafts to account for corrosion of construction materials. Source (and sink) terms for L/ILW and HLW are distributed equally across all caverns and drifts in the model. Heat sources are assigned only in the HLW emplacement drifts, in every other element along each drift.

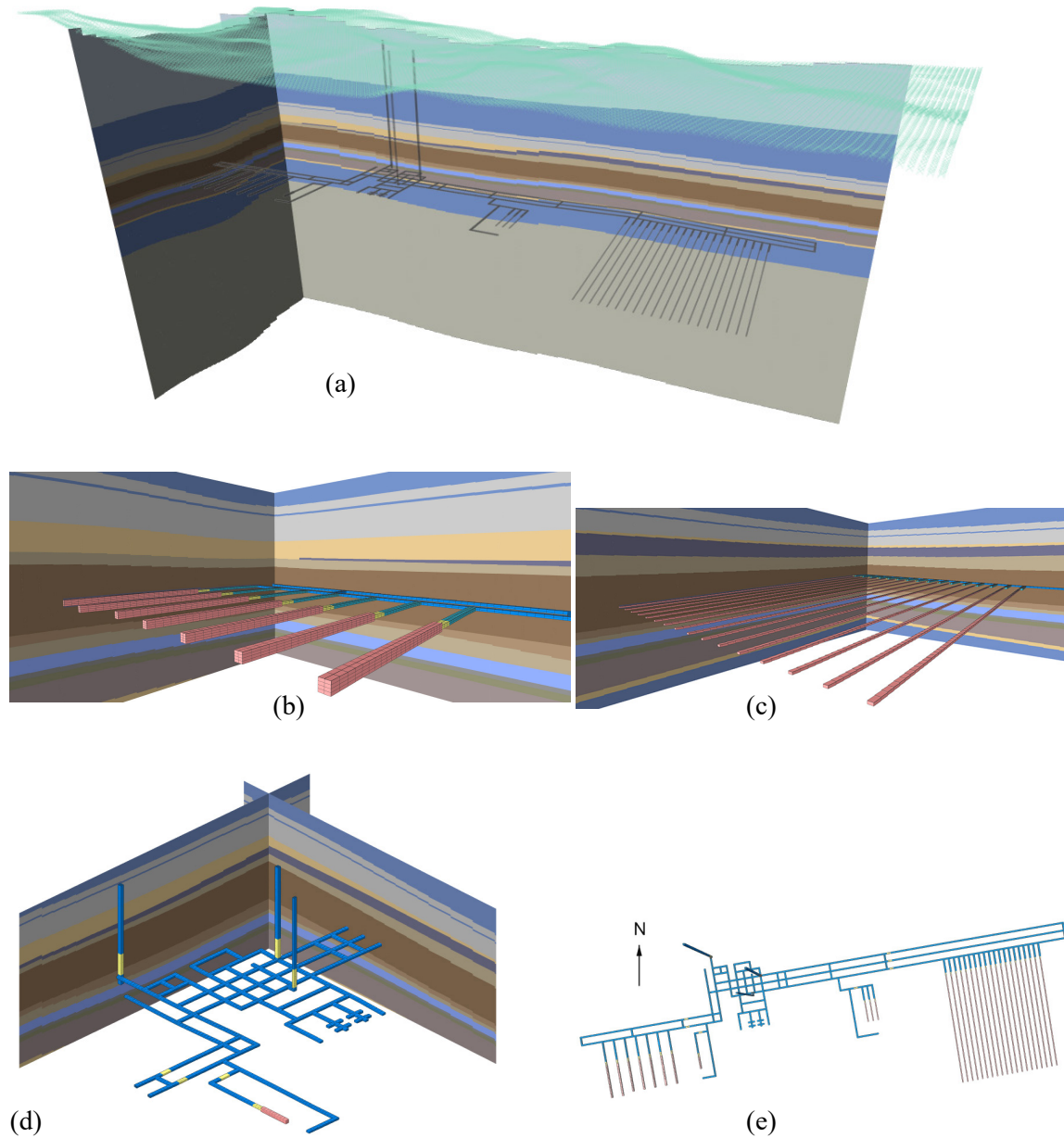


Fig. 4-6: Geometry of the combined repository model

(a) 3D view of the entire combined repository with a stack of geological formations; (b) close-up of L/ILW emplacement caverns (in pink) with sealing sections (in yellow) and branching/operations tunnels (in blue); (c) close-up of HLW emplacement drift (in pink) with sealing sections (in yellow) and branching/operations tunnels (in blue); (d) close-up of central area and facilities for EUU; (e) plan view of all repository structures.

It should be noted that the geometry of the combined repository model is based on a provisional design may be refined and modified in future stages of the project.

Tab. 4-6: Hydraulic and two-phase flow parameters assigned to the repository components

Repository tunnel^{1,2}	Porosity (-)	Int. perm. (m²)	Pore compr. (1/Pa)	vG P0 (Pa)	vG n (-)	vG Slr⁴ (-)
HLW drifts	0.25	3.0E-20	3.0E-09	1.0E07	1.54	0.00
HLW V1 seals (incl. pilot)	0.30	1.0E-20	3.0E-09	2.2E07	1.67	0.00
HLW branching tunnels (incl. pilot repository)	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30
HLW operations tunnel (excl. V2)	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30
HLW ventilation tunnel (excl. V2)	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30
HLW construction tunnel (excl. V2)	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30
HLW connecting tunnels	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30
HLW operations tunnel for pilot repository (excl. V2)	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30
HLW observation drift	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30
HLW pilot repository drift	0.25	3.0E-20	3.0E-09	1.0E07	1.54	0.00
L/ILW caverns	0.20	1.0E-15	5.0E-10	2.1E05	2.00	0.05
L/ILW caverns V1 seals ³ (incl. Pilot repository)	0.30	5.0E-18	1.0E-09	4.0E03	2.50	0.20
L/ILW branching tunnels (excl. pilot repository)	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30
L/ILW operations tunnel (excl. V2)	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30
L/ILW ventilation tunnel (excl. V2)	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30
L/ILW connecting tunnels	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30
L/ILW operations tunnel for pilot repository (excl. V2)	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30
L/ILW observation drift	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30
L/ILW pilot repository cavern	0.20	9.7E-15	5.0E-10	2.1E05	2.00	0.05

Tab. 4-6: Cont.

Repository tunnel ^{1,2}	Porosity (-)	Int. perm. (m ²)	Pore compr. (1/Pa)	vG P0 (Pa)	vG n (-)	vG Slr ⁴ (-)
Central area	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30
Access tunnel	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30
V3 (all shafts)	0.30	1.0E-20	3.0E-09	2.2E07	1.54	0.00
V2-HLW	0.30	1.0E-20	3.0E-09	2.2E07	1.67	0.00
V2-L/ILW ³	0.30	5.0E-18	1.0E-09	4.0E03	2.50	0.20
Access shaft (excl. V3)	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30
Ventilation shaft (excl. V3)	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30
Construction shaft (excl. V3)	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30
Facilities for EUU	0.35	1.0E-15	1.0E-09	4.0E03	2.50	0.30

¹ Specific heat: 964 (J/kg/°C) in HLW emplacement drifts, V1-HLW, V2-HLW, V3; 920 (J/kg/°C) in all the rest.

² Residual gas saturation assumed to be zero in all materials.

³ Alternative values may be considered as: n = 1.5 and Slr = 0.05.

⁴ Value for relative permeability (value for capillary pressure in all tunnels: 0.01).

Remaining parameters: values from granular bentonite material (GBM) in HLW emplacement drifts, V1-HLW, V2-HLW, V3; values from S/B in all the rest.

4.4 Assumptions and conservatism

The modelling workflow elaborated in the previous sections is used for the model-based assessment presented in Chapter 5. In general, the objectives of the assessment (Sections 1.1.1 and 4.1) are formulated for a real physical system, namely the deep geological repository, but are addressed using modelled representations thereof. In this process, assumptions are necessary and must be chosen such that they add conservatism to the assessment or, at a minimum, negligibly impact it.

The assessment of effects associated with geometric abstraction is inherent in the current workflow through the integration of and comparisons between repository- and component-scale models summarised in Tab. 4-7 (see also Section 4.2.2). Differences in model results must be traceable and justifiable with the assumptions, boundary conditions and geometric representations used in each case (Nagra 2024e). Due to their level of detail, component models in general allow more detailed appraisal of state variables, especially when these may exhibit contrasts at material interfaces, such as saturation. One example is the HLW disposal canister surface and adjacent bentonite. However, from a mathematical viewpoint, the principle of superposition inherent in the component-scale models of emplacement rooms implies an infinite number of emplacement rooms positioned next to each other. This is of particular significance for HLW repository modelling, as pressure estimates for single-drift models can be overly conservative (Nagra 2024e).

Moreover, the component model for HLW is based on the inherent assumption that all drifts, and in extension all waste, are identical (e.g., of the same type of SF). This model is therefore used to evaluate nearfield saturation and temperature at the canister and bentonite but not for pressure buildup. Similarly, pressure estimates in L/ILW single-cavern models depend on the gas storage volume connected to the cavern and require appropriate consideration as described in Section 4.3.2.1. On the other hand, repository-scale modelling represents the entire, finite disposal area with the surrounding rock mass and tunnels connected to it. The drawback in this case is the averaged representation of materials, and therefore state variables, within the emplacement rooms (Nagra 2024e).

Tab. 4-7: Overview of gas transport models used in this report

	Gas transport models				
	Total system	Components			
Model aspect	Repository	L/ILW	HLW	V2-L/ILW	V3
Size (L×W×H)	6,700×3,240 m (vertical extent variable)	643.6×40×11 m	1,037×20×112 m	100×54×310 m	400×226×317 m
Stratigraphy considered	Permo-Carboniferous to Tertiary	Opalinus Clay	Opalinus Clay (Permo-Carboniferous to Tertiary with 1D elements)	Argillaceous Lias to Malm	Argillaceous Lias to Malm
Operational phases	0-21 years: ventilation central area up to V2 seals	-	-	-	0-96 years: ventilation
	21-36 years: ventilation all tunnels except HLW emplacement tunnels	21-36 years: ventilation	-	21-56 years: ventilation	
	36-46 years: ventilation HLW tunnels, backfilled L/ILW caverns	36 years: backfilled	36-46 ² years: ventilation		
	46-56 years: backfilled HLW tunnels		46 ² years: backfilled		
	56-96 years: backfilled L/ILW and HLW disposal areas up to V2 seals			96 years: backfilled	
	96 years: backfill of remaining tunnels				
# elements	~ 437,000	~ 189,000 ¹	~ 154,000	~ 51,000	~ 134,000

¹ model version with operations tunnel up to V2-L/ILW

² simulations implemented in terms of time relative to emplacement, e.g., 0-2 years

Abstraction through homogenisation is common in and inherent to modelling workflows. Even on the component level, where finer discretisation is feasible, it is assumed that materials emplaced in the repository and the surrounding rock formations can be represented as homogeneous porous media with effective hydraulic, transport and thermal properties. The EDZ surrounding the repository structures is also homogenised and represented in the models in a stylised fashion as shown in the model descriptions in Section 4.3.2.

As discussed in Section 4.1, in this report, uncertainty is addressed in a deterministic fashion. Comprehensive probabilistic assessment of propagation of uncertainty from homogenisation is addressed separately in the performance assessment (Nagra 2024e).

Process abstraction relates to the approximation of physical processes in mathematical and numerical models. In the present analyses, gas transport modelling is performed using the EOS5 equation-of-state module of TOUGH3 (Jung et al. 2018). This module assumes that all gases in the repository have the properties of hydrogen. Conservatively for pressure, molecular diffusion is deactivated in the simulations, unless stated otherwise in the description. Furthermore, the corrosion and degradation of materials in the present analyses are conservatively decoupled from the availability of water for the reactions. In reality, gas generation ceases in dry conditions or at low relative humidity, as water availability is considered to be the most important limiting factor for all processes that generate gas (e.g., degradation of organics and corrosion of metals). Similarly, it is conservatively assumed that gas generation from the L/ILW repository section starts immediately after emplacement, despite the highly alkaline near-field conditions decreasing corrosion and inhibiting microbial activities. The duration of the operational or ventilation phases, respectively, is also simplified in the model implementations. These are, however, chosen such that they provide consistency across the workflow and, in particular, between the component models and the repository model as shown in Tab. 4-7.

Additional assumptions related to individual assessment cases are provided in Section 5.2.

5 Model-based assessment

5.1 Overview

The model-based assessment is performed using the modelling workflow described in Chapter 4 to reach objectives *Obj2* to *Obj4* (Sections 1.1.1 and 4.1). It is implicit in all three objectives that the overall analysis requires appraisal of system perturbations, which can be postulated by synthesising individual assessments of system variants. In the present analysis, a so-called *base case* is formulated and enveloped by deterministic variants. The base case is defined as the expected evolution of the system, under the phenomenological consideration and best estimates of input data used in the analysis (see Chapter 4). The deterministic variants in the present analysis do not aim to capture and evaluate explicitly every possible perturbation in the system. Instead, they are a subset selected to demonstrate the functionality and robustness of the repository system in terms of gas transport and hydraulic evolution. The complete list of cases and specifications used in each case is given in Section 5.2.

5.2 Specifications of base case and assessment cases

As introduced in Chapter 4, the assessments can be conceptualised such that they can be implemented in the simulation variants by means of simplified configurations and inputs. An overview of all cases presented in this report is given in Tab. 5-1. These comprise 12 cases evaluated from a total of 33 model simulations. These are elaborated in more detail below.

Base case (Case 1)

In the base case, material parameters correspond to their reference values listed in Tab. 4-1, Tab. 4-2, Tab. 4-3, Tab. 4-4, Tab. 4-5, Tab. 4-6 and Tab. 4-7. Gas generation rates are calculated from the best estimate values of corrosion and degradation rates. Each transport model introduced in Chapter 4 provides one simulation that contributes to the base case results: the L/ILW near-field and V1-L/ILW model (described in Section 4.3.2.1), the HLW near-field and V1-HLW model (Section 4.3.2.2), the V2-L/ILW model (Section 4.3.2.3), the V3 model (Section 4.3.2.4), and the repository model (Section 4.3.2.5). The simulations with the repository and near-field models account for generation of gas (L/ILW, HLW) and heat (HLW) based on the best-estimate rates. In the repository model, the heat source corresponds to the average heat rates per canister type. The repository model simulation provides gas inflow at the upstream boundary of the V2 and V3 models (see also Chapter 4). In particular for the L/ILW near-field model, both model variants described in Section 4.3.2.1 are used: the first version assuming a permeable operations tunnel extending until an impermeable V2-L/ILW seal and the second assuming a permeable operations tunnel extending all the way to an impermeable V2-HLW seal. In the HLW near-field model, three heat generation rates are explicitly considered for the HLW disposal canisters, namely for those containing PWR-MOX, PWR-UO₂, and BWR waste types. The results of the base case are provided in Section 5.3.1.

Case 2

In Case 2, the generation of gas is neglected, and all gas source terms are set to zero. Heat generation (HLW section) is also set to zero. As in the base case, material parameters correspond to their reference values, and each model from the available portfolio is used to contribute a simulation to the analysis. The results of Case 2 are provided in Section 5.3.2.

Case 3

In Case 3, the upper bound estimates are taken for the corrosion and degradation rates used to calculate the gas source terms, resulting in the highest estimate of gas generation rate in the repository. All models used in the base case are modified accordingly. Conservatively for gas pressure buildup, the L/ILW near-field model version corresponding to an impermeable V2-L/ILW seal is used. Note that this simulation assumes a fixed inventory of metallic and organic materials that generate gas. As such, gas generation rates, which are initially higher than the base case, tail off earlier in the post-closure phase due to the materials corroding or degrading completely more quickly. The results of Case 3 are provided in Section 5.3.3.

Case 4

In Case 4, the lower bound estimates are taken for the corrosion and degradation rates used to calculate the gas source terms, resulting in the lowest estimate of gas generation rate in the repository. All models used in the base case are modified accordingly. Note that, due to the assumption of a fixed inventory of degradable and corrodible materials, in this simulation the gas generation rates, which are initially lower than in the base case, persist longer in the post-closure phase. The results of Case 4 are provided in Section 5.3.4.

Case 5

In this case, the corrosion rate of iron and carbon steel for $\text{pH} \geq 10.5$ is increased from 6 nm/a to 250 nm/a. Note that this metal group corresponds to 77% of all metals in the L/ILW inventory (Fig. 2-3). In comparison, the upper bound value used in Case 3 is 20 nm/a. All other corrosion and degradation rates are kept at their best estimate values. Only the L/ILW near-field model is used for this assessment. For more conservatism, the assessment is carried out with the model version assuming impermeable V2-L/ILW. Regarding the gas generation rate, see final note at the end of Case 3 description, which applies similar for this case. The results of Case 5 are provided in Section 5.3.5.

Case 6

In addition to gas generation, this case considers the consumption of water associated with corrosion of metallic materials. The mass of water consumed is approximated from the mass of generated hydrogen (from all metals or corrosion reactions, respectively), using the stoichiometry coefficients of the corrosion reaction for iron and carbon steel (Section 3.1.2). Following a similar approach as that used for gas generation, water consumption in the model is not implicitly coupled to state variables (see also Section 4.2.2). In practical terms, in this simplified approach, the water sink is imposed at the waste packages regardless of pressure and saturation. The assessment is performed using the L/ILW near-field model (model version for impermeable V2-L/ILW). The results of Case 6 are provided in Section 5.3.6.

Case 7

This case combines the best estimates of gas generation rates with the reference values for all material parameters except the permeability for the sealing element (S/B) of the V1-L/ILW seal, which is decreased to $1.E-19 \text{ m}^2$. Only the L/ILW near-field model assuming an impermeable V2-L/ILW is used for this assessment. The results of Case 7 are provided in Section 5.3.7.

Case 8

This case combines the best estimates of gas generation rates with the reference values for all material parameters except the permeability for the sealing element (S/B) of the V2-L/ILW seal, which is decreased to $1.E-19 \text{ m}^2$. The repository model and the V2 model are used for this assessment. The results of Case 8 are provided in Section 5.3.8.

Case 9

This case combines the best estimates of gas generation rates with the reference values for all material parameters except the permeability for the sealing element (compacted bentonite) of the V3 seal, which is increased to $1.E-19 \text{ m}^2$. The repository model and the V3 model are used for this assessment. The results of Case 9 are provided in Section 5.3.9.

Case 10

In Case 10, the porosities of M1 mortar, LC-86H container's walls, waste packages, Dorodur, liner and concrete in the L/ILW cavern are reduced by 20%. All other material parameters and gas generation rates correspond to their reference values. Only the L/ILW near-field model assuming an impermeable V2-L/ILW is used for this assessment. The results of Case 10 are provided in Section 5.3.10.

Case 11

This case focuses on the HLW near-field for conservative estimates of heat generation from the SF types. The gas source term is identical in all three cases, corresponding to the best estimate rates for the reference steel canister. The heat source term per canister is varied, using a representative maximum value for each PWR-MOX, PWR- UO_2 and BWR canister type, respectively. This assessment case therefore incorporates 3 simulations using the HLW near-field and HLW-V1 model. The results of Case 11 are provided in Section 5.3.11.

Case 12

This case modifies Case 4 (lower bound corrosion rates) by decreasing the intrinsic permeability of the sealing element (S/B) of the V1-L/ILW to $1.E-20 \text{ m}^2$ after 10,000 years. In addition, molecular diffusion is activated in the simulation. Only the L/ILW near-field model is used for this assessment (model version for impermeable V2-L/ILW). The results of Case 12 are provided in Section 5.3.12.

Tab. 5-1: Overview of assessment cases

Case #	Description of assessment cases Conceptualisation and input used	Models
1	Base case: expected evolution of the repository system - material parameter values according to reference values (Chapter 4) - best-estimate gas generation rates	Repository
		L/ILW+V1 ^{1,2} (×2)
		HLW+V1 ³ (×3)
		V2
		V3
2	Repository resaturation: evolution without gas sources - material parameter values same as Case 1 - no gas generation, no heat generation	Repository
		L/ILW+V1 ²
		HLW+V1
		V2
		V3
3	Repository evolution for upper bound gas generation - material parameter values same as Case 1 - upper bounding values gas generation rate	Repository
		L/ILW+V1 ²
		HLW+V1 ³
		V2
		V3
4	Repository evolution for lower bound gas generation - material parameter values same as Case 1 - lower bounding values gas generation rate	Repository
		L/ILW+V1 ²
		HLW+V1 ³
		V2
		V3
5	L/ILW cavern with extreme carbon steel corrosion - material parameter values same as Case 1 - best estimate gas generation rates except for carbon steel, which is fixed at 250 nm/a for pH ≥ 10.5	L/ILW+V1 ²
6	L/ILW cavern evolution with water consumption - material parameter values same as Case 1 - best estimate gas generation rates w. water consumption	L/ILW+V1 ²
7	Low-permeability variant V1-L/ILW seal - intrinsic permeability S/B in V1: 1.E-19 m ² - best-estimate gas generation rates	L/ILW+V1 ²
8	Low-permeability variant V2-L/ILW seal - intrinsic permeability S/B in V2: 1.E-19 m ² - best-estimate gas generation rates	Repository
		V2
9	High-permeability variant V3 seal - intrinsic permeability compacted bentonite in V3: K=1.E-19 m ² , P ₀ = 7 MPa - best-estimate gas generation rates	Repository
		V3

Tab. 5-1: Cont.

Case #	Description of assessment cases Conceptualisation and input used	Models
10	L/ILW cavern with low porosity - porosity of M1, LC-86H, waste packages, Dorodur, liner and concrete reduced by 20% - best-estimate gas generation rates	L/ILW+V1 ²
11	HLW near-field evolution for different heat outputs - representative maximum heat generation - best estimate gas generation rates	HLW+V1 ⁴ (×3)
12	Extreme V1 permeability change in post-closure phase - lower bounding values gas generation rate - with molecular diffusion - restart after 10,000 years with intrinsic permeability S/B in V1-L/ILW: 1.E-20 m ²	L/ILW+V1 ²

¹ assuming operations tunnel extends to V2-HLW

² assuming impermeable V2-L/ILW

³ representative average heat generation from PWR-MOX, PWR-UO₂, BWR disposal canisters

⁴ representative maximum heat generation from PWR-MOX, PWR-UO₂, BWR disposal canisters

5.3 Model-based assessments

Most of the simulations are performed for a period of 100,000 years as this period is generally sufficient to demonstrate peak pressure and safety-relevant hydraulic effects in the repository. The base case is simulated until 1,000,000 years. As described in Section 4.2.2, the first component of the modelling workflow is the calculation of gas generation rates from the corrosion and degradation of materials in the repository. The results from the gas generation tool are shown in Fig. 5-1, with three estimates provided: the upper bound values, used in assessment Case 3, the lower bound values, used in Case 4, and the best estimate (reference) values, used in the remaining assessment cases except Case 2 (that assumes there is no gas and heat generation). These are accordingly tied to the upper bound, best estimate, and lower bound corrosion and degradation rates discussed in Chapter 3 (see Tab. 3-1 and Tab. 3-2). The rates are provided as volume of gas (in m³ standard ambient temperature and pressure) generated per emplacement room in the L/ILW and HLW sections of the combined repository, respectively, per year (Fig. 5-1a; b), and cumulative (Fig. 5-1c).

In the L/ILW emplacement caverns, the upper bound value is initially approximately 5 times higher than the best estimate but decreases at later times and becomes lower than the best estimate due to the faster depletion of materials when corrosion rates are higher. Conversely, the lower bound values are between 1 and 2 orders of magnitude lower than the best estimate values and, as such, gas generation persists longer than in the base case (not shown in Fig. 5-1).

In the HLW emplacement drifts, there are only two sources of gas generation: the steel canisters and the tubing ("tunnel F10" in Fig. 5-1). Gas generation from the corrosion of the HLW disposal canisters in compacted bentonite is constant until the canisters breach, which for the purposes of modelling is assumed to occur at 10,000 years for all canisters simultaneously. Once the HLW disposal canisters have breached, gas generation increases with the corrosion of the spent fuel assemblies and internal canister components not in contact with bentonite (see Tab. 3-1).

The upper bound corrosion rates result in the canister corroding entirely within $\sim 25,000$ years, compared to $\sim 115,000$ years in the base case.

The rate of gas generation in the L/ILW emplacement caverns is overall much higher compared to that in the HLW emplacement drifts. In the first 10,000 years, before the HLW canisters are assumed to breach in the model, the difference is between two and three orders of magnitude. After 1 million years, the cumulative volume of gas generated in the L/ILW emplacement caverns is nearly 3 times higher than that generated in the HLW emplacement drifts.

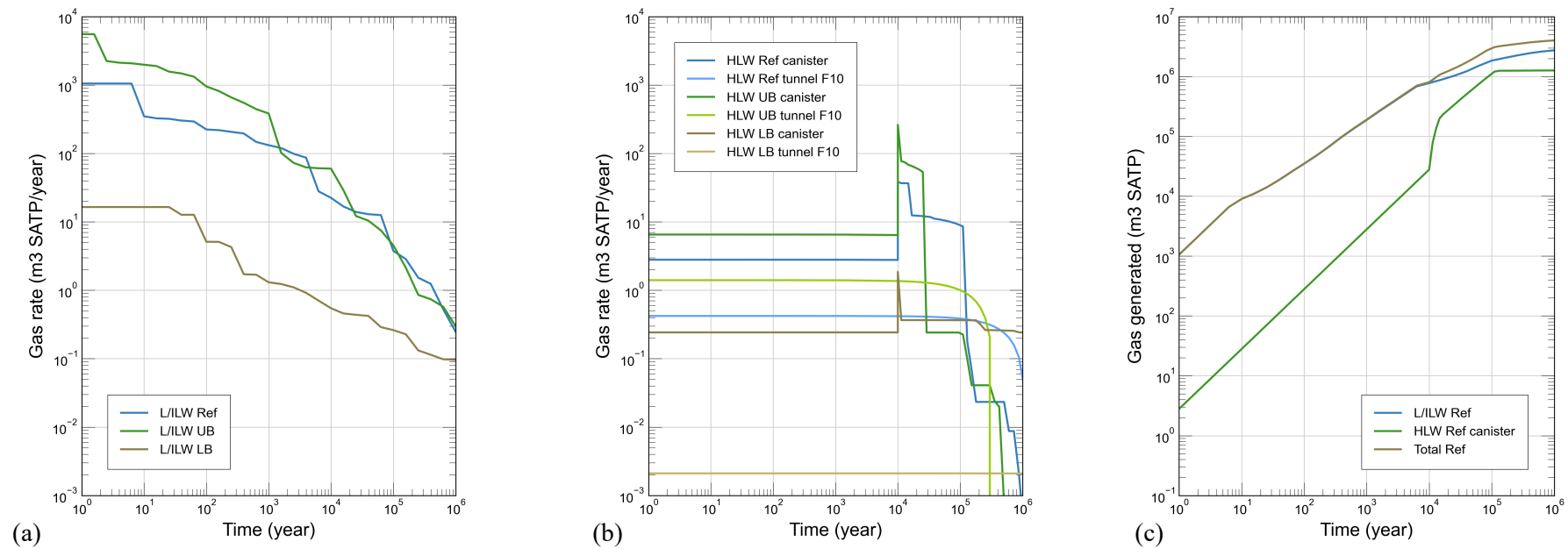


Fig. 5-1: Best estimate (Ref), upper bound (UB), and lower bound (LB) values of gas generation rates calculated per emplacement room with the gas generation tool for the (a) L/ILW, (b) HLW repository sections, and (c) respective cumulative volume

In general, the models can provide user-defined output of state variables (e.g., saturation, pressure, temperature) in space and time. Two main types of output are used in the present report:

- Spatial plots of gas saturation distributions at selected timesteps;
- Transients of gas saturations, pressures, and temperatures at selected locations.

Pressure corresponds to gas pressure when a gas phase is present, and liquid pressure when only water is present, respectively. The spatial plots of saturation essentially provide isolated snapshots of the hydraulic evolution. In that sense, their use in this report is limited, with the primary aim of helping the reader to visualise the problem under consideration rather than deriving quantitative conclusions. They complement the quantitative assessments which are predominantly based on the time-series plots of state variables. These comprise multiple observation points in the models that are deemed relevant to deliver key outcomes of the assessment. The observation points, shown in Fig. 5-2, are the following:

Repository model (Fig. 5-2a)

L/ILW cav: in the central L/ILW emplacement cavern (cavern 4);

V1 L/ILW: in the V1 seal of the central L/ILW emplacement cavern;

OT L/ILW: in the operations tunnel directly connected to the L/ILW emplacement caverns, before the V2 seal;

V2 L/ILW: in the V2 seal of the L/ILW repository section;

L/ILW cav pilot: in the pilot L/ILW emplacement cavern in the pilot repository;

OT central (L/ILW): in the operations tunnel between the V2-L/ILW seal and the facilities for the EUU;

HLW can: in the central HLW emplacement drift, within an element containing a heat source;

HLW bent: in the central HLW emplacement drift, within an element not containing a heat source;

V1 HLW: in the V1 seal of the central HLW emplacement drift;

OT HLW: in the operations tunnel directly connected to the HLW emplacement drifts, before the V2 seal;

V2 HLW: in the V2 seal of the HLW repository section;

HLW can pilot: in the emplacement drift of the HLW pilot repository, within an element containing a heat source;

HLW bent pilot: in the emplacement drift of the HLW pilot repository, within an element not containing a heat source;

OT central: in the operations tunnel between the V2-HLW seal and the facilities for the EUU;

OPA above HLW: in the Opalinus Clay, 30 m directly above the centre of the HLW disposal area.

All observation points in the repository model are taken from the same model layer. This corresponds to the third layer (bottom to top) out of four layers in the L/ILW emplacement caverns, and the second layer (top layer) out of two layers in the operations tunnels and sealing sections.

L/ILW near-field and V1-L/ILW model (Fig. 5-2b)

M1, waste top: in the M1 mortar, halfway between the top of the top disposal container and the roof of the emplacement cavern, between disposal container stacks 7 and 8 (counting from mouth of the cavern);

M1, waste bot: in the M1 mortar, between the bottom disposal containers stacks 7 and 8;

M1, mouth top: same as *M1, waste top* but between disposal container stacks 1 and 2 (counting from mouth of the cavern);

M1, mouth bot: same as *M1, waste bot* but between disposal container stacks 1 and 2;

S/B top: in the S/B sealing element of the V1 seal, top element at tunnel roof;

S/B bot: in the S/B sealing element of the V1 seal, bottom element at tunnel invert;

Trans. top: in the middle transition layer between sealing element and abutment, top element at tunnel roof;

Trans. bot: in the middle transition layer between sealing element and abutment, bottom element at tunnel invert;

Abut. top: in the abutment, top element at tunnel roof;

Abut. bot: in the abutment, bottom element at tunnel invert.

All observation points are located axially or at the centre of the tunnel, respectively.

HLW near-field and V1-HLW model (Fig. 5-2c)

CAN 2 top: at the second canister (counting from mouth of the emplacement drift);

PELL above CAN 2: in the bentonite directly adjacent to the second canister (5 cm from canister);

PELL mid: in the bentonite halfway between the second canister and the liner wall;

PELL top: in the bentonite directly adjacent to the liner wall;

PELL btw. CAN 2&3: in the bentonite between second and third canister, middle of emplacement drift;

LINER: in the liner above the second canister;

V1 branch side: in the bentonite of the V1 adjacent to the outer transition layer, middle of emplacement drift;

CAN 10 top: same as *CAN 2 top*, but at the tenth canister (counting from mouth of the emplacement drift);

OPA 20 m lateral: in the Opalinus Clay, at 20 m laterally from the tenth canister;

OPA 20 m above: in the Opalinus Clay, at 20 m directly above the tenth canister;

OPA 50 m above: in the Opalinus Clay, at 50 m directly above the tenth canister.

All observation points are located axially or at the centre of the tunnel, respectively.

V2-L/ILW model (Fig. 5-2d)

S/B top: in the S/B sealing element of the V2 seal, top element at cavern roof;

S/B bot: in the S/B sealing element of the V2 seal, bottom element at cavern invert;

EDZ: in the EDZ above *S/B top*;

VF1 top: in the VF1 backfill towards the caverns, top element at cavern roof;

VF1 bot: in the VF1 backfill towards the caverns, bottom element at cavern invert;

Liner: in the liner above *VF1 top*;

VF2 top: in the VF2 backfill towards the EUU, top element at cavern roof;

VF2 bot: in the VF2 backfill towards the EUU, bottom element at cavern invert;

Trans t.: in the transition layer between abutment and VF2 backfill, top element at cavern roof;

Trans b.: in the transition layer between abutment and VF2 backfill, bottom element at cavern invert.

All observation points are located axially or at the centre of the tunnel, respectively.

V3 model (Fig. 5-2e)

Seal: in the middle compartment of the bentonite sealing element of the V3 seal;

EDZ at seal: in the EDZ next to the seal;

Abutment: in the middle of the abutment above the sealing element;

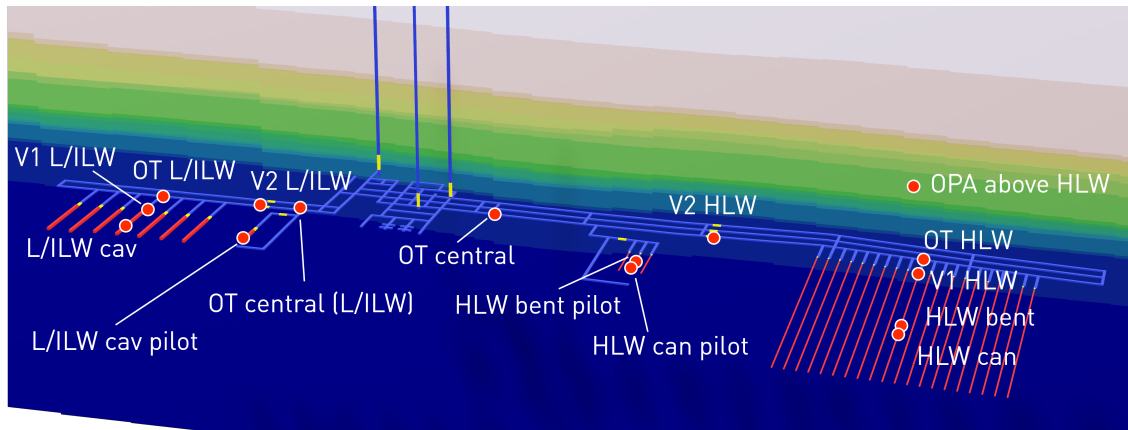
Shaft above seal: at the bottom of the shaft directly above the abutment;

Trans. below seal: in the transition layer below the sealing element;

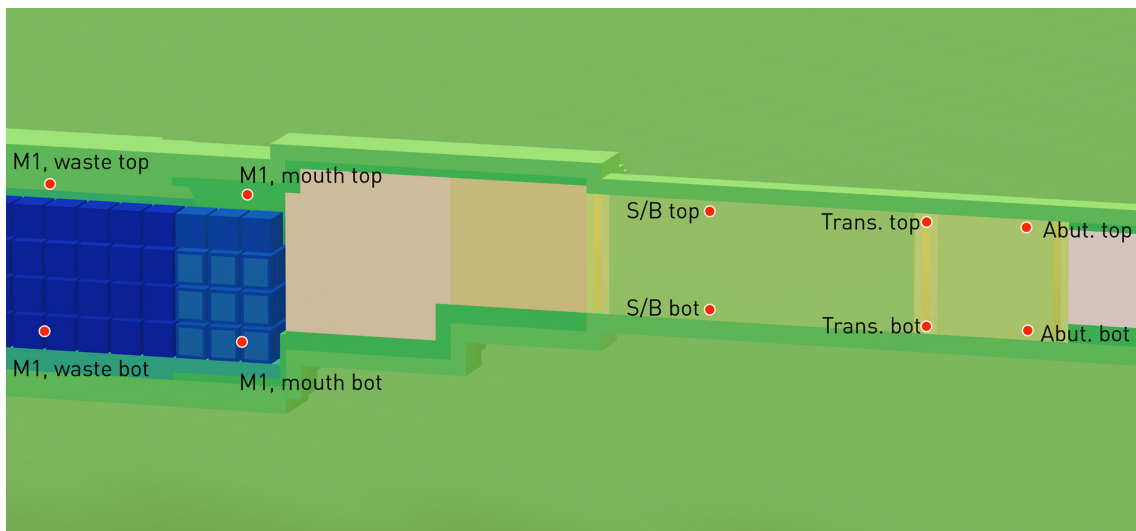
Shaft bot: in the shaft sump;

Access tunnel: in the access tunnel leading to the base of the shaft.

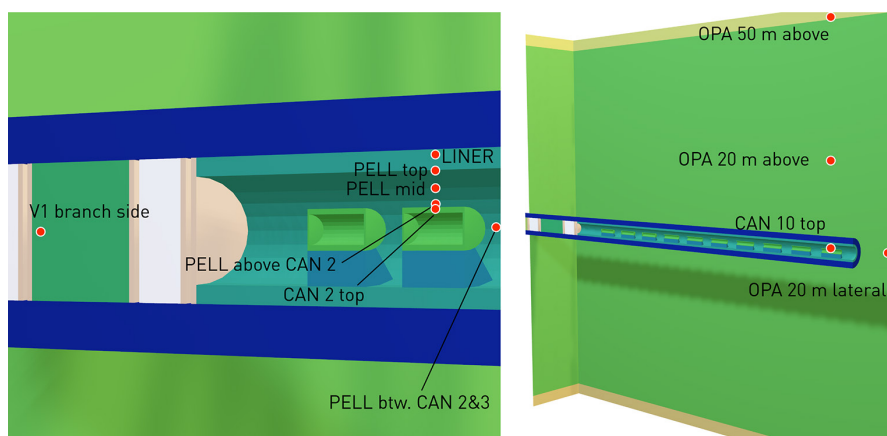
All observation points are located axially or at the centre of the shaft and access tunnel, respectively.



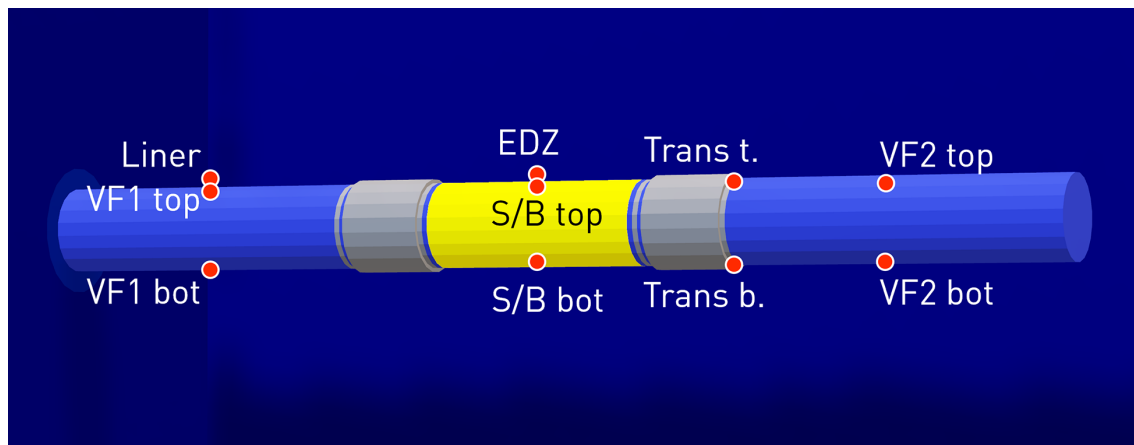
(a)



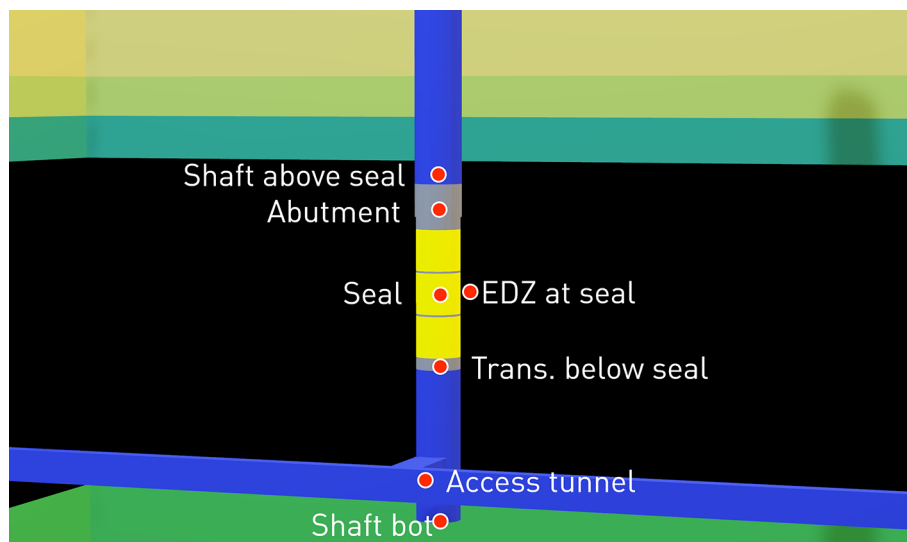
(b)



(c)



(d)



(e)

Fig. 5-2: Observation points used for simulated transients in the (a) repository model, (b) L/ILW near-field and V1-L/ILW model, (c) HLW near-field and HLW-V1 model, (d) V2-L/ILW model, and (e) V3 model

5.3.1 Case 1: Base case

The assessment for the base case draws on results from the repository model, as well as the component models as shown in Fig. 5-3 through Fig. 5-7. In general, the simulation results are consistent with the qualitative description of the repository evolution given in Section 4.1. Two distinct phases can be discerned. The first phase coincides with the early post-closure phase (hundreds of years) and is marked by the development of a thermal pulse extending radially (or taking an ellipsoid shape) around the HLW repository section from the heat released by the waste. The increasing temperature in the HLW emplacement drifts and surrounding rock results in a porewater pressure increase caused by the difference between the expansivity of porewater and of the pores, referred to as *differential thermal expansion*. Differential thermal expansion is mitigated when heat (and water) is transported away from the repository and, to some extent, when the affected porous materials are partially saturated with a more compressible gas.

The second phase of the evolution coincides with the late post-closure phase (thousands to tens of thousands of years) and is marked by the accumulation of gas in the L/ILW and HLW repository sections. The increasing gas mass in the repository structures also increases the pressure as gas compresses in the available pore volume, referred to as *gas pressure buildup*. Note that, as introduced in Section 4.1, the pore volume available to gas is also coupled to porewater exchange with the surrounding rock. In general, gas pressure buildup is mitigated when the generated gas can transport into sufficient pore volume and when it dissolves into the porewater of the host rock. As shown in Fig. 5-1, the rate of gas generated in the L/ILW caverns is orders of magnitude higher than that in the HLW drifts of the repository. The materials in the L/ILW and HLW repository sections are tailored accordingly. In the L/ILW section, materials are chosen so that gas generated in the emplacement caverns can be transported along the network of repository tunnels and in this way stored over larger volumes. In the HLW section, the gas generation rate is lower, and gas dissipates by radial transport and dissolution through the nearfield and surrounding Opalinus Clay.

A snapshot of this evolution is shown in the 3D spatial plot of gas saturation after 5,000 years shown in Fig. 5-3a. Overall, the repository structures are partially saturated, with higher gas saturations observed in the upper part of the tunnels. Gas saturations exceed 50% in most of the operations and access tunnels except some segments in the HLW repository section. The HLW emplacement drifts and all bentonite seals (V1-HLW, V2-HLW, V3) show gas saturations below 1%, whereas the shafts above the V3 seals are fully saturated with porewater.

The transients of temperature simulated in the L/ILW and HLW repository sections with the repository model are shown in Fig. 5-3b and Fig. 5-3c, respectively. The sharp temperature drops from ambient temperature (ca. 43 °C) to ventilation temperature (28 °C) during the first decades indicate the instantaneous opening of the respective repository structures at these times. After emplacement and backfilling, the temperature in the L/ILW repository structures starts to increase and equilibrate with the temperature of the surrounding rock after ~ 3,000 years. Due to the relatively small magnitude of temperature changes over this long period (assuming a ventilation and emplacement temperature of 28 °C), thermally induced effects on the hydraulic evolution of the L/ILW repository section are practically negligible. In the HLW repository section, the temperature increases sharply after emplacement owing to the heat sources, reaching a peak temperature of ~ 137 °C at the heat-generating elements. As discussed in Chapter 4, this value is only an approximation given the level of abstraction adopted in the repository model.

The transients of pressure simulated in the L/ILW and HLW repository sections with the repository model are shown in Fig. 5-3d and Fig. 5-3e, respectively. Note that in this figure and subsequent figures in this report, the pressure drop at the beginning of the ventilation phase corresponds to the decrease from the hydrostatic to atmospheric pressure in the repository tunnels. During the early post-closure phase of the L/ILW repository section, pressures increase faster in the emplacement caverns than in the operations tunnels due to the gas generation from the waste. This pressure gradient results in axial gas transport from the emplacement caverns to the adjacent tunnels, which is a key feature of the L/ILW repository section. After ~ 5,000 years, pressures equilibrate across the L/ILW structures while remaining below hydrostatic. From that time until the end of the simulation, all tunnels in the L/ILW repository section have approximately the same pressure at any given time, indicating that there is effective hydraulic connection across the tunnels with sufficient gas transport capacity to distribute the gas in the available pore volume. Hydrostatic pressure is reached in the L/ILW repository section after ~ 20,000 years. Pressures then continue to increase for ~ 70,000 years, when they reach a peak value of ~ 9.3 MPa before decreasing again towards the hydrostatic value as gas generation gradually diminishes. In the early post-closure phase of the HLW section of the repository, pressure first increases in the host rock surrounding the emplacement drifts due to the differential thermal expansion in the low-permeable rock. At the selected location ~ 30 m above the centre of the repository, pressure reaches ~ 13 MPa after 200 years.

Note that the thermally induced peak pressure will vary in location and time around the repository. In comparison, the thermally induced pressures in the emplacement drifts increase to nearly hydrostatic values after $\sim 2,000$ years, owing to the depressurisation and partial saturation of the near-field at the time of emplacement. Pressure then continues to increase due to gas accumulation in the HLW emplacement drifts, reaching ~ 10.5 MPa shortly after canister breach. Due to additional corrosion of the canister from inside (not in contact with bentonite), pressure continues to increase and reaches a maximum of ~ 11.8 MPa when the canister corrodes entirely after $\sim 115,000$ years. Note that the associated maximum gas-induced pressure in the Opalinus Clay (30 m above the tunnels) is ~ 10.5 MPa. Contrary to the thermally induced pressures that reach maximum values in the rock surrounding the tunnels, gas-induced pressures are higher at the gas source and dissipate in the rock away from the tunnels. After the corrosion of the steel canisters completes, pressures decrease steeply owing to the decline in the gas generation rate.

The transients of gas saturation simulated in the L/ILW and HLW repository sections with the repository model are shown in Fig. 5-3f and Fig. 5-3g, respectively. After the L/ILW repository section is backfilled, gas saturation increases continuously in the upper part of the operations and ventilation tunnels until the end of the simulation, owing to the buoyant gas migrating from the emplacement rooms and accumulating at the roof of the tunnels. In the middle of the L/ILW emplacement caverns, gas saturations decrease as porewater flows into the cavern for $\sim 10,000$ years and then increases with the accumulation of waste-generated gas until the end of the simulation. Overall, the gas saturation transients show a continuous path for gas in the L/ILW repository section, sustained by the axial transport of gas through the repository structures. Accordingly, the partially saturated tunnels contribute to the interface to the surrounding host rock that is available for dissolution of gas in porewater. Gas saturations in the HLW repository section vary depending on the location and backfill material, respectively. The operation and ventilation tunnels show overall increasing gas saturation similar to that of the tunnels in the L/ILW section of the repository. On the other hand, the emplacement drifts fully saturate with water within hundreds of years owing to the high suction of the bentonite material. As discussed in Chapter 4, these saturation values are indicative estimates due to the homogenisation applied in the repository model (see also Tab. 4-6). Some gas migrates through the Opalinus Clay above the repository at later times (i.e., $\sim 40,000$ years at 30 m above the HLW repository with gas saturations that remain below 1%).

Additional insights into the near-field evolution are gained with modelling on the component scale. Simulation results from the L/ILW and HLW near-field models are shown in Fig. 5-4 and Fig. 5-5, respectively. A snapshot of gas saturation after 1,000 years in the L/ILW emplacement cavern and V1-L/ILW seal is shown in Fig. 5-4a. At that time, water has accumulated in the lower part of the cavern, while gas has accumulated in the upper part and throughout the V1 seal due to buoyancy. Note that (high) gas saturation in the M1 mortar (which fills the gaps between waste packages and has high porosity and low capillary strength) is not shown in this spatial plot to enhance the visualisation of the waste packages. In general, porewater from the M1 will be taken up by disposal containers owing to their higher capillary strength. The waste packages show variable degrees of saturation depending on their elevation in the cavern and their interface area with the water-supplying M1. In that sense, a relatively dry mortar layer surrounding the LC-86H containers may form a low-capillarity barrier around the waste, limiting liquid transport between the waste and the surrounding environment. Furthermore, the array of high-porosity mortar between the containers constitutes a connected network of pathways with high effective gas permeabilities. Transients of gas saturation are shown in Fig. 5-4b; c for the model version assuming an impermeable V2-L/ILW seal. These indicate a temporary resaturation of the lower part of the emplacement cavern with porewater (after ~ 300 years) before pressure, shown in Fig. 5-4d, exceeds hydrostatic conditions and displaces porewater back into the surrounding rock. As a result of this, the lower part of the cavern becomes filled with gas after $\sim 8,000$ years. The upper part of the cavern maintains high (and increasing) gas saturations throughout the simulation.

The impact of an effective gas pathway is also depicted in gas saturation transients in the V1 seal. Fig. 5-4c shows that, although the lower part of the abutments saturates with water temporarily after ~ 600 years owing to the capillary strength of concrete (see also Tab. 4-3), a continuous gas path is sustained throughout the entire S/B element and at least in the upper parts of the transition layers and abutments. In accordance with this observation, the pressure transients in the L/ILW emplacement cavern show that pressure equilibrates instantly throughout the cavern (Fig. 5-4d), indicating the absence of any significant local effects of gas entrapment and accumulation. With the assumption of an impermeable V2-L/ILW seal, peak pressure in the cavern corresponds to ~ 10.1 MPa after 70,000 years (Fig. 5-4d). For comparison, a pressure transient from the model version assuming a permeable V2-L/ILW seal is shown in the same figure and is very similar to that obtained with the repository model.

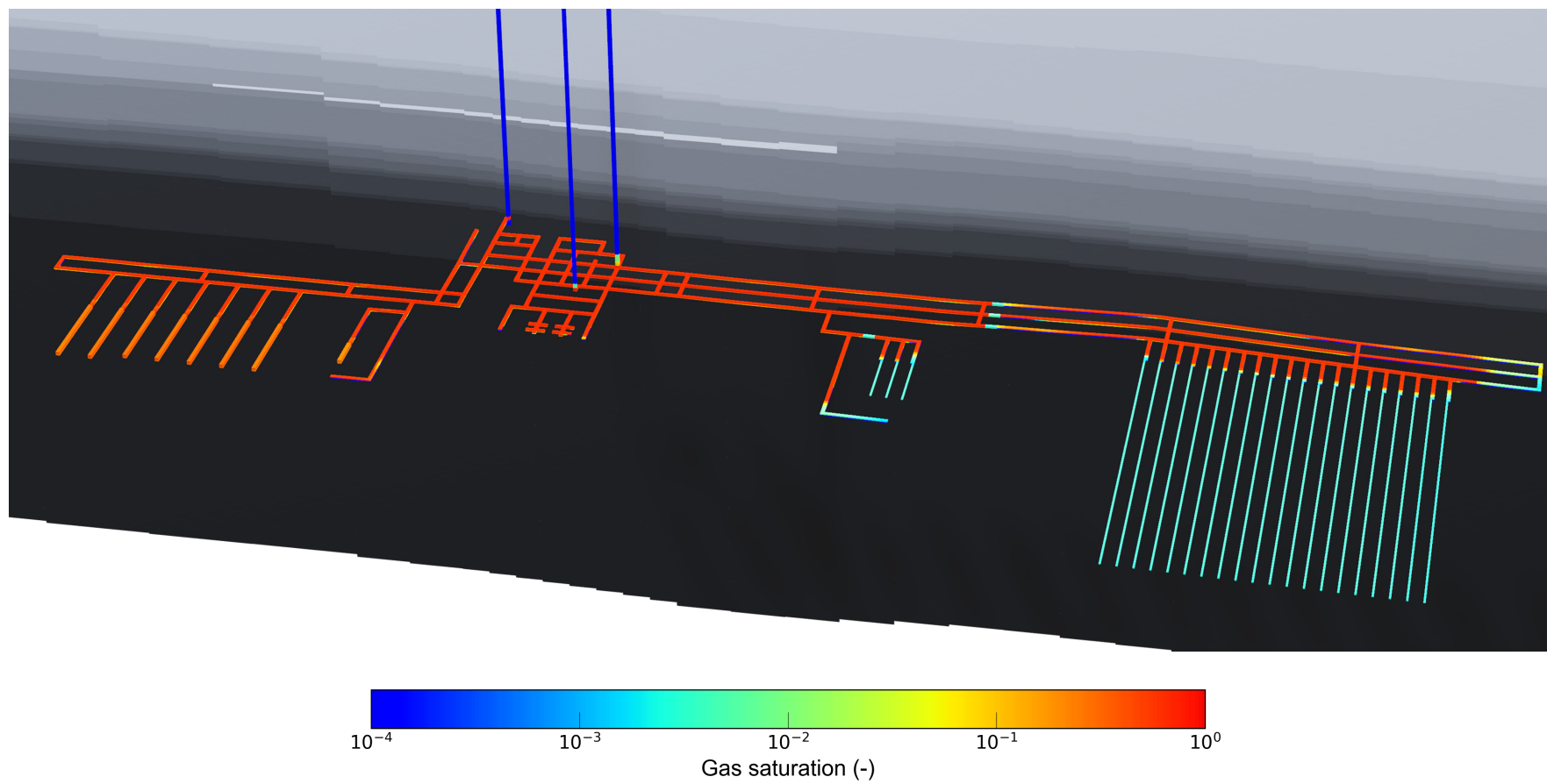
A snapshot of gas saturation after 2,000 years in the HLW emplacement drift and V1-HLW seal is shown in Fig. 5-5a. At that time, the bentonite buffer has already resaturated with porewater from the host rock, whereas gas generated at the canisters results in some gas saturation (ca. 2%) spreading radially around the canisters. Note that (low) gas saturation in the buffer is not shown in this spatial plot to enhance the visualisation of the disposal canisters. The resaturation of the buffer with porewater after emplacement occurs radially, mainly driven by two effects: the high capillary strength of the partly saturated bentonite (see also Tab. 4-4) that creates suction gradient from the surrounding rock, and the thermally induced pressure increase in the surrounding host rock that, combined with the lower pressure in the emplacement drift, creates an additional hydraulic gradient towards the drift. These effects are depicted in Fig. 5-5b; c; d that shows transients of gas saturation around canisters containing three types of SF. The outer part of the bentonite next to the liner begins to saturate with water directly after emplacement ($t = 2$ years). The porewater front moves inwards and reaches the middle part of the bentonite after ~ 20 years. The bentonite next to the canister shows a slight increase in gas saturation after 10 years due to water evaporation at the canister surface. This effect is nonetheless temporary, and water saturations next to the canister increase after ~ 40 years. Finally, porewater reaches the bentonite at the centre of the emplacement drift between the canisters after ~ 60 years. Full water saturation is reached at all observation points in the bentonite around the canisters after 200 years (Fig. 5-5b;c;d). In comparison, full saturation at the middle of the V1 seal close to the branching tunnel is reached after ~ 300 years. Note that the thermally induced gradient towards the tunnel is less pronounced in the sealing section compared to the waste section but that, at the same time, the compacted bentonite of the sealing section has higher capillary strength (see also Tab. 4-5). The bentonite buffer and the V1 seal remain fully saturated for 10,000 years when the HLW disposal canisters are assumed to breach in the model. As a consequence, axial gas transport in the HLW repository section is very limited and gas dissipates through radial transport and dissolution in the surrounding rock. Associated with an increase in gas generation, the canister breaching results in the formation of gas with saturations reaching $\sim 4\%$ and $\sim 2\%$ between the canisters and, in the seal, respectively (Fig. 5-5b; c; d). Temperature transients in the HLW near-field are shown for the same canister types in Fig. 5-5e; f; g. Canister temperature reaches approximately 136°C after 5 years. Temperature in the bentonite within 5 cm of the canisters reaches approximately 130°C . The middle and outer parts of the bentonite show significantly lower maximum temperatures of 108°C and 83°C , respectively. Temperature in the liner and the V1 seal remains below 80°C . Overall, the thermo-hydraulic evolution in the canister near-field is similar for all three types of SF (Fig. 5-5b;c;d;e;f;g). As explained in Section 4.4, pressure transients in the component model for HLW are not used in the present assessment. However, for the sake of completeness, they are provided in App. F.

In a similar fashion, component-scale modelling offers more insight into the hydraulic evolution of the sealing sections. Simulation results from the V2 and V3 seal models are shown in Fig. 5-6 and Fig. 5-7, respectively.

A snapshot of gas saturation after 10,000 years in the V2-L/ILW seal is shown in Fig. 5-6a. The saturation distribution shows a connected gas phase throughout all components of the seal and the adjacent operations tunnel on both sides. Due to buoyancy, higher gas saturations are observed in the upper part of the structures. The bottom part of the VF2 backfill and the adjacent abutment of the seal (towards the central area of the repository) has saturated fully with porewater. The evolution over time is captured in the gas saturation transients shown in Fig. 5-6b. During the ventilation phase (21 to 56 years), the EDZ and liner desaturate due to vapour suction imposed on the ventilation tunnel. Once the tunnel backfill and seal components are in place, the EDZ and liner take up some porewater through suction from the emplaced materials with lower capillary strength, namely the S/B sealing element, the transition layers, and the VF1 and VF2 backfill on each side of the seal (see also Tab. 4-5). Soon after emplacement, gravity-driven redistribution of water and gas within the gallery and the seal is also visible. The VF1 and VF2 backfill remains partially saturated throughout the entire simulation (Fig. 5-6b). The lower part of the S/B sealing element saturates with water for a period between 400 and 7,000 years, and then gradually desaturates as transport of waste-generated gas takes place through the seal. The upper part of the S/B sealing element maintains a gas saturation between 40% and 70% throughout the entire simulation, forming the main path for gas release through the seal. Similarly, transition layers and abutments only reach full water saturation in their respective lower parts (Fig. 5-6b). The connectivity of the gas path determining gas pressures across the sealing section is also depicted in the pressure transients shown in Fig. 5-6c. Similar to the observations made in the repository-scale results, pressures initially increase faster in the VF1 due to gas coming from the emplacement caverns but after $\sim 5,000$ years they equilibrate across the sealing section and adjacent tunnel and remain approximately uniform in all observation points at any given time (Fig. 5-6c).

In Fig. 5-7a, three snapshots of gas saturation (after 1,000, 10,000, and 20,000 years) are shown for the V3 seal and adjacent access shaft. The saturation distribution after 1,000 years shows that porewater from the surrounding formations has already fully saturated the shaft as well as the abutment and the upper compartment of the bentonite seal. Note that the gas present in the middle and lower compartments of the seal at that time is residual gas from the emplacement of the seal and is not generated by the waste. After 10,000 years, the entire bentonite seal is fully saturated with porewater. After 20,000 years, gas arriving from the operations tunnels has entered the bentonite seal, resulting in some gas saturation (ca. 0.5%) in the lower half of the seal. Note that, based on the gas generation rates and transport regimes in the repository sections discussed earlier, gas reaching the seal originates from the L/ILW repository section. The transients of gas saturation are shown in Fig. 5-7b. The shaft above the seal and the abutment at the top of the bentonite seal saturate almost instantly after emplacement with porewater from the formations overlying the Opalinus Clay (note that a constant pressure boundary is assigned at the top model boundary resp. bottom of the Malm aquifer). On the other hand, the transition layer below the seal accumulates gas due to its low suction. The centre of the bentonite seal and the EDZ surrounding it reach full water saturation after $\sim 3,000$ years. Once gas breaks through the V3 seal ($\sim 39,000$ years, see also Fig. 5-29), it does not cause appreciable gas saturations in the shaft until the end of the simulation (Fig. 5-7b).

Similar to the other repository components, pressure transients can be used to deduce information on gas pathways through the V3 seal and shaft, as shown in Fig. 5-7c. Due to the high permeability of the access tunnels until the bottom of the seal, pressures at the shaft sump follow those in the central area of the repository (which are prescribed at the end of the access tunnel in the model). On the other hand, pressure in the abutment equilibrates to hydrostatic pressure within 100 years after emplacement and remains constant until the end of the simulation (Fig. 5-7c). The pressure difference imposed by the low-permeable seal between the shaft sump and the shaft above the seal indicates a limited hydraulic connection between these components.



(a)

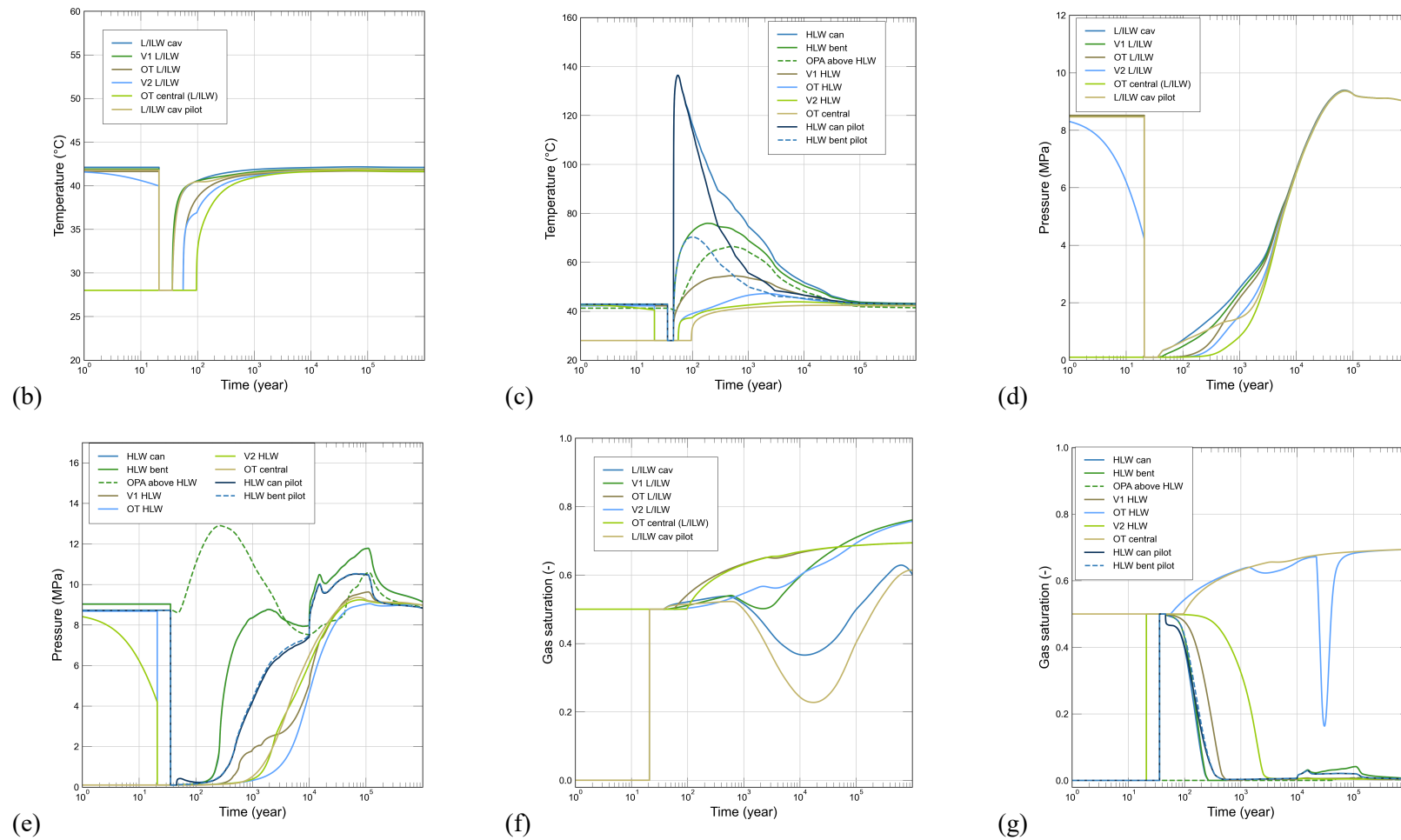


Fig. 5-3: Base case, repository model

(a) 3D snapshot of saturation distribution after 5,000 years; transients of temperature (b) in the L/ILW and (c) in the HLW repository; transients of pressure (d) in the L/ILW and (e) in the HLW repository; transients of gas saturation (f) in the L/ILW and (g) in the HLW repository.

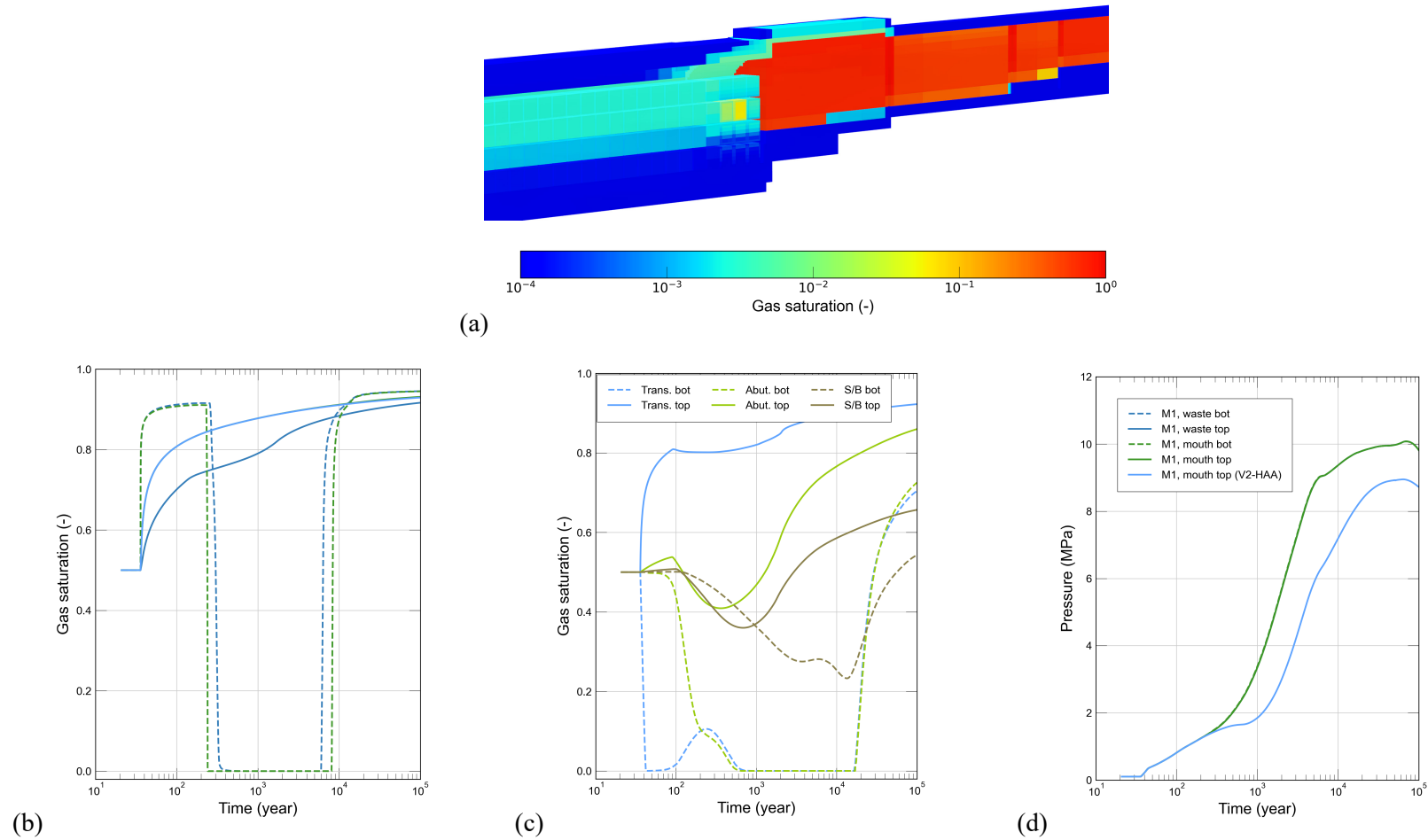
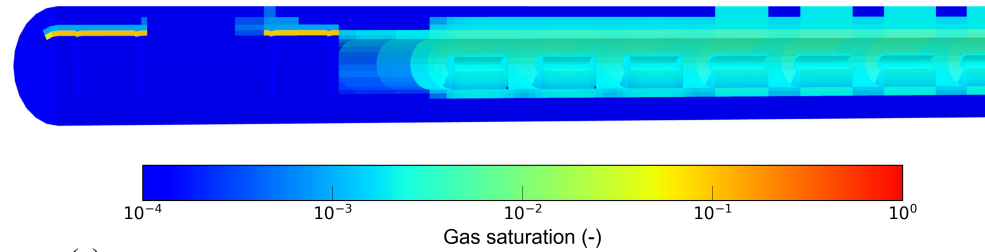
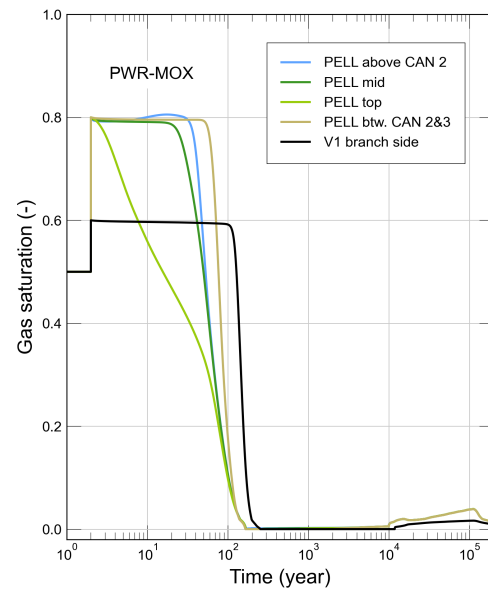


Fig. 5-4: Base case, L/ILW & V1 model

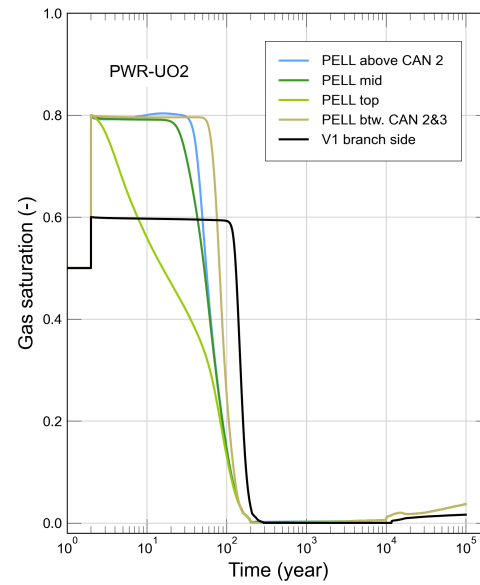
(a) 3D snapshot of saturation distribution after 1,000 years; transients of gas saturation in the (b) L/ILW emplacement cavern and (c) V1-L/ILW seal; and (d) transients of pressure in the V1-L/ILW cavern. Legend for (b) shown in (d).



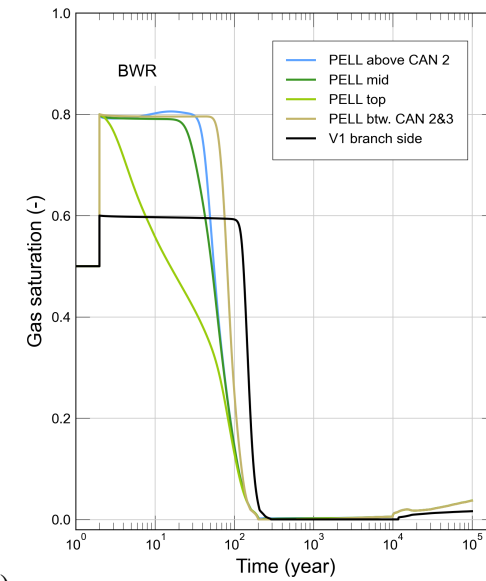
(a)



(b)



(c)



(d)

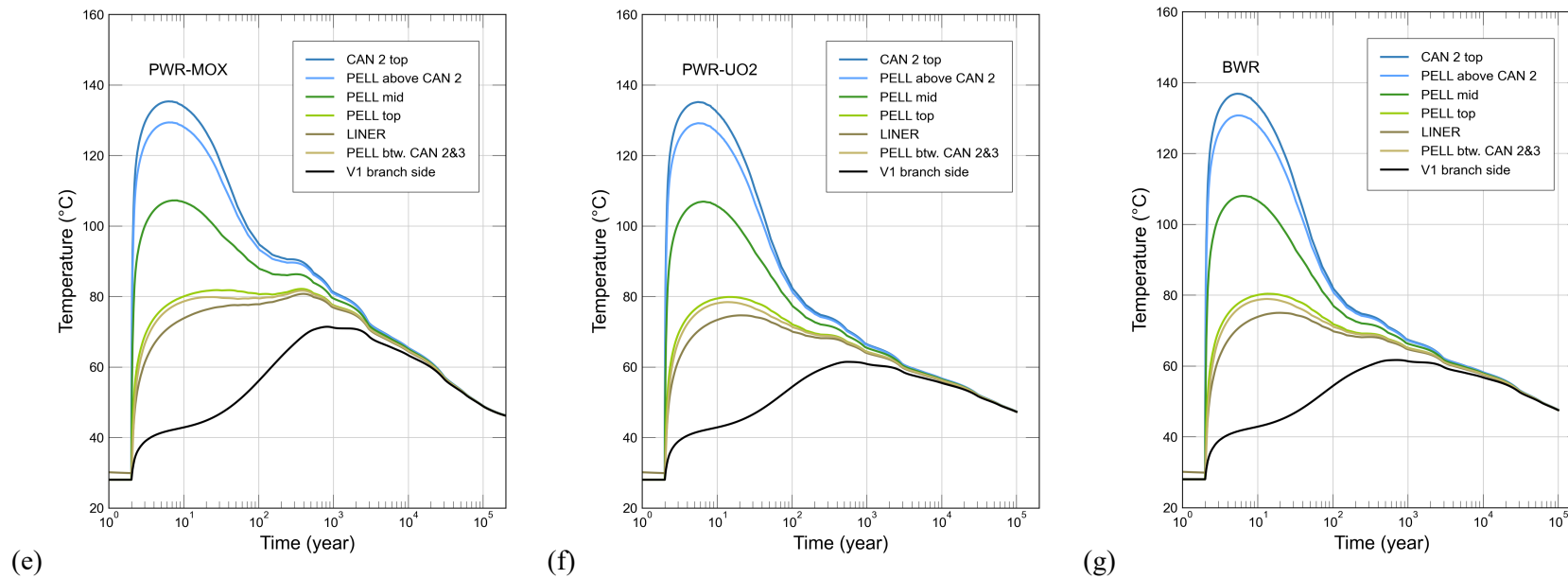


Fig. 5-5: Base case, HLW & V1 model

(a) 3D snapshot of saturation distribution after 2,000 years; transients of gas saturation around representative canister of type (b) PWR-MOX, (c) PWR-UO₂, (d) BWR; and transients of temperature around a representative canister of type (e) PWR-MOX, (f) PWR-UO₂, (g) BWR.

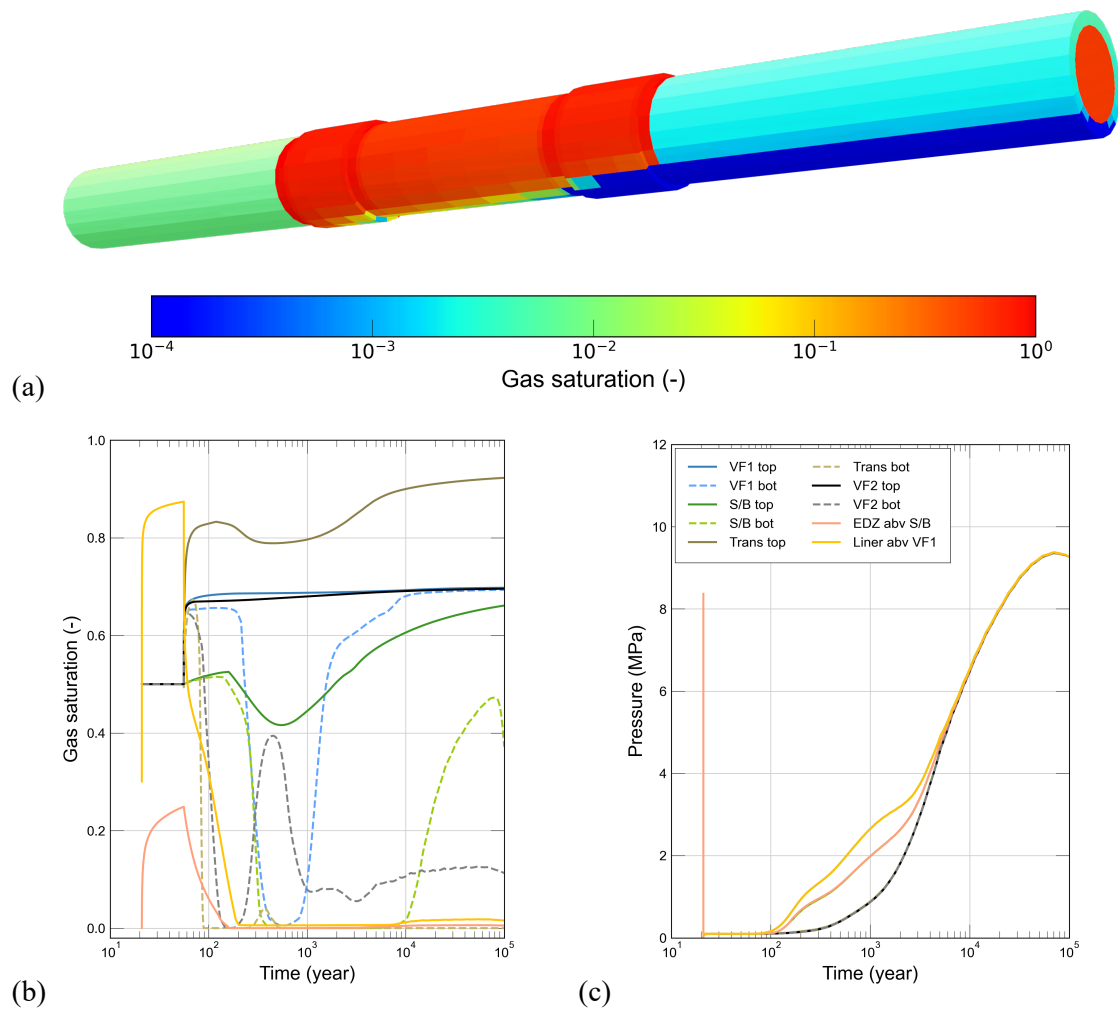


Fig. 5-6: Base case, V2-L/ILW model

(a) 3D snapshot of saturation distribution after 10,000 years; transients of (b) gas saturation and (c) pressure in the V2 seal and operations tunnel.

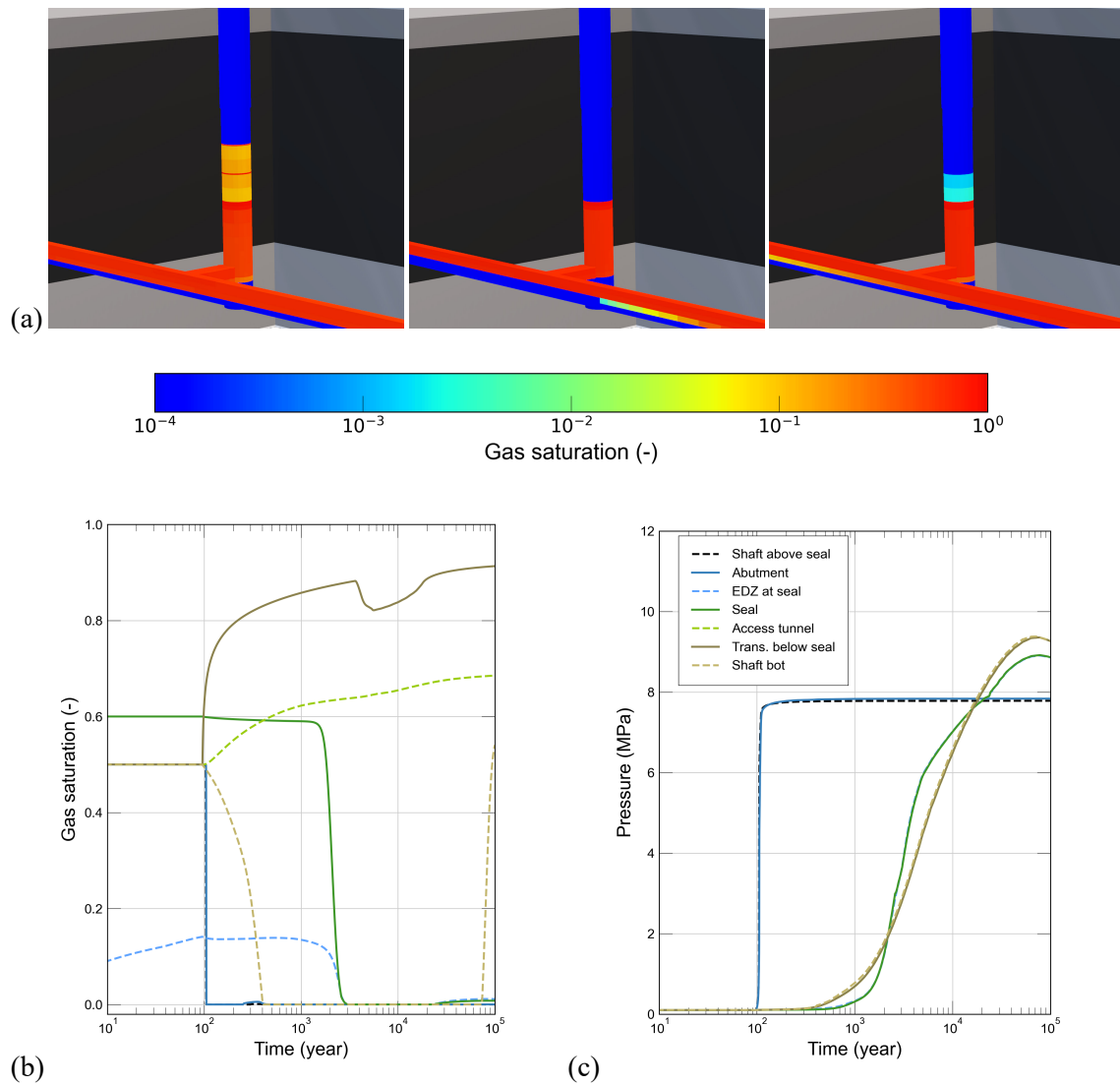


Fig. 5-7: Base case, V3 model

(a) 3D snapshot of saturation distribution after 1,000, 10,000 and 20,000 years (from left to right); transients of (b) gas saturation and (c) pressure in the V3 seal and shaft.

5.3.2 Case 2: Resaturation without gas sources

The second assessment case aims to evaluate the hydraulic evolution of the repository under the assumption that gas (and heat) sources in it are negligible. In this case, all gas found in the repository comes from the materials partially saturated upon emplacement and the partial desaturation of the rock during the ventilation of the repository structures. The analysis is carried out with a spatial plot of gas saturation at the repository scale, complemented with transients of gas saturation and pressure at selected observation points in the component models.

Gas saturation simulated after 5,000 years with the repository model without gas sources is shown in Fig. 5-8. The emplacement rooms in the HLW repository section, including those in the pilot repository, have become fully saturated with porewater from the surrounding rock. In the L/ILW emplacement caverns there is still some residual gas, however at lower gas saturations compared to the base case (Fig. 5-3). The operations and access tunnels leading to the central area are mostly water-saturated in their lower portions, and partially saturated in their upper portions. The highest gas saturations are observed in the tunnels in the central area around the shafts. Note that the same emplacement schedule is used as in the base case simulation, which implies that tunnels closest to the shafts have been ventilated the longest. The more extensive depressurisation of the Opalinus Clay (unmitigated by the generation of gases), combined with the relatively low capillary strength of the backfilled tunnels, results in slower resaturation. The shafts are fully saturated with porewater both due to inflow from more permeable overlying formations and to the high capillary suction imposed by the compacted bentonite of the V3 seal.

Transients of gas saturation at selected locations (defined in Fig. 5-2) of the component models are illustrated in Fig. 5-9a and show an overall similar behaviour to the repository-scale analysis. The shaft above the V3 seal resaturates practically instantly after backfilling. In the absence of pressure buildup in the repository, the centre point of the V3 seal resaturates in less than 3,000 years. On the other hand, the absence of thermally induced overpressures around the HLW emplacement drifts delays the full resaturation of the buffer to approximately 400 years. The mortar in the L/ILW emplacement caverns saturates from the bottom after 300 years to the roof after 10,000 years (note that the disposal containers and concrete saturate earlier due to capillary suction). Finally, the bottom of the S/B element in the V2 seal saturates after 800 years, whereas the top part maintains some amount of gas until the end of the simulation. All observation points in the repository components indicate that, once full saturation is reached, it remains unchanged until the end of the simulation.

Transients of pressure at the same locations are shown in Fig. 5-9b. The shaft above the seal reaches hydrostatic pressure soon after emplacement, as in the base case. The L/ILW emplacement cavern and V3 seal reach hydrostatic pressure after ~ 40,000 years. The V2-L/ILW seal reaches hydrostatic pressure after ~ 100,000 years. Pressure increase in the HLW emplacement drifts initiates earlier due to the suction of the bentonite, with hydrostatic conditions reached towards the end of the simulation.

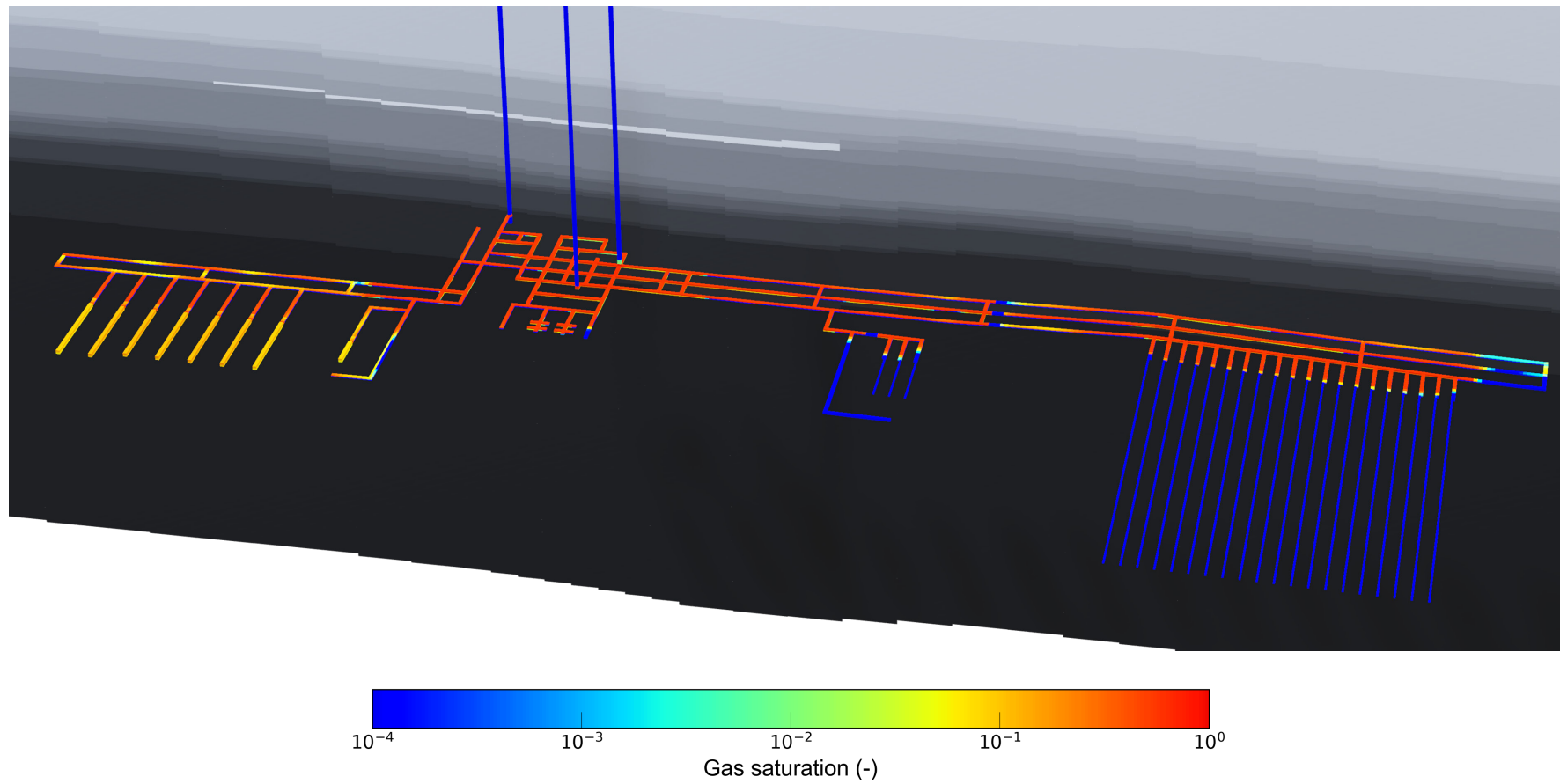


Fig. 5-8: Case 2, repository model: 3D snapshot of saturation distribution after 5,000 years

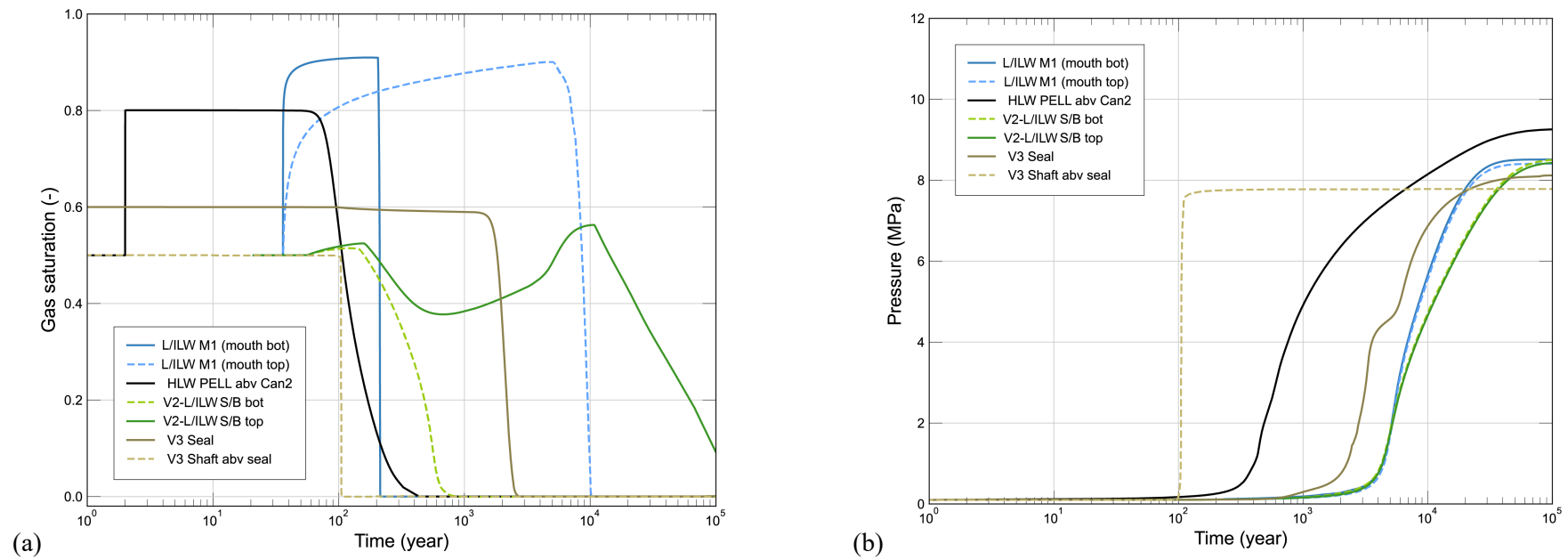


Fig. 5-9: Case 2, component models

Transients of (a) gas saturation pressure and (b) pressure in different parts of the combined repository.

5.3.3 Case 3: Upper bound gas rates

The third assessment case is implemented using the upper bound values of gas source terms. The outcomes are discussed in terms of selected metrics, namely transients of pressure, gas saturation, and (for the HLW near-field model) temperature.

Transients of pressure simulated with the repository model in the L/ILW section are shown in Fig. 5-10a. Similar to the base case, pressure first increases in the emplacement caverns and then in the V1 seal and operations tunnels, before it equilibrates across all L/ILW emplacement caverns after $\sim 5,000$ years. After that, roughly uniform pressures are observed throughout the L/ILW repository section, reaching the hydrostatic value after $\sim 10,000$ years and a maximum value of slightly below 10 MPa after $\sim 70,000$ years. Pressure transients in the HLW repository section are shown in Fig. 5-10b. Similar to the base case, the thermally induced pressure peak approaches the hydrostatic pressure after $\sim 2,000$ years. Gas-induced pressures reach 12.5 MPa at 10,000 years, when the canisters were assumed to breach in the model, and increase to a maximum of 14.4 MPa when all canisters corrode entirely after $\sim 25,000$ years. Pressures consequently decrease until the end of the simulation.

Transients of gas saturation simulated with the near-field L/ILW model are shown in Fig. 5-11a; b. Note that these results are obtained with the model variant that additionally assumes an impermeable V2-L/ILW seal. Partial saturation conditions prevail in the M1 mortar in the upper part of the emplacement cavern as gas saturation increases continuously until the end of the simulation. In the bottom part, gas saturations temporarily decrease between 300 and 1,000 years (notably reaching full water saturated conditions only near the mouth of the cavern) and then increase until the end of the simulation (Fig. 5-11a). Similarly, the transients in the V1 seal, shown in Fig. 5-11b, indicate the presence of a gas phase in all components of the seal practically throughout the simulation. Hydrostatic pressure is reached after $\sim 1,000$ years, whereas peak pressure from the accumulation of gas reaches a maximum of ~ 11.7 MPa after $\sim 12,000$ years (Fig. 5-11c, note that all curves fall on top of each other). The pressure decrease after that coincides with increasing gas saturation in the bottom part of the seal.

The results from the HLW near-field model are shown in Fig. 5-12. For practical reasons, a single SF type (PWR-MOX) is adopted for the analysis. The resaturation of the bentonite buffer with porewater is practically identical to that observed in the base case. The bentonite and V1 seal remain fully saturated after 10,000 years, when the canisters are assumed to breach in the model. After the canister breaching, gas saturation in the bentonite is higher compared to the base case, reaching up to $\sim 10\%$ in the pitch between the canisters. Gas saturation in the middle of the V1 seal next to the branching tunnel reaches $\sim 4\%$. Near-field temperatures are practically identical to the base case throughout the entire simulated time. Pressure transients are provided for the sake of completeness in App. F.

The evolution of gas saturation in the V2-L/ILW seal, shown in Fig. 5-13a, is overall similar to the base case (see Fig. 5-6a). Higher gas saturation is observed in the lower parts of the seal components, due to the higher inflow of gas from the emplacement caverns. The gas path is also depicted in the pressure transients shown in Fig. 5-12b, with earlier and higher pressure increases in the VF1 backfill in the first 2,000 years (compared to the base case) and equilibration of pressure across both sides of the sealing section after $\sim 5,000$ years.

Gas saturation transients simulated with the V3 model are shown in Fig. 5-14a. Similar to the base case, the shaft above the seal and the abutment at the top of the bentonite sealing element saturate with porewater directly after backfilling. However, in this case the resaturation of the sealing element with porewater is slower due to the higher gas pressure in the repository. The middle point of the sealing element saturates with porewater after $\sim 7,000$ years (compared to $\sim 3,000$ years in the base case). Gas that breaks through the V3 seal ($\sim 16,000$ years, refer to Fig. 5-30) does not result in any appreciable gas saturation in the shaft until the end of the simulation.

Similar to the base case, the pressure transients shown in Fig. 5-14b point to the hydraulic separation of the shaft above the sealing element from the rest of the repository, albeit with slightly higher peak pressures.

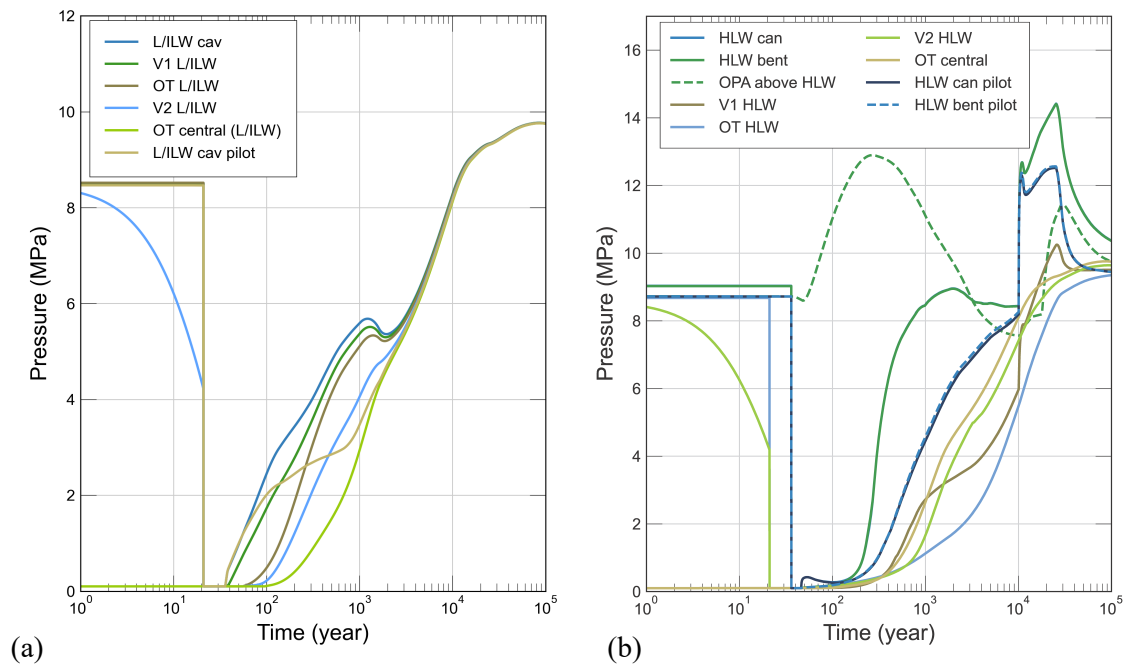


Fig. 5-10: Case 3, repository model: transients of pressure (a) in the L/ILW and (b) in the HLW repository

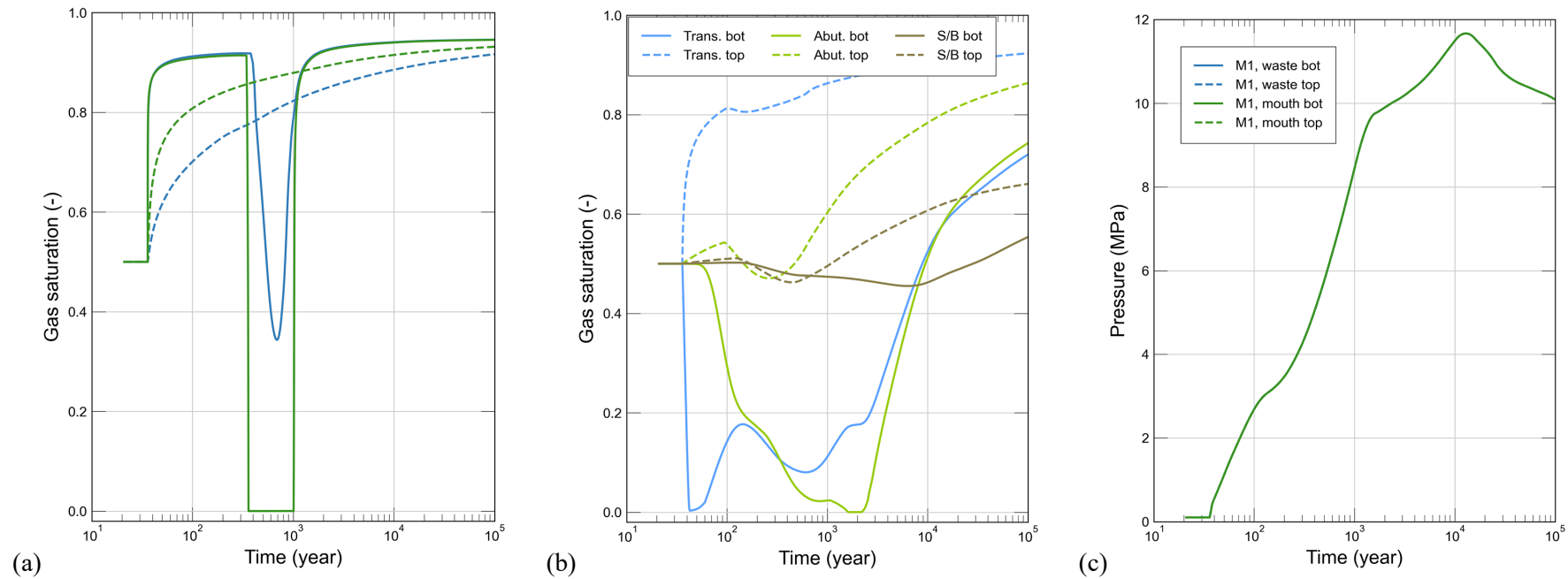


Fig. 5-11: Case 3, L/ILW & V1 model

Transients of gas saturation in the (a) L/ILW emplacement cavern and (b) V1-L/ILW seal; and (c) transients of pressure in the L/ILW emplacement cavern. Legend for (a) shown in (c).

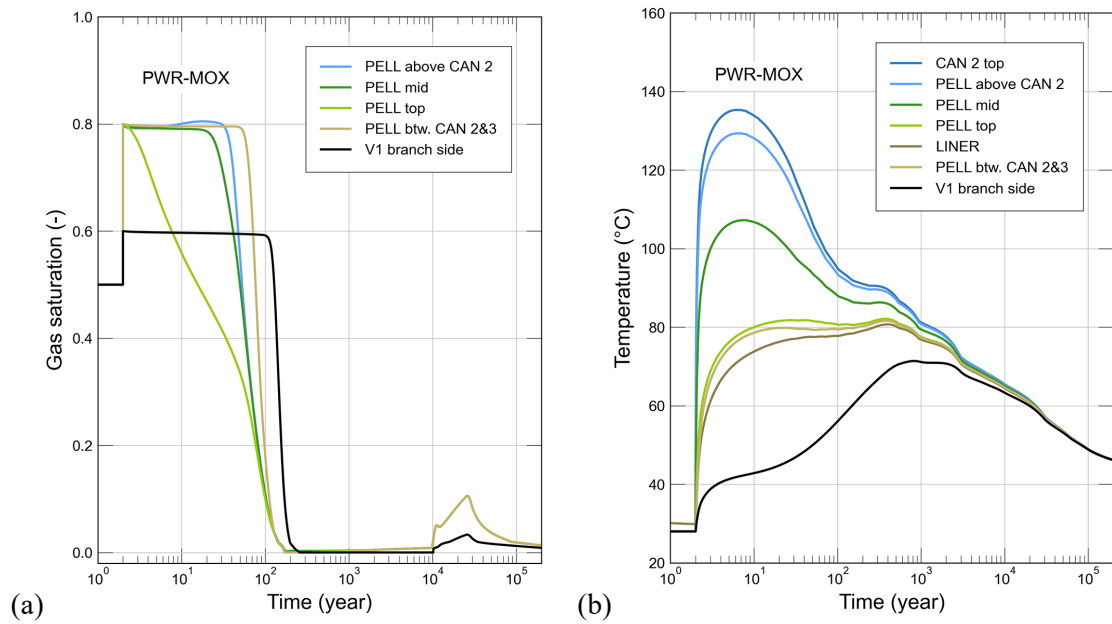


Fig. 5-12: Case 3, HLW & V1 model

Transients of (a) gas saturation and (b) temperature around a representative canister of type PWR-MOX.

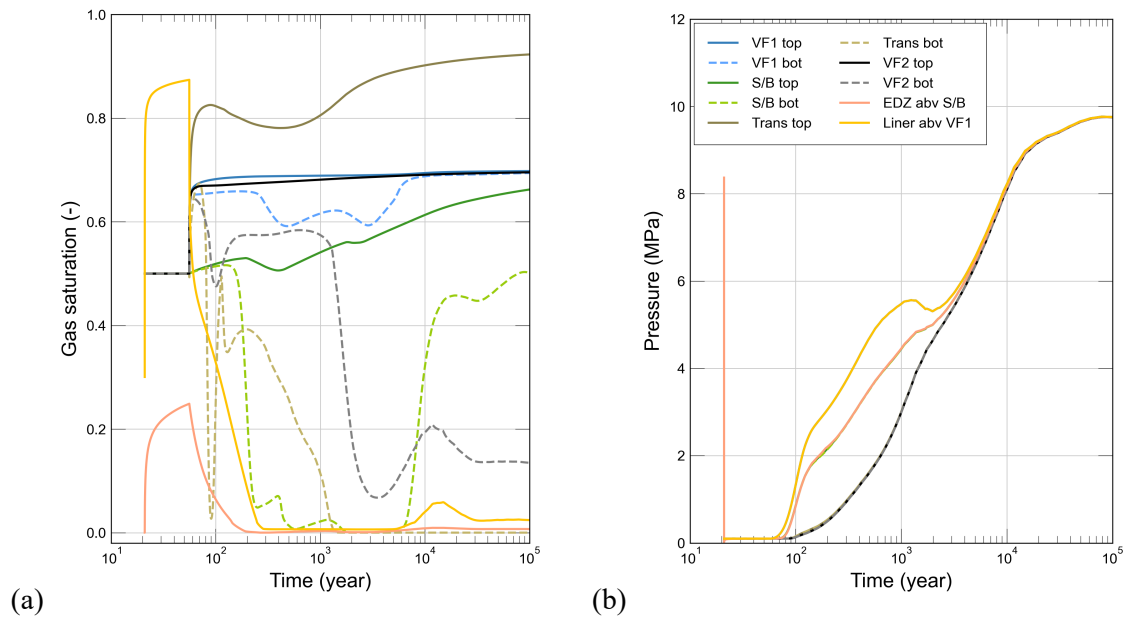


Fig. 5-13: Case 3, V2-L/ILW model

Transients of (a) gas saturation and (b) pressure in the V2 seal and operations tunnel.

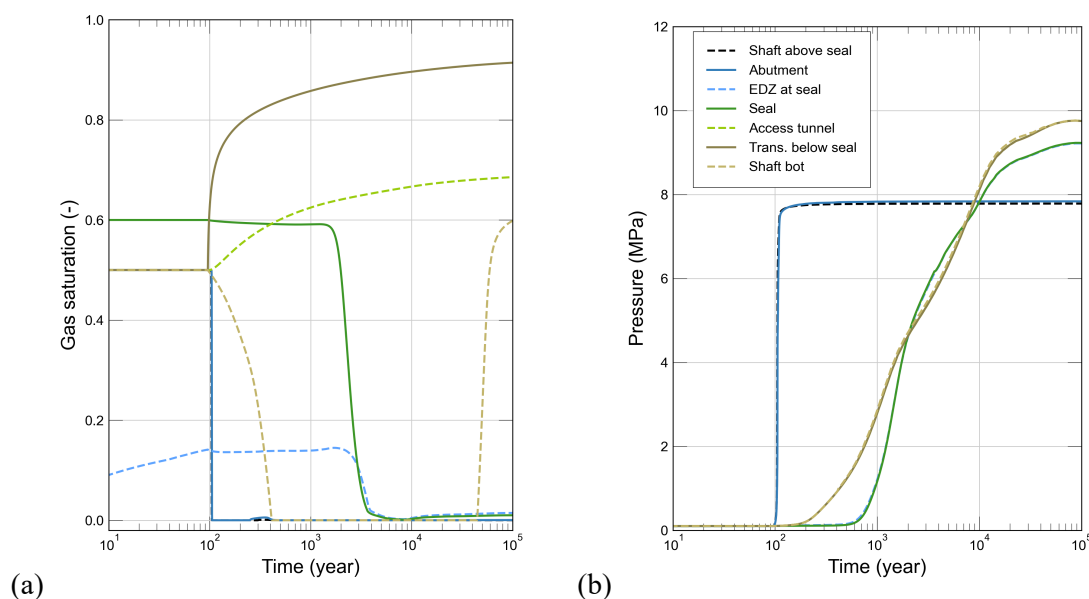


Fig. 5-14: Case 3, V3 model

Transients of (a) gas saturation and (b) pressure in the V3 seal and shaft.

5.3.4 Case 4: Lower bound gas rates

The assessment assuming the lower bound gas generation rates in the repository evolution is undertaken in a similar fashion. Transients of pressure and gas saturation are provided by all models, with the addition of temperature transients from the HLW near-field model.

The pressure transients obtained with the repository model in the L/ILW and HLW repository sections are shown in Fig. 5-15a and Fig. 5-15b, respectively. In comparison to the base case (see Fig. 5-3), the post-closure pressure increase in the L/ILW repository section is slower due to the slower accumulation of gas. Accordingly, pressure equilibrates across the emplacement and operations tunnels after ~10,000 years. The maximum pressure is very close to the hydrostatic value reached towards the end of the simulation (Fig. 5-15a). In the HLW repository section, thermally induced pressure develops in a similar way to the base case (see Fig. 5-3e). In the late post-closure phase, pressure increases slowly and plateaus at hydrostatic pressure at the end of the simulation (Fig. 5-15b).

Gas saturation transients obtained with the near-field L/ILW model are shown in Fig. 5-16a; b. The lower part of the M1 mortar in the cavern saturates with porewater after ~300 years and remains fully saturated until the end of the simulation. The upper part saturates after ~10,000 years maintaining very low gas saturations (~2%) in the inner part of the emplacement cavern and higher saturations (reaching ~90%) at the mouth of the cavern. Similar to the repository model, pressures do not exceed hydrostatic conditions until the end of the simulation (Fig. 5-16c).

Gas saturation and temperature transients from the HLW near-field model are shown in Fig. 5-17a and Fig. 5-17b, respectively. Similar to the previous case, a PWR-MOX-type canister is selected for the SF waste. The resaturation of the bentonite in the early post-closure phase is very similar to the base case (see Fig. 5-3g). After 10,000 years, when the canisters are assumed to breach in the model, fully water-saturated conditions remain in the bentonite surrounding the canisters and in the sealing element of the V1 seal, as the amount of gas released stays below solubility limits

in the surrounding porewater. Near-field temperatures are practically identical to the base case throughout the entire simulated time (see Fig. 5-3c).

Gas saturation transients in the V2-L/ILW seal, shown in Fig. 5-18a, point to an evolution similar to the base case but with overall lower gas saturations in the lower portions of the components of the seal and adjacent tunnels (see Fig. 5-6a). The upper part of the sealing element remains partially saturated until the end of the simulation when hydrostatic pressure is reached. Pressure initially increases faster in the VF1 backfill (albeit with overall less pressurisation as compared to the base case) and equilibrates across the seal after $\sim 7,000$ years, so that the same pressure values are observed on both ends of the sealing section until the end of the simulation (Fig. 5-18b).

Gas saturation transients in the V3 seal, shown in Fig. 5-19a, indicate full saturation at the centre of the sealing element in less than 3,000 years, which is similar to the resaturation case without gas sources in the repository (see Fig. 5-9a). Gas that breaks through the V3 seal ($\sim 80,000$ years, see also Fig. 5-31) does not result in any significant gas saturation in the shaft. Similar to the previous cases, the pressure transients, shown in Fig. 5-19b, point to effective hydraulic isolation of the shaft above the seal from the rest of the repository, with slightly lower peak pressures compared to those of the base case.

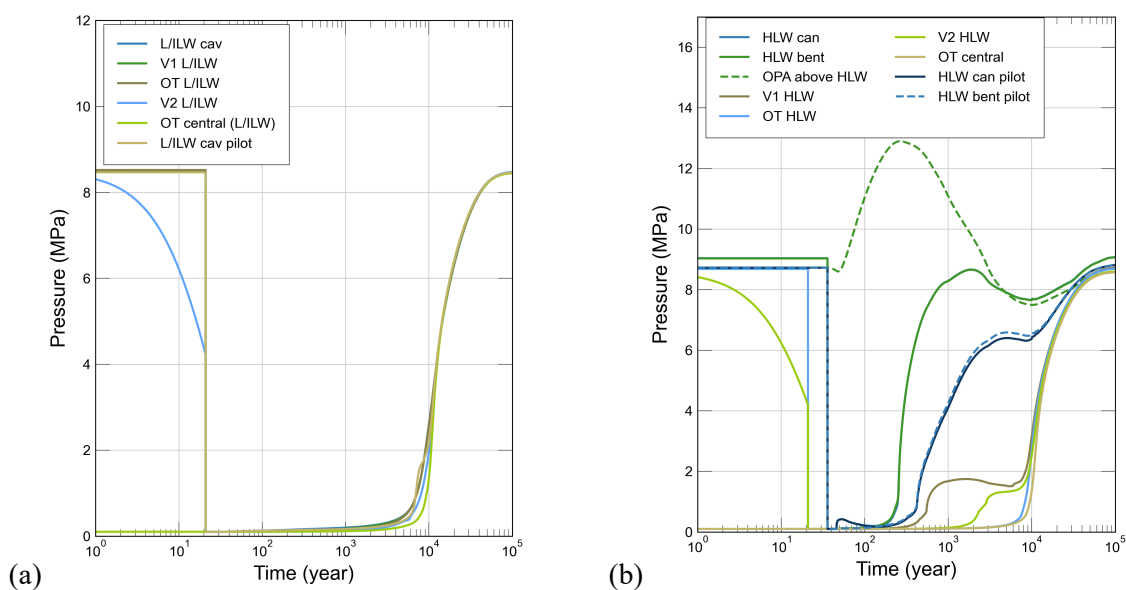


Fig. 5-15: Case 4, repository model

Transients of pressure (a) in the L/ILW and (b) in the HLW repository.

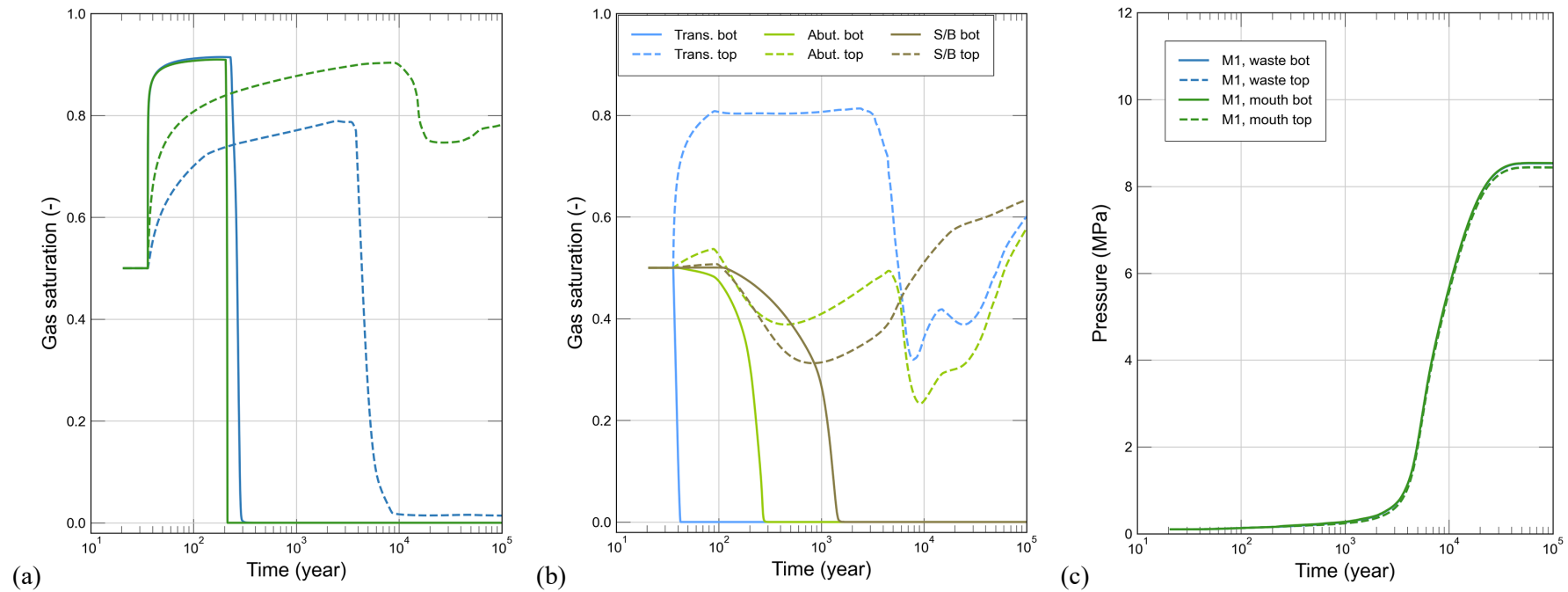


Fig. 5-16: Case 4, L/ILW & V1 model

Transients of gas saturation in the (a) L/ILW emplacement cavern and (b) V1-L/ILW seal; and (c) transients of pressure in the L/ILW emplacement cavern. Legend for (a) shown in (c).

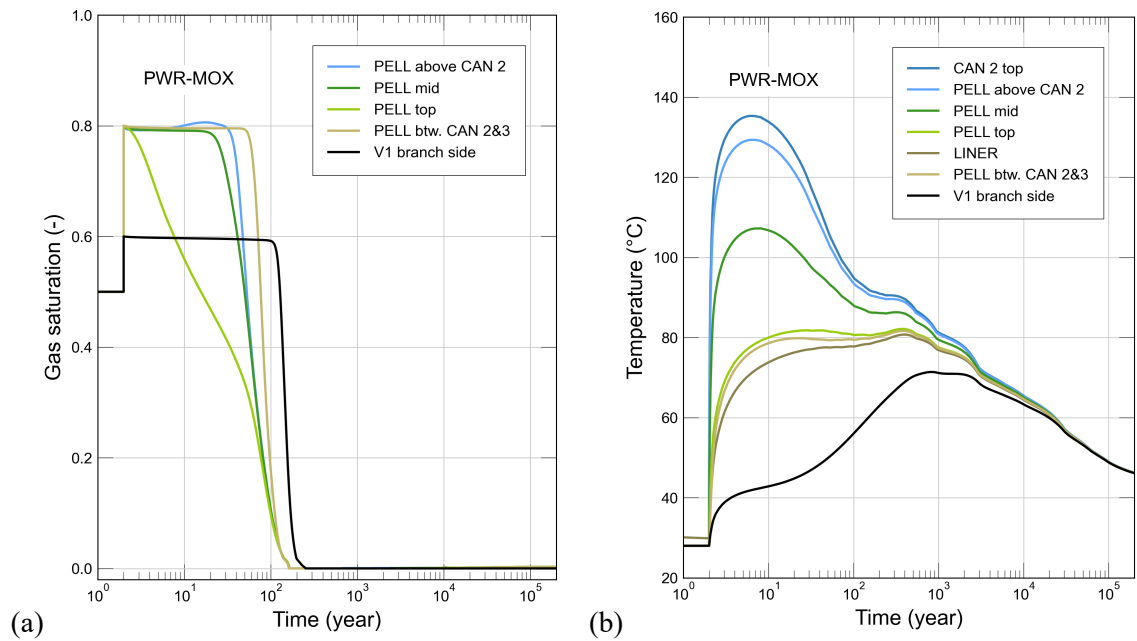


Fig. 5-17: Case 4, HLW & V1 model

Transients of (a) gas saturation and (b) temperature around a representative canister of type PWR-MOX.

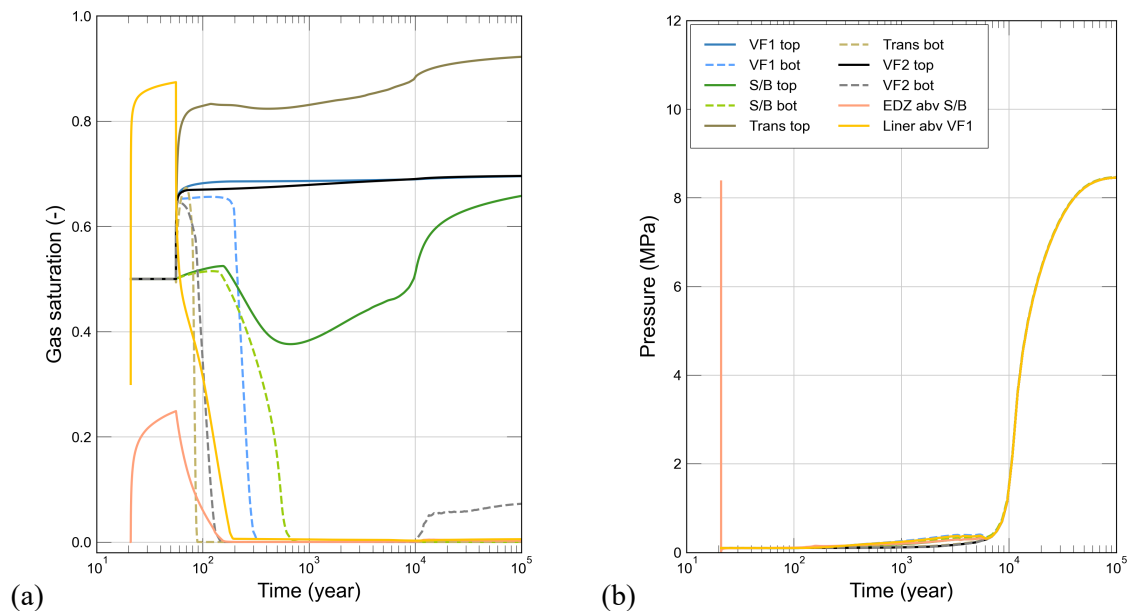


Fig. 5-18: Case 4, V2-L/ILW model

Transients of (a) gas saturation and (b) pressure in the V2 seal and operations tunnel.

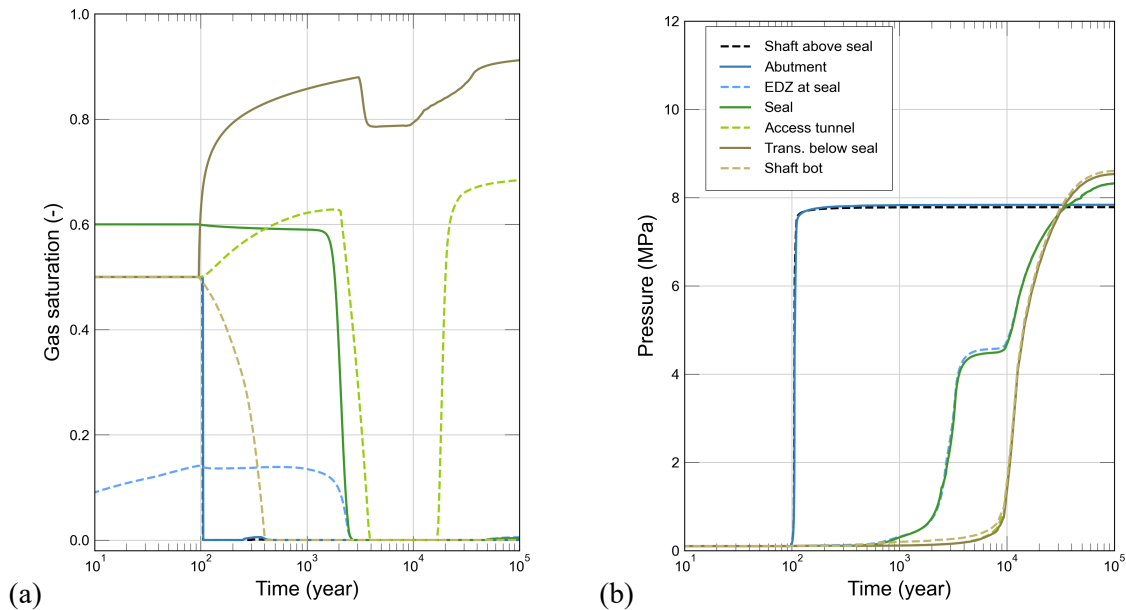


Fig. 5-19: Case 4, V3 model

Transients of (b) gas saturation and (c) pressure in the V3 seal and shaft.

5.3.5 Case 5: L/ILW cavern with extreme iron and carbon steel corrosion

The assessment assuming a hypothetical, extreme value for carbon steel corrosion (250 nm/a for $\text{pH} \geq 10.5$) is performed with the L/ILW near-field and V1-L/ILW model assuming an impermeable V2-L/ILW seal.

Transients of gas saturation in the L/ILW emplacement cavern are shown in Fig. 5-20a. It is shown that the lower part of the mouth of the cavern fully saturates with water between ~ 300 and $\sim 1,000$ years. The duration of this effect is shorter compared to the base case (see Fig. 5-4b) due to the faster release and accumulation of gas associated with corrosion. Accordingly, the entire sealing section remains partially saturated throughout the simulation, with the exception of the bottom part of the transition layer shortly after emplacement, as shown in Fig. 5-20b. The higher gas saturations in the V1 seal compared to the base case indicate more gas flow through the seal, which results from the cavern pressure buildup shown in Fig. 5-20c. Hydrostatic pressure is reached much sooner compared to the base case (see Fig. 5-4d), namely shortly after 1,000 years. The peak pressure of ~ 13.6 MPa is reached after $\sim 5,000$ years. The high corrosion rate leads to faster depletion of iron and carbon steel materials. Consequently, gas pressure decreases continuously until the end of the simulation.

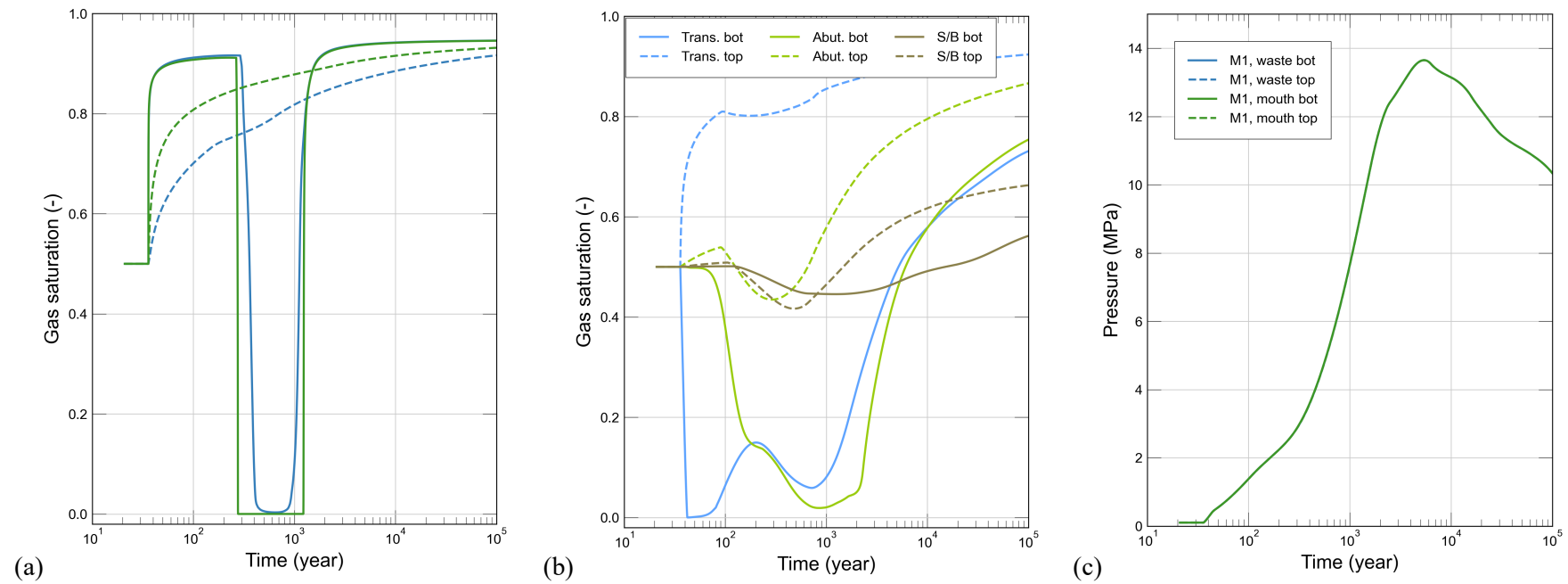


Fig. 5-20: Case 5, L/ILW & V1 model

Transients of gas saturation in the (a) L/ILW emplacement cavern and (b) V1-L/ILW seal; and (c) transients of pressure in the L/ILW emplacement cavern. Legend for (a) shown in (c).

5.3.6 Case 6: Water consumption

Case 6 demonstrates the effect of water consumption associated with the corrosion of metals using the L/ILW near-field and V1-L/ILW model under the assumption of an impermeable V2-L/ILW seal. The water consumption rate is calculated from the rate of gas generation and the stoichiometries of corrosion reactions as discussed in Section 3.1. In the current model implementation, the water sink term is not coupled to water and vapor availability.

Transients of gas saturation in the L/ILW emplacement cavern are shown in Fig. 5-21a. The saturation evolution in the early post-closure phase is overall similar to that of the base case (see Fig. 5-4), with gas accumulating in the upper part of the cavern while the lower part saturates with porewater after a few hundred years. The desaturation of the lower part in the case with water consumption takes place earlier, after $\sim 5,000$ years, earlier than the $\sim 8,000$ years required in the base case. In the previous assessment cases, higher gas saturations in the emplacement cavern are typically associated with more gas accumulation and accordingly higher pressure in the cavern. Here, the sink term applied to water results in an increase of the portion of porosity occupied by gas at lower pressure. Similarly, gas saturation transients in the V1 seal, shown in Fig. 5-21b, show increased resaturation of the seal materials with porewater from the surrounding rock until hydrostatic pressure is reached after $\sim 10,000$ years, as shown in Fig. 5-21c. The pressure increases to maximum of about 0.5 MPa above the hydrostatic value after $\sim 20,000$ years. As the ongoing consumption of water continues to dry out the mortar surrounding the disposal containers, the pressure decreases and eventually (after $\sim 40,000$ years) dips below the hydrostatic pressure. This introduces a pressure gradient from the rock into the branching tunnel and emplacement cavern, again increasing the water saturation in the bottom part of the seal and the M1 mortar after $\sim 40,000$ years as shown in Fig. 5-21a. The renewed water supply at the bottom of the cavern once more increases the pressure towards hydrostatic conditions after 100,000 years (Fig. 5-21c).

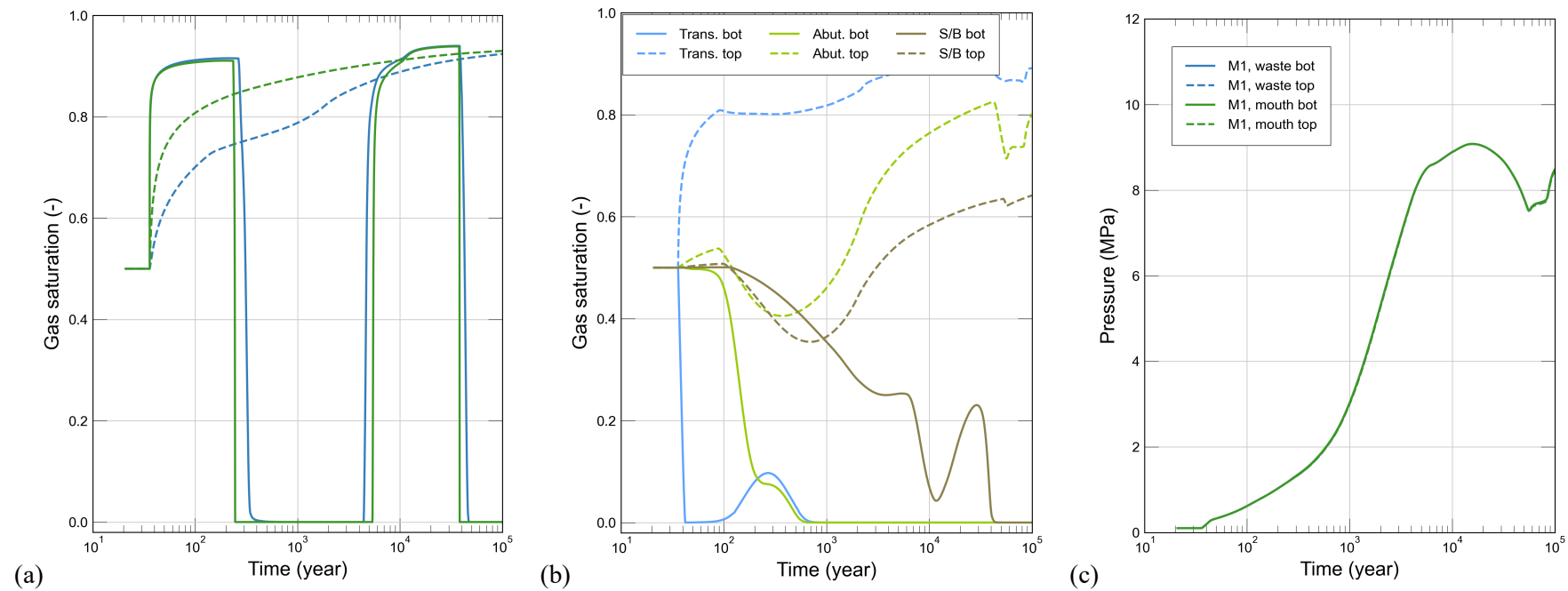


Fig. 5-21: Case 6, L/ILW & V1 model

Transients of gas saturation in the (a) L/ILW emplacement cavern and (b) V1-L/ILW seal; and (c) transients of pressure in the L/ILW emplacement cavern. Legend for (a) shown in (c).

5.3.7 Case 7: Low-permeability seal V1-L/ILW

Case 7 is assessed with the L/ILW near-field and V1-L/ILW model, thus combining two conservative assumptions with regard to gas pressure buildup: V1 seal having low permeability (see Tab. 5-1) and an impermeable V2 seal in the L/ILW repository.

Transients of gas saturation in the L/ILW emplacement cavern are shown in Fig. 5-22a. Overall, the evolution of saturation is very similar to the base case (see Fig. 5-4), except for the duration of the full saturation in the M1 mortar surrounding the bottom row of disposal containers, which is more than 4,000 years shorter in this case. The duration of full water saturation of the bottom parts of the transition layer and abutment in the V1 seal are also somewhat shorter, as shown in Fig. 5-22b. The overall higher gas saturation in the L/ILW emplacement cavern and sealing section is due to the decreased amount of gas released through the seal. This is also inferred from the pressure transients shown in Fig. 5-22c. Hydrostatic pressure is reached after $\sim 3,000$ years. Pressure then continues to increase, reaching a maximum of ~ 10.1 MPa after $\sim 70,000$ years. In comparison to the base case (see Fig. 5-4d), the pressure increase is somewhat faster (e.g., higher pressures are noted after 10,000 years) but the peak pressure in the late post-closure phase is similar.

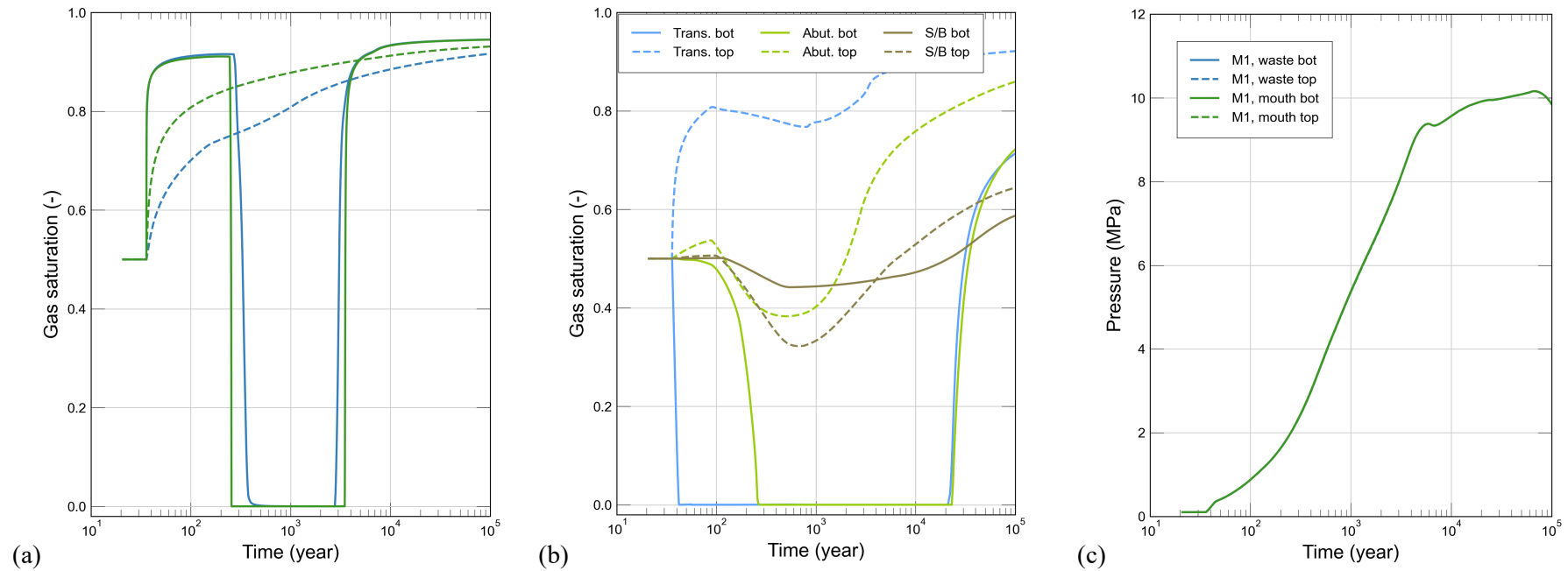


Fig. 5-22: Case 7, L/ILW & V1 model

Transients of gas saturation in the (a) L/ILW emplacement cavern and (b) V1-L/ILW seal; and (c) transients of pressure in the L/ILW emplacement cavern. Legend for (a) shown in (c).

5.3.8 Case 8: Low-permeability seal V2-L/ILW

In some of the modelling results presented in the previous cases, an implicit assumption of the model was that the V2-L/ILW seal is impermeable to gas and water transport. Case 8 focuses on the evolution of the seal itself under the assumption that the S/B element has 15 times lower permeability compared to the base case (see Tab. 5-1). The assessment is performed with the V2-L/ILW component model using gas inflow (at the upstream boundary of the VF1) and gas pressure (at the downstream boundary of the VF2) computed by the repository model with the same input.

Transients of gas saturation simulated with the V2-L/ILW model are shown in Fig. 5-23a. Similar to the base case (see Fig. 5-6), the bottom part of the transition layer becomes saturated with porewater shortly after emplacement, while the top part shows increasing gas saturation until the end of the simulation. The transients at the lower and upper parts of the S/B element indicate a continuous gas path across the entire seal throughout the simulation. Similarly, the transients in the VF1 backfill of the adjacent operations tunnel show more gas accumulating upstream of the seal compared to the base case. Pressure transients, shown in Fig. 5-23b, show the hydraulic separation imposed by the low-permeable V2 seal, with distinct pressure differences across the seal during the entire simulated period. Peak pressure, however, does not exceed 10 MPa, and is slightly lower than the estimate obtained in Case 1 using the L/ILW near-field model that assumed an impermeable V2 seal (see also Fig. 5-4).

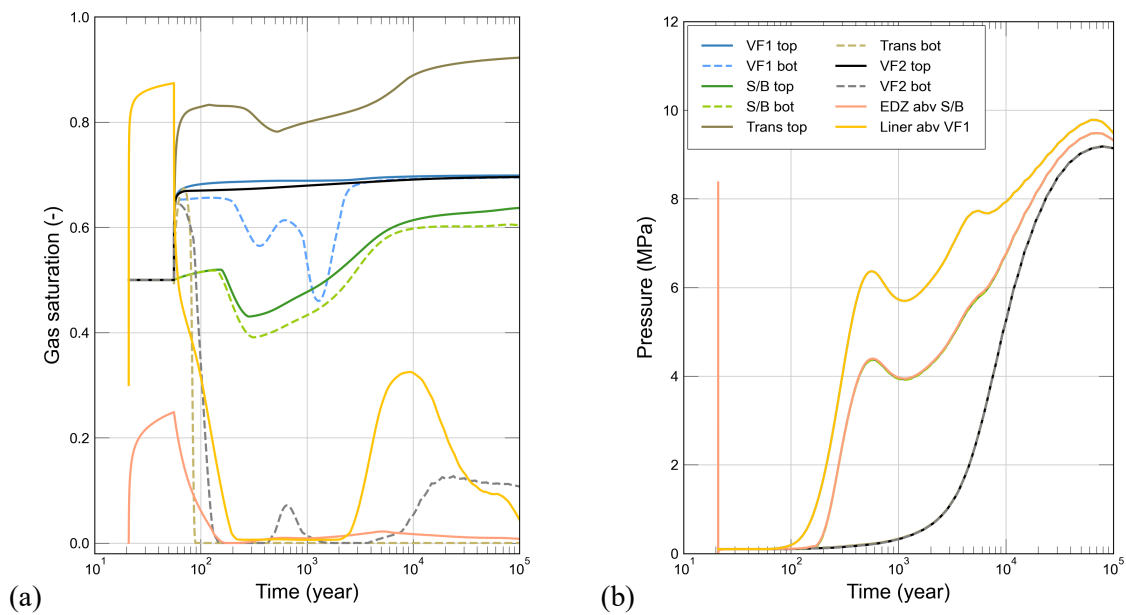


Fig. 5-23: Case 8, V2-L/ILW model

Transients of (a) gas saturation and (b) pressure in the V2 seal and operations tunnel.

5.3.9 Case 9: High-permeability seal V3

Assessment Case 9 focuses on the evolution of the V3 seal under the assumption that the compacted bentonite seal is more permeable than in the base case. For this, the intrinsic permeability of the sealing element is increased by a factor of 10 to $1.E-19 \text{ m}^2$ and the capillary strength is decreased to 7 MPa from the base case value of 22 MPa. The assessment is performed with the V3 component model using gas inflow (at the upstream boundary of the access tunnel) and gas pressure (at the downstream boundary of the access tunnel) computed by the repository model with the same input.

The simulated gas saturation transients are shown in Fig. 5-24a. Similar to the previous cases, the shaft above the seal and the abutment at the top of the bentonite element saturates with porewater once the shaft is backfilled. The resaturation of the sealing element is faster than in the previous cases due to its higher permeability. The middle point of the sealing element fully saturates with porewater after ~ 900 years. Gas breakthrough from the seal to the shaft ($\sim 25,000$ years, refer to Fig. 5-31) does not change the saturation in the shaft appreciably. Similar to the previous cases, pressure in the shaft does not indicate any perturbation from gas pressure buildup in the repository (see Fig. 5-24b), despite the higher permeability of the sealing element.

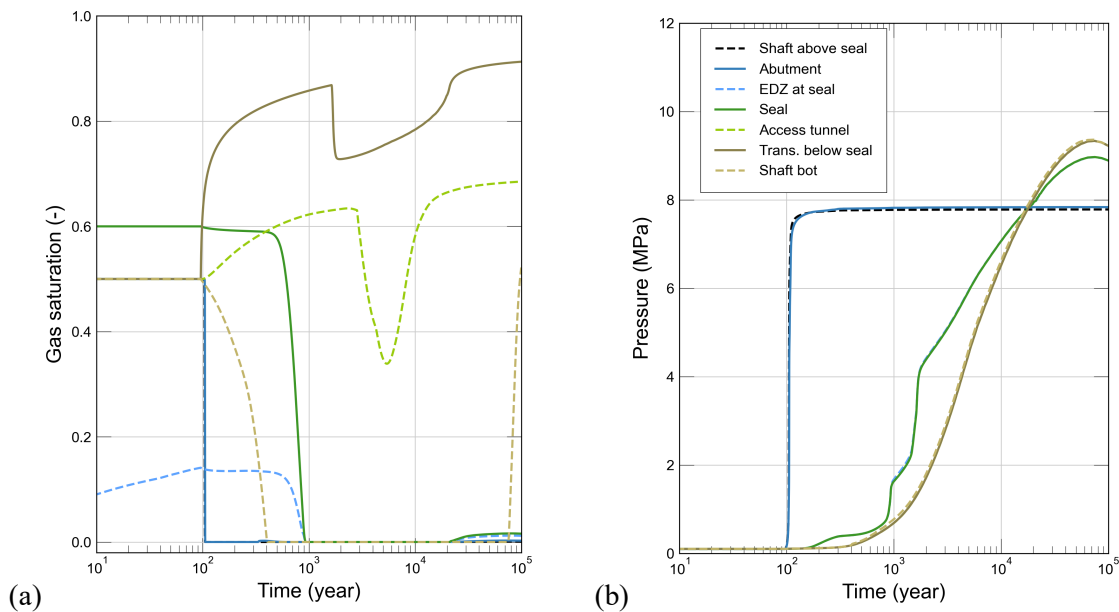


Fig. 5-24: Case 9, V3 model

Transients of (a) gas saturation and (b) pressure in the V3 seal and shaft.

5.3.10 Case 10: L/ILW cavern with low porosity

Assessment Case 10, which reduces the porosities of materials in the L/ILW emplacement cavern, is performed with the L/ILW near-field and V1-L/ILW model. Conservatively for gas pressure buildup, the model variant selected for the assessment assumes an impermeable V2-L/ILW seal.

The saturation evolution of the emplacement cavern, shown in the transients of Fig. 5-25a, is overall similar to the base case (see Fig. 5-4) with the distinct temporary resaturation of the lower part of the M1 mortar in the first few hundreds of years. Due to the reduced pore volume available for gas storage, the mortar then becomes filled with gas earlier (after ~ 6,000 years) compared to the base case (which occurred after ~ 8,000 years). The gas saturation transients in the V1 seal, shown in Fig. 5-25b, show negligible changes from the base case (see Fig. 5-4c), except for the somewhat earlier desaturation of the bottom part of the S/B sealing element after pressure exceeds hydrostatic. The pressure evolution, shown in Fig. 5-25c, shows a faster pressure increase, particularly in the first 20,000 years. The peak pressure reached after 70,000 years is only slightly higher than that of the base case (see Fig. 5-4d).

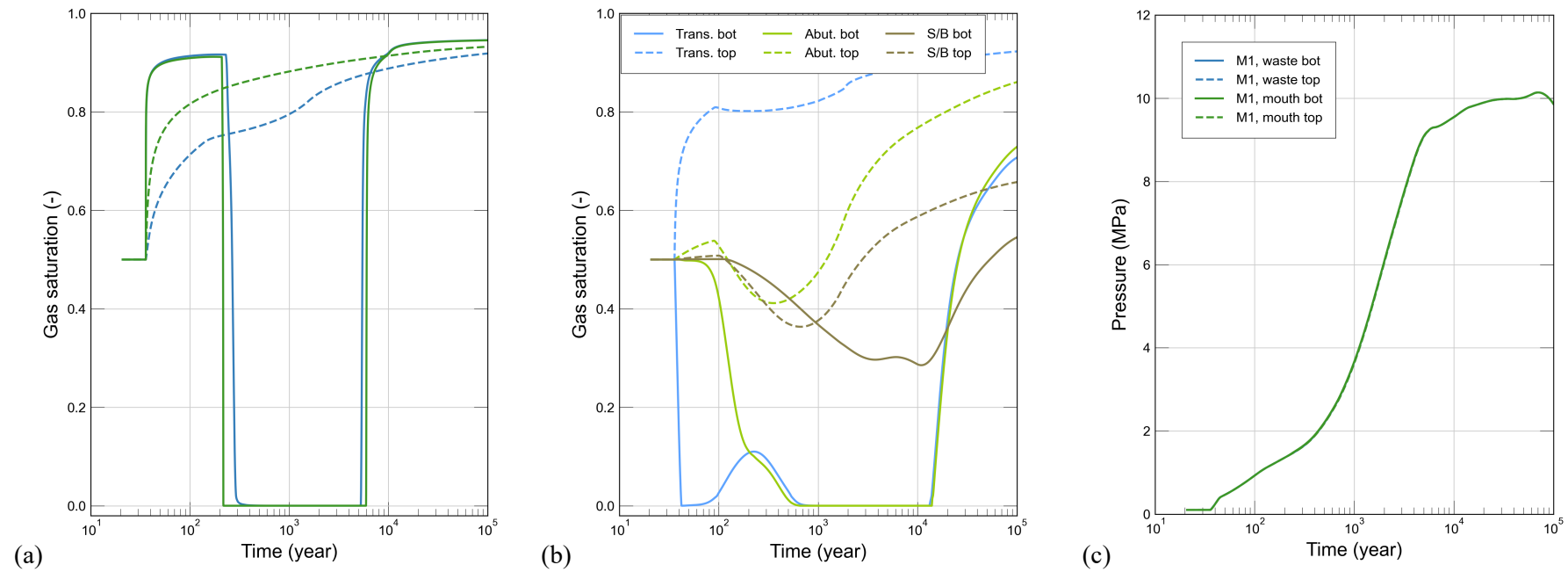


Fig. 5-25: Case 10, L/ILW & V1 model

Transients of gas saturation in the (a) L/ILW emplacement cavern and (b) V1-L/ILW seal; and (c) transients of pressure in the L/ILW emplacement cavern. Legend for (a) shown in (c).

5.3.11 Case 11: Heat output HLW disposal canister

Assessment Case 11, focusing on the near-field hydraulic evolution for conservative estimates of heat generation rates at the HLW disposal canister, is performed using the HLW near-field and V1-HLW model. The assessment period in this case is reduced to 200 years to focus on near-field temperature and the bentonite resaturation with porewater. The results from the simulations using a so-called representative maximum heat output for PWR-MOX, PWR-UO₂, and BWR (see also App. E) are presented in terms of gas saturation at the bentonite directly next to the corresponding canister and the midpoint between the canister and the liner and, in terms of temperatures, at the canister and in the bentonite at the midpoint between the canister and the liner (see also Fig. 5-2).

The gas saturation transients are shown in Fig. 5-26a. Overall, the resaturation of the buffer with porewater is very similar to the base case (see Fig. 5-5), with the bentonite becoming fully water saturated within 200 years in all simulations. Minor differences are observed in the bentonite next to the PWR-MOX drying through evaporation in the first 30 years, resulting in a slightly higher gas saturation next to the canister. This is due to vapor transport associated with the temperature at the canister, shown in Fig. 5-26b, that is overall higher around the PWR-MOX canister. Peak canister temperatures however remain below 150 °C in all cases, while the bentonite temperature at the middle of the buffer reaches ~ 110 °C. Pressure transients are provided for the sake of completeness in App. F.

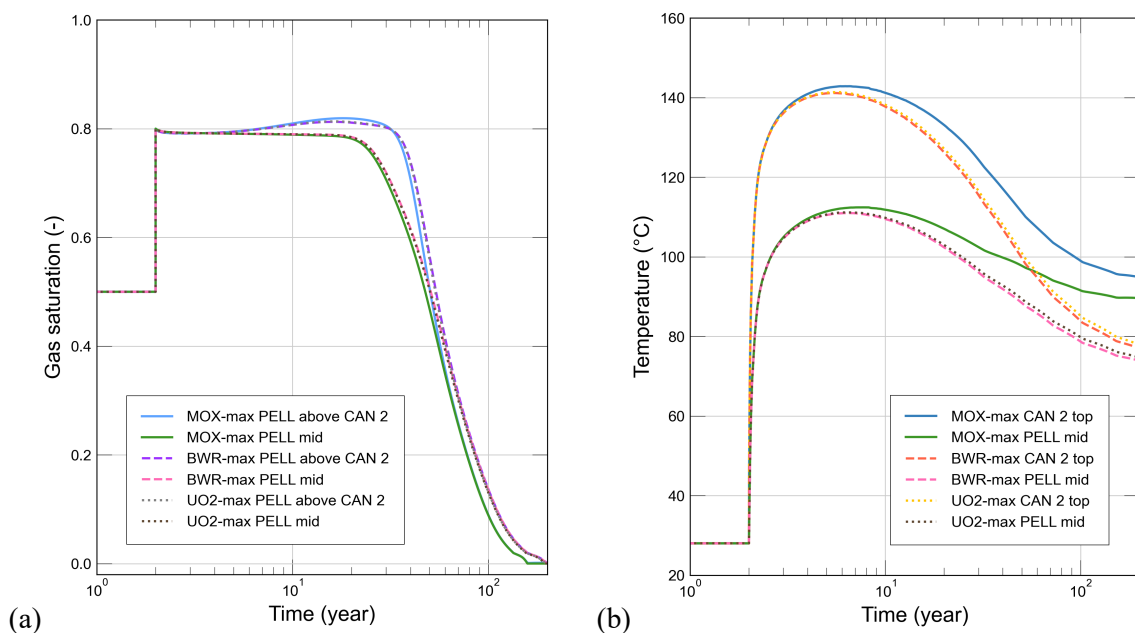


Fig. 5-26: Case 11, HLW & V1 model

Transients of (a) gas saturation in the bentonite adjacent to the disposal canister and at the middle between the canister and the liner; and (b) temperature at the disposal canister and in the bentonite at the middle between canister and liner.

5.3.12 Case 12: Extreme permeability decrease in the V1-L/ILW seal

In Case 12, the Case 4 simulation (with lower bound gas generation rates) is repeated but includes molecular diffusion using the hydrogen and water diffusion coefficients provided in Nagra (2024e). In addition, the permeability of the S/B in the V1-L/ILW seal is decreased to $1.0\text{E-}20\text{ m}^2$ (base case: $5.0\text{E-}18\text{ m}^2$) after it becomes fully saturated with water ($\sim 10,000$ years, see also Fig. 5-27a). The assessment is performed with the L/ILW near-field and V1-L/ILW model.

The simulated transients of gas saturation in the L/ILW cavern are shown in Fig. 5-27a. The bottom part of the M1 mortar saturates with porewater after ~ 400 years. The remaining gas at the roof of the cavern entirely dissolves in water after $\sim 6,000$ years (note that at that time the only difference to Case 4 is the molecular diffusion). Around that time, all components of the V1 seal, including the S/B sealing element, also become fully saturated with water, as indicated in Fig. 5-27b. After the permeability of the seal decreases after 10,000 years, there is no change in saturation, and both the emplacement cavern and the seal remain fully saturated with water. Pressures increase gradually until they reach hydrostatic conditions after $\sim 40,000$ years (Fig. 5-27c). From that time until the end of the simulation, pressures and saturations remain unchanged (Fig. 5-27a; b; c), indicating that all gas generated in the emplacement cavern dissolves in porewater and diffuses into the surrounding rock.

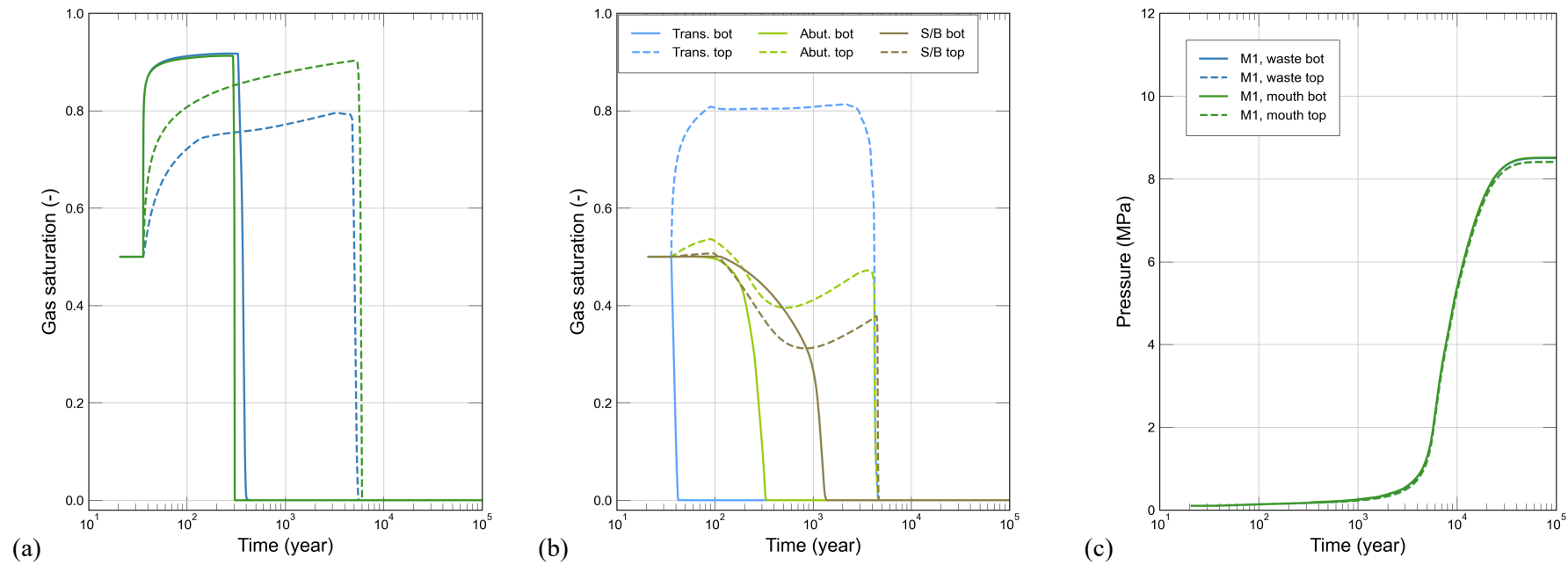


Fig. 5-27: Case 12, L/ILW & V1 model

Transients of gas saturation in the (a) L/ILW emplacement cavern and (b) V1-L/ILW seal; and (c) transients of pressure in the L/ILW emplacement cavern. Legend for (a) shown in (c).

5.4 Synthesis of results

Results from the 12 assessment cases presented in the previous sections are compared to each other to assess the hydraulic evolution, demonstrate the functionality of the provisional design with respect to gas, and assess the associated uncertainties in a deterministic manner (objectives *Obj2* and *Obj3*, Sections 1.1.1 and 4.1).

L/ILW emplacement cavern

Cavern pressures simulated with the L/ILW near-field model are shown in Fig. 5-28a. In Fig. 5-28b, the same cases are compared in terms of gas saturation in the M1 mortar at the top of the cavern (above the stack of waste packages) and at the bottom of the cavern (between the lowermost waste packages, solid curves).

Three assessment cases, namely Cases 1 (model version with operations tunnel reaching the V2-L/ILW), 7 and 10, result in overall similar pressure evolution with a peak pressure of ~ 10.1 MPa after $\sim 70,000$ years. All three cases are based on the conservative assumption that the operations tunnel attached to the emplacement cavern extends only to the V2-L/ILW seal, which is represented as an impermeable boundary. Case 7 additionally assumes lower permeability in the V1-L/ILW seal, whereas Case 10 assumes lower porosity in the cavern materials. When comparing to Case 1, these conservative assumptions result in a somewhat higher pressures during the first 30,000 years but have negligible impact at later times when the peak pressures has been reached. Moreover, as shown in Fig. 5-28b, they result in the earlier desaturation of the lower part of the mortar (i.e., more gas storage in the emplacement cavern).

Two assessment cases, namely Cases 1 (model version with operations tunnel reaching the V2-HLW) and 6, adopt less conservative model assumptions that could be considered in the assessments. Case 1 with this model version assumes that the operations tunnel extends without interruption to the V2-HLW seal, which is represented as an impermeable boundary, providing larger volume for gas storage. Case 6 includes the consumption of water associated with corrosion of metals (but still combined with the impermeable V2-L/ILW seal). In both cases, the resulting peak pressures are decreased to ~ 9 MPa. In comparison, the base case with the repository model resulted in a peak pressure of ~ 9.5 MPa (no water consumption and reference parameters for V2 seals).

Three assessment cases, i.e., Cases 2, 4 and 12, are based on lower gas generation rates. All three cases conservatively assume an impermeable V2-L/ILW seal. Case 4 is based on lower bound gas generation rates. Case 12 additionally combines molecular diffusion of gas with a change of the V1-L/ILW seal permeability to a very low value after 10,000 years. Case 2 sets gas generation to zero. In all three cases, no overpressure is observed at any time during the simulation. Cases 12 and 2 (no gas generation) are the only cases that result in full saturation of the mortar at the roof of the cavern after several thousands of years.

Finally, Case 3 is based on upper bound gas generation rates and Case 5 assumes an extreme corrosion rate for iron and carbon steel, which constitute 70% of metals in the L/ILW inventory. Both cases conservatively assume an impermeable V2-L/ILW seal. Peak pressure of ~ 13.6 MPa occurs after $\sim 5,000$ years in Case 5, and of ~ 11.7 MPa occurs after $\sim 15,000$ years in Case 3. Both cases result in overall higher gas saturations in the emplacement caverns.

V1-L/ILW and V2-L/ILW seals

Gas saturation transients simulated at the top of the S/B in the V1-L/ILW and V2-L/ILW seals are shown in Fig. 5-29a and Fig. 5-29b, respectively.

All cases result in partially saturated conditions at the top of the V1 sealing element with increasing gas saturations after ~ 1,000 years until the end of the simulated time, except Cases 2 and 12 where pressures do not exceed hydrostatic conditions (note that in Case 2 there is no gas generation, and in Case 12 molecular diffusion is included and combined with the lower bound gas generation rates). In Case 12 the seal saturates with water faster than in Case 2 due to the enhanced vapor transport. The highest gas saturation values are observed in Cases 3 and 5 (high corrosion rates). These also resulted in the highest gas pressure values.

Similarly, all cases result in partially saturated conditions at the top of the V2 sealing element with increasing gas saturation after ~ 1,000 years until the end of the simulation, except Case 2 that has no gas sources. The highest gas saturation values are observed in Cases 3 and 8 with upper bound gas generation and lower permeability of the V2 seal, respectively.

HLW emplacement drift

Temperature transients simulated at the canister (depicted with dashed curves) and at the bentonite next to the canister (depicted with solid curves) are shown in Fig. 5-30a. Gas saturation transients simulated at the bentonite between canisters (depicted with solid curves) and in the V1 seal next to the branching tunnel (depicted with dashed curves) are shown in Fig. 5-30b.

Canister temperatures are highest in Case 11, which assumes the representative maximum heat output per SF canister type (see also App. E). In all cases, the peak canister temperatures are observed within the first 8 years after emplacement and are below 145 °C, whereas the peak temperatures in the bentonite next to the canister are below 136 °C. In general, the peak temperatures differences when using representative average and maximum heat output (Case 1 and Case 11, respectively) are ~ 8 °C. Cases 3 and 4 (with the upper and lower bound gas generation) show no appreciable change from the base case.

Accordingly, the resaturation with porewater of the bentonite between the canisters and of the bentonite of the V1 seal is very similar in all cases. The bentonite between the canisters fully saturates within the first 200 years, whereas the V1 seal takes ~ 400 years. The only exception is Case 2 which has no sources of heat or gas. After the assumed canister breaching time, Case 3 results in an overall higher gas saturation in the bentonite buffer and in the V1 seal. Cases 1 and 11, meanwhile, result in the same gas saturation evolution after canister breaching.

V3 seal and shaft

Gas saturation transients at the centre of the V3 seal and at the bottom of the shaft directly above the seal are shown in Fig. 5-31a. The flow rates of gas release from the V3 seal to the shaft are shown in Fig. 5-31b. The bottom of the shaft above the seal saturates practically immediately after backfilling in all cases.

Case 4, with lower bound gas generation rates, results in water resaturation of the middle of the bentonite sealing element that is similar to the base case (~ 2,800 years), and a later breakthrough of gas to the shaft above the seal (~ 80,000 years). In Case 3, with upper bound gas generation rates, the seal takes longer to resaturate with water (~ 7,000 years for the middle compartment) and a small amount of gas remains in the bentonite (~ 1% gas saturation). Accordingly, this case shows the fastest gas breakthrough at the top of the seal, namely after ~ 16,000 years.

On the other hand, in Case 9 (higher permeability and lower capillary strength of bentonite), the middle of the bentonite sealing element saturates with water faster, after ~ 900 years, and gas breakthrough to the shaft occurs after $\sim 25,000$ years. After gas breakthrough, a gas path is reestablished with gas saturations around 1–2% in the sealing element in Cases 3 and 9, whereas no gas saturation is observed in the shaft above the seal in any of the cases. Note that molecular diffusion, which is conservatively not included in these cases, would result in lower gas saturations and significantly delayed gas breakthrough.

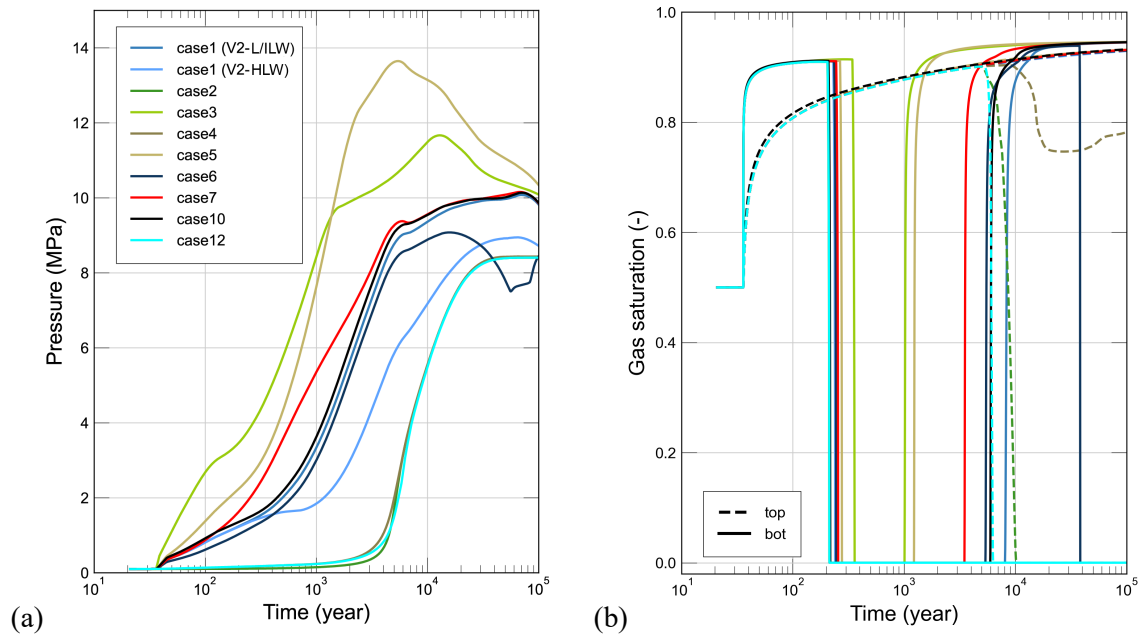


Fig. 5-28: Comparison of (a) pressure in the L/ILW near-field, and (b) gas saturation in the M1 mortar at the top and bottom of the array of disposal containers, simulated in the assessment cases

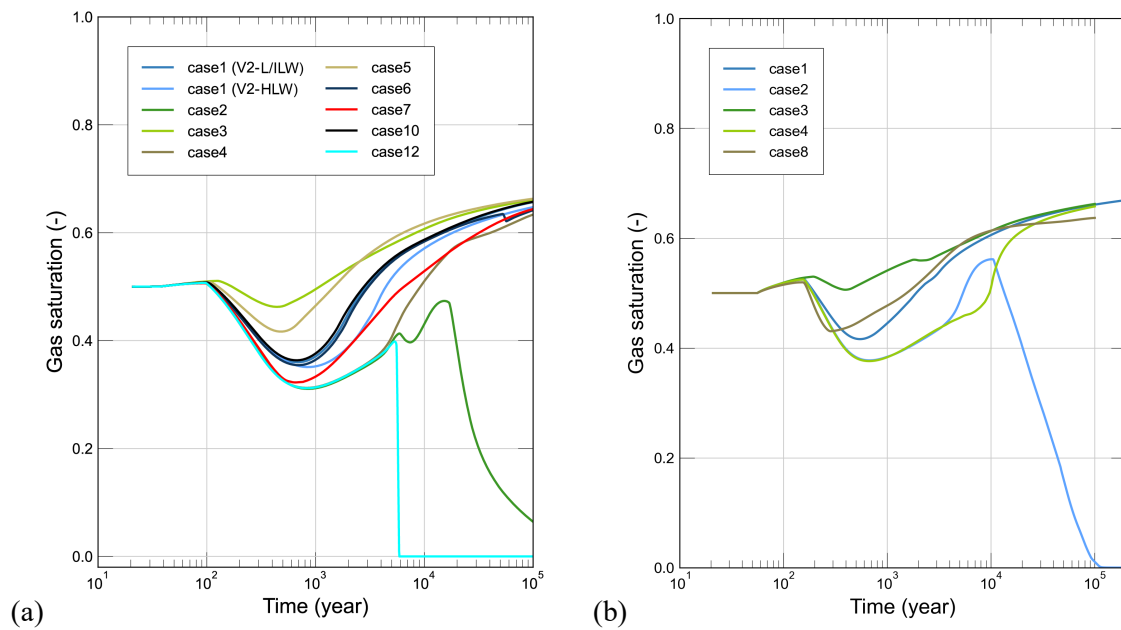


Fig. 5-29: Comparison of gas saturation simulated in the assessment cases (a) at the top of the S/B sealing element of V1-L/ILW, and (b) at the top of the S/B sealing element of V2-L/ILW

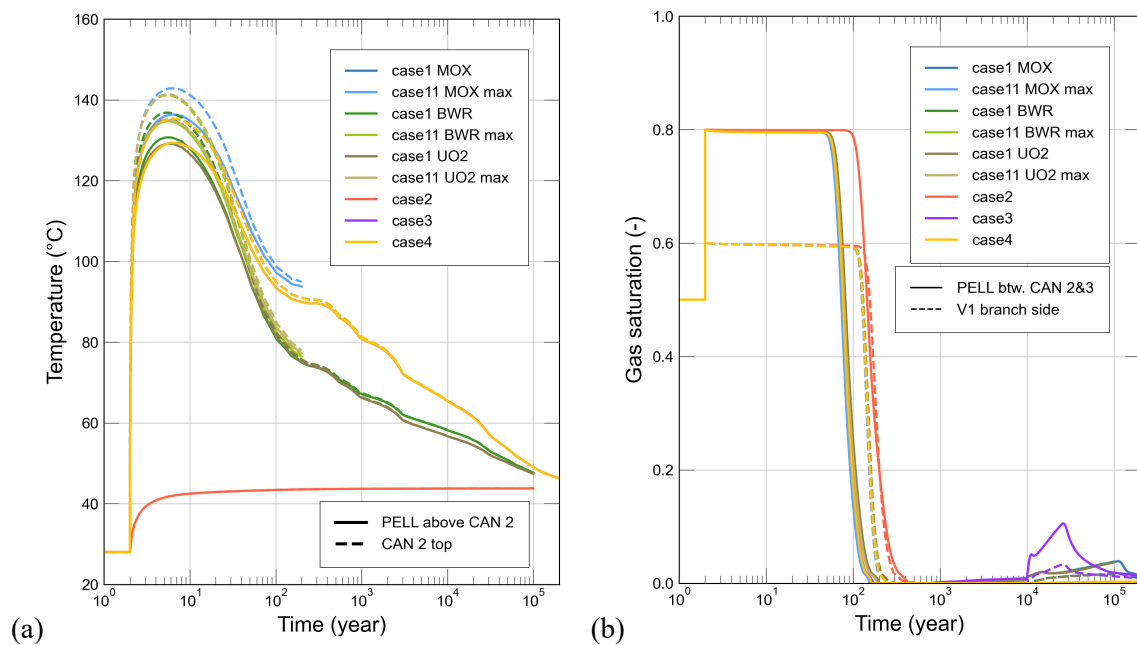


Fig. 5-30: Comparison of (a) the temperature at the SF disposal canister and adjacent bentonite, and (b) gas saturation in the bentonite between the canisters and in the bentonite sealing element of the V1-HLW seal, simulated in the assessment cases

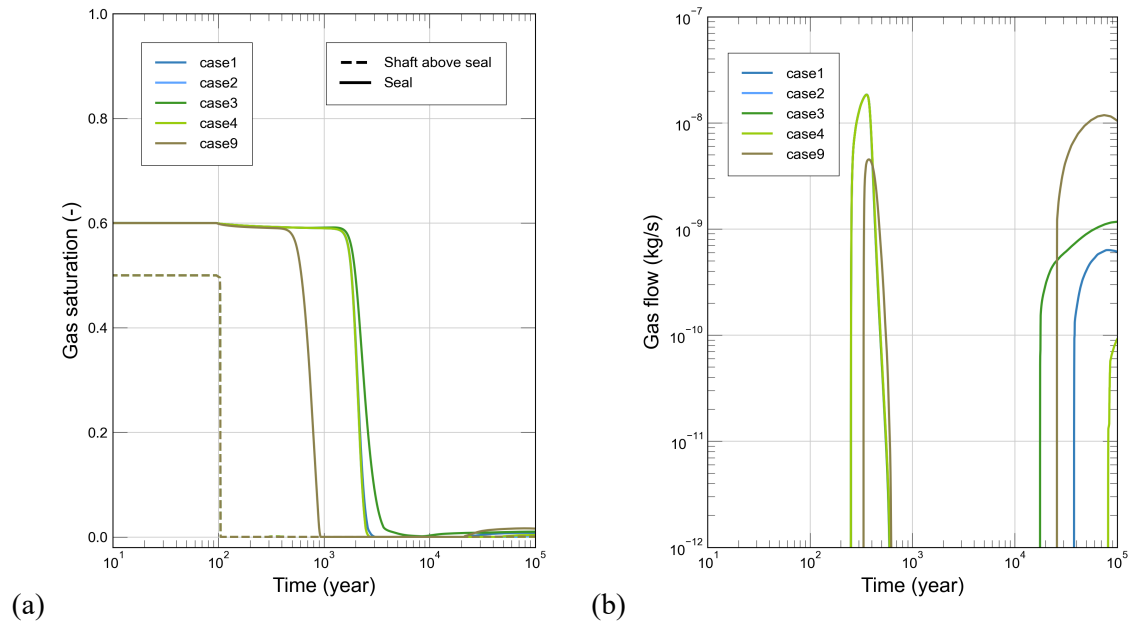


Fig. 5-31: Comparison of (a) gas saturation at the middle of the seal and at the bottom of the shaft above the seal, and (b) gas flow from the seal to the shaft, simulated in the assessment cases

6 Conclusions

The key messages and outcomes of this report are summarised below.

Methodology

The approach used to achieve a comprehensive description of the TH² hydraulic evolution of the repository as part of the PA follows four objectives:

- Obj1: a comprehensive synthesis of the repository components and processes relevant to the production and fate of gases in the deep geological repository;
- Obj2: a quantitative assessment of the hydraulic evolution of the repository under consideration of accumulation and transport of gases in the repository structures;
- Obj3: a demonstration of the functionality of the provisional design with respect to gas including a deterministic assessment of associated uncertainties affecting the hydraulic evolution of the repository;
- Obj4: underlying argumentation basis for the PA of the repository, the subsequent derivation of safety scenarios, and the analysis of radiological consequences from the release, retention and transport of volatile radionuclides through the repository barriers.

The report is structured accordingly and comprises (i) the synthesis of materials and processes that determine the production and fate of gases in the repository, and (ii) the model-based assessment of gas generation and transport in the repository and surrounding environment.

Materials are synthesised from MIRAM-RBG (Nagra 2023c) with the changes they will undergo over time as described in the phenomenological evolution of the repository (Nagra 2024f). The model conceptualisation and abstraction is part of the abstraction workflow implemented in the PA (Nagra 2024e). The workflow integrates the repository- and component-scale models and allows to elaborate a range of assessment cases that draw a comprehensive picture of the hydraulic evolution of the repository. The assessment cases are formulated generically as part of a deterministic sensitivity analysis. A so-called *base case* is defined, corresponding to the expected evolution of the repository, enveloped by deterministic variants. The variants are a subset of possible perturbations in the system, demonstrating the functionality and robustness of the repository system in terms of gas transport and hydraulic evolution.

Hydraulic evolution – expected performance

The excavation and ventilation of the repository structures causes depressurisation and partial desaturation of the EDZ and the surrounding rock. After emplacement and backfilling of the repository structures, gas is generated from the corrosion (HLW and L/ILW) and degradation (L/ILW only) of materials in the repository. The rate of gas generated in the L/ILW emplacement caverns is orders of magnitude higher than that in the HLW emplacement drifts of the repository. At the same time, water redistributes locally depending on the balance of capillary, viscous and gravity forces associated with the emplaced materials in each section. In general, materials with large pores, and accordingly low capillary suction, favour viscous- and gravity-driven over capillary-driven transport of gas and water.

Gas generation from L/ILW is highest directly after emplacement and decreases with time. Backfill and sealing materials in the L/ILW section of the repository are overall characterised by high porosities and low capillary strengths. This is a key feature of the repository with regard to gas and is currently designed to allow the axial transport of gas through the repository structures.

Thanks to this feature, pressure gradients generated from gas accumulation in the emplacement caverns result in advective flow of gas into the adjacent tunnels and along the network of tunnels in the repository. As a result, gas spreads to a larger storage volume, which mitigates the increase of gas pressures. At the same time, there is gas transport radially around the tunnels into the surrounding rock that, due to the very low permeability and high capillary suction of the Opalinus Clay, is dominated by dissolution and diffusion in porewater. Through the advective spreading of gas along the repository tunnels, the interface area for gas dissolution in porewater also increases, further mitigating overpressures. With this provisional design that combines axial and radial transport of gas, the increase of pressure in the expected evolution of the repository takes place gradually over several thousands of years, and hydrostatic conditions are reached after $\sim 20,000$ years. The accumulation of gas in the backfill results in peak pressures of ~ 9.3 MPa after $\sim 70,000$ years in the L/ILW repository section. Gas saturations during that time are overall high, particularly in the upper portions of the backfill and the materials used in the seals (V1-L/ILW and V2-L/ILW). This forms a connected pathway for gas that accumulates in the upper part of the emplacement caverns and therewith facilitates the transport of gas through the L/ILW section of the repository and the central area. The gas saturation transients simulated with the models show that this pathway is maintained for hundreds of thousands of years. During that time the resaturation of the L/ILW section of the repository with porewater, including the emplacement caverns, occurs gradually from the bottom to the top. This process is determined on the one hand by gas pressure in the tunnels that counteracts the inflow of porewater and on the other hand by gravity in the high-porosity backfill that drives water to the tunnel invert and gas to the tunnel roof.

The early post-closure phase of the HLW section of the repository is marked by heat output by the HLW. The heat output is highest directly after emplacement and decreases with time. Temperatures at the PWR-MOX, PWR-UO₂ and BWR canisters reach ~ 136 °C after 5 years. Temperatures in the bentonite within 5 cm of the canisters reach ~ 130 °C. The thermal pulse results in pressure increase caused by thermal expansion of porewater in the rock surrounding the HLW disposal area (for example ~ 13 MPa at 30 m above the disposal area), that dissipates after few hundreds of years. During that period, the bentonite surrounding the canisters takes up porewater due to its high suction and the thermal gradient, reaching full water saturation after ~ 200 years. Similarly, the bentonite of the V1-HLW sealing element saturates with porewater after ~ 300 years. Combined with the low permeability and high capillary suction of the Opalinus Clay, this creates a low-permeable barrier in the HLW section of the repository where gas transport is dominated by capillary suction, dissolution and diffusion in porewater. As opposed to the L/ILW section, gas transport axially through the tunnels in the HLW section is very limited. However, gas generation from HLW occurs very slowly so that radial transport and dissolution are sufficient to dissipate gas. Gas generation is constant until the time when the canisters are assumed to breach (in the present model conceptualisation this is assumed to occur simultaneously for all canisters after 10,000 years; the effect of canister breaching times on repository pressure is discussed in Nagra 2024e). After canisters have breached, gas generation increases temporarily until the canisters have corroded entirely ($\sim 115,000$ years). Accordingly, gas pressure reaches ~ 10.5 MPa shortly after the assumed canister breaching time and a maximum of ~ 11.8 MPa when the canisters corrode entirely.

After backfilling, the shafts saturate with porewater from the surrounding rock formations. Full saturation of the shaft sections in the Passwang formation is reached almost immediately. The middle compartment of the bentonite seal in the access shaft saturates with porewater after $\sim 3,000$ years (in comparison, the top and bottom bentonite compartments take less than 1,000 years and 10,000 years, respectively). The seal thereby acts as a hydraulic barrier, limiting the release of gas to the overlying shaft. Gas breakthrough from the V3 seal occurs after pressure in the repository has exceeded hydrostatic conditions (in this case, after $\sim 39,000$ years). The release of gas does not result in any appreciable gas saturation in the shaft above the seal.

Note that molecular diffusion, which is conservatively not included in this case, would result in lower gas pressures and saturations and significantly delay the breakthrough of gas through the V3 seal.

Hydraulic evolution – deviations from expected performance

The synthesis of the assessment cases representing deviations is based on direct comparison between these in terms of selected model metrics in the L/ILW repository section, the HLW repository section, and the access shaft.

In terms of gas pressure in the L/ILW section of the repository, the key aspect is the balance between the rate of gas generation and the volume that is readily accessible for gas storage. The latter is determined by hydraulic properties assigned to materials in the backfill and seals. Cases that adopt conservative assumptions related to the gas generation rates (UB gas rates), or properties of materials that limit gas transport along the repository structures (permeabilities of seals and porosities of emplacement caverns), result in moderate peak pressures of ~ 10 MPa. Peak pressures increase more in cases that combine such conservative assumptions (i.e., ~ 11.7 MPa when UB gas rates are used in a model that also assumes an impermeable V2-L/ILW seal) or very pessimistic scenarios (i.e., ~ 13.6 MPa when extreme corrosion rates for iron and carbon steel are used in the same model). Cases that adopt the LB gas rates do not result in any overpressure in the L/ILW section of the repository, even when combined with an impermeable V2-L/ILW seal, as the dissolution and diffusion of gas through the surrounding host rock provide sufficient transport capacity. A case with significantly decreased permeability (combined with increased capillary strength) of the V1-L/ILW seal after the latter has fully saturated with water also does not result in any overpressure. These observations are also depicted in gas saturations in the L/ILW repository section. All cases show water accumulating at the lower part of the L/ILW caverns at least until hydrostatic conditions are reached. At the same time, gas accumulates at the upper part of the cavern for at least 100,000 years, except in cases with LB or zero gas generation that result in overall higher water saturations. Cases with high gas generation, and accordingly more pressure buildup, result in more water displacement and accordingly overall higher gas saturations in the L/ILW nearfield. The saturation evolution is similar in the V1-L/ILW and V2-L/ILW sealing sections. All cases result in partially saturated conditions at the upper portions of the sealing elements for at least 100,000 years, except in cases with LB or zero gas generation. Cases with high gas generation result in overall higher gas saturations in the sealing elements and their adjacent components.

In the HLW section of the repository, temperatures in the nearfield increase by only few degrees Celsius when representative maximum canister heat outputs are used (peak temperatures below 145°C and 136°C at the canister and in the bentonite next to the canister, respectively). For the same cases, resaturation of the bentonite surrounding the canisters and of the bentonite of the V1-HLW seal is very similar to the base case. Cases that adopt the LB and UB gas rates also do not change the times required to reach full water saturation in the bentonite of the emplacement tunnels and V1-HLW seal. Peak pressures induced by gas generation after all canisters are assumed to breach simultaneously vary from hydrostatic (LB gas rates) to 14.4 MPa (UB gas rates).

All cases show very fast water resaturation of the shaft section in the Passwang formation after backfilling, similar to the base case. On the other hand, the bentonite sealing element saturates with water slower compared to the base case when conservative gas generation rates are adopted (UB gas rates). Gas breakthrough from the V3 seal occurs earlier in the case of UB and later in the case of LB gas rates (between $\sim 16,000$ and $\sim 80,000$ years if molecular diffusion is conservatively not taken into account). No gas saturation is observed in the shaft above the seal in any of the cases.

Key outcomes

The synthesis of results demonstrates sensitivities of the hydraulic evolution to the deviations considered in the assessment cases, and key processes underpinning the phenomenological evolution of the repository. Gas generation occurs at much higher rates in the L/ILW than in the HLW repository section, and the provisional repository design and prevailing transport regimes are tailored accordingly. The main outcome of the analysis is a consistent hydraulic evolution of the repository that adheres to the provisional design principles and associated transport regimes for all considered cases.

In the L/ILW section, gas transport occurs axially and advective along the repository tunnels and radially into the surrounding rock. Through the operations tunnels and sealing sections, gas generated in the L/ILW caverns spreads through the entire L/ILW section and central area of the repository. The storage volume for gas available in these structures provides significant robustness, resulting in moderate gas pressures even in very conservative cases of gas generation and material properties. A significant observation therein concerns the self-regulating nature of gas pressure in the repository: an increase in the amount of gas in the pores of the emplaced materials results in a higher effective permeability for gas, which increases gas transport along the repository structures and decreases pressure build-up. The analysis shows that partially saturated conditions will sustain gas pathways in the emplacement caverns, the sealing sections, and through the repository structures such that significant overpressures are mitigated.

By contrast, axial gas transport in the HLW section of the repository is very limited. The HLW near-field saturates with water within few hundreds of years in all assessment cases, due to the high suction and thermal gradient. The saturated bentonite material forms a hydraulic barrier to gas flow away from the corroding canisters. However, due to the low corrosion rate of the carbon steel canister under repository conditions, radial gas transport and dissolution in porewater are sufficient to dissipate gas. The resulting gas pressure build-up in the HLW drifts is not significant unless extremely conservative assumptions are made.

Gas reaching the shaft has therefore its origins mainly in the L/ILW repository section. However, gas release to the shaft is limited by the hydraulic barrier imposed by the V3 seal. This function is maintained even in conservative cases of gas generation and seal properties. Notably, gas generated in the combined repository is essentially contained within the underground structures (or dissolved in the surrounding rock) without introducing significant overpressures thanks to the storage volume (and interface to surrounding rock) provided by the repository.

PA modelling employs conservatism where assumptions and simplifications need to be made. For example, the corrosion and degradation of materials are conservatively decoupled from the availability of water for these reactions. In reality, gas generation ceases in dry conditions, or at low relative humidity, as water availability is the most important limiting factor for the degradation of organics and corrosion of metals. As a further example, it is conservatively assumed that gas generation from the L/ILW repository section starts immediately after waste emplacement, despite the highly alkaline near-field conditions, which, in reality, are expected to decrease corrosion and to inhibit microbial activity. Gas-induced overpressures could be further reduced by gas-consuming microorganisms, which are not accounted for in the present calculations, or, if it were to prove necessary, by further tailoring the sealing system.

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App. A Schematic illustrations of components of the repository

A.1 Emplacement rooms and operations tunnels

A schematic illustration of the unloading and waste transfer area of the L/ILW emplacement cavern is shown in Fig. A-1. The corresponding tunnel dimensions for the L/ILW branching tunnel, unloading area, waste transfer area, and L/ILW emplacement cavern are shown in Fig. A-2. The dimensions of the HLW emplacement drift are shown in Fig. A-3.

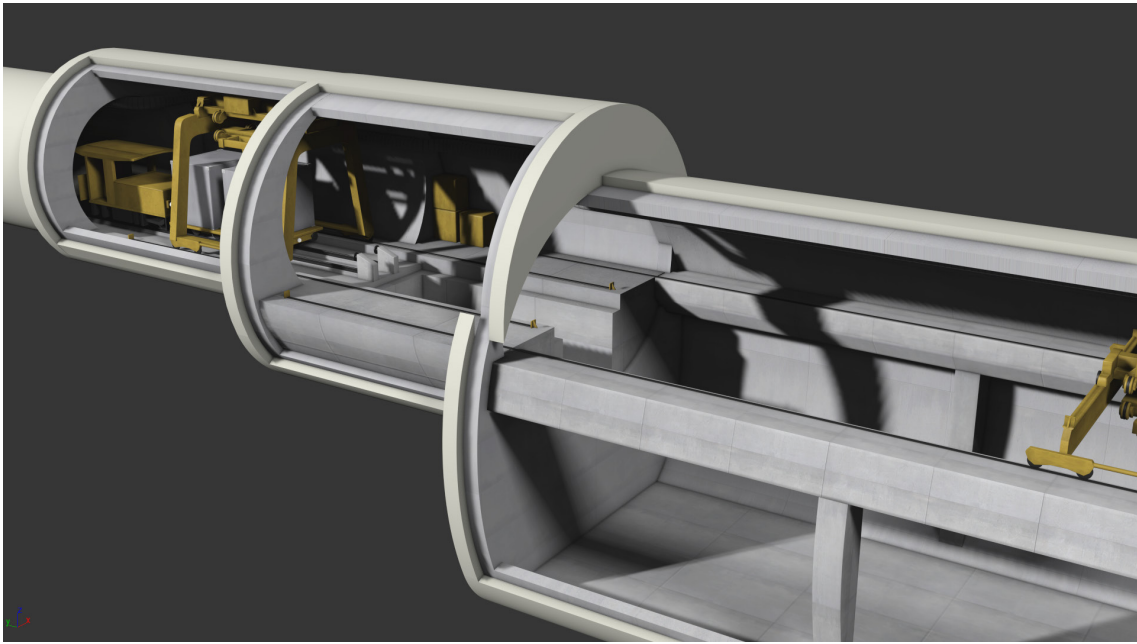


Fig. A-1: Schematic illustration of the mouth of an L/ILW emplacement cavern with the unloading and waste transfer area

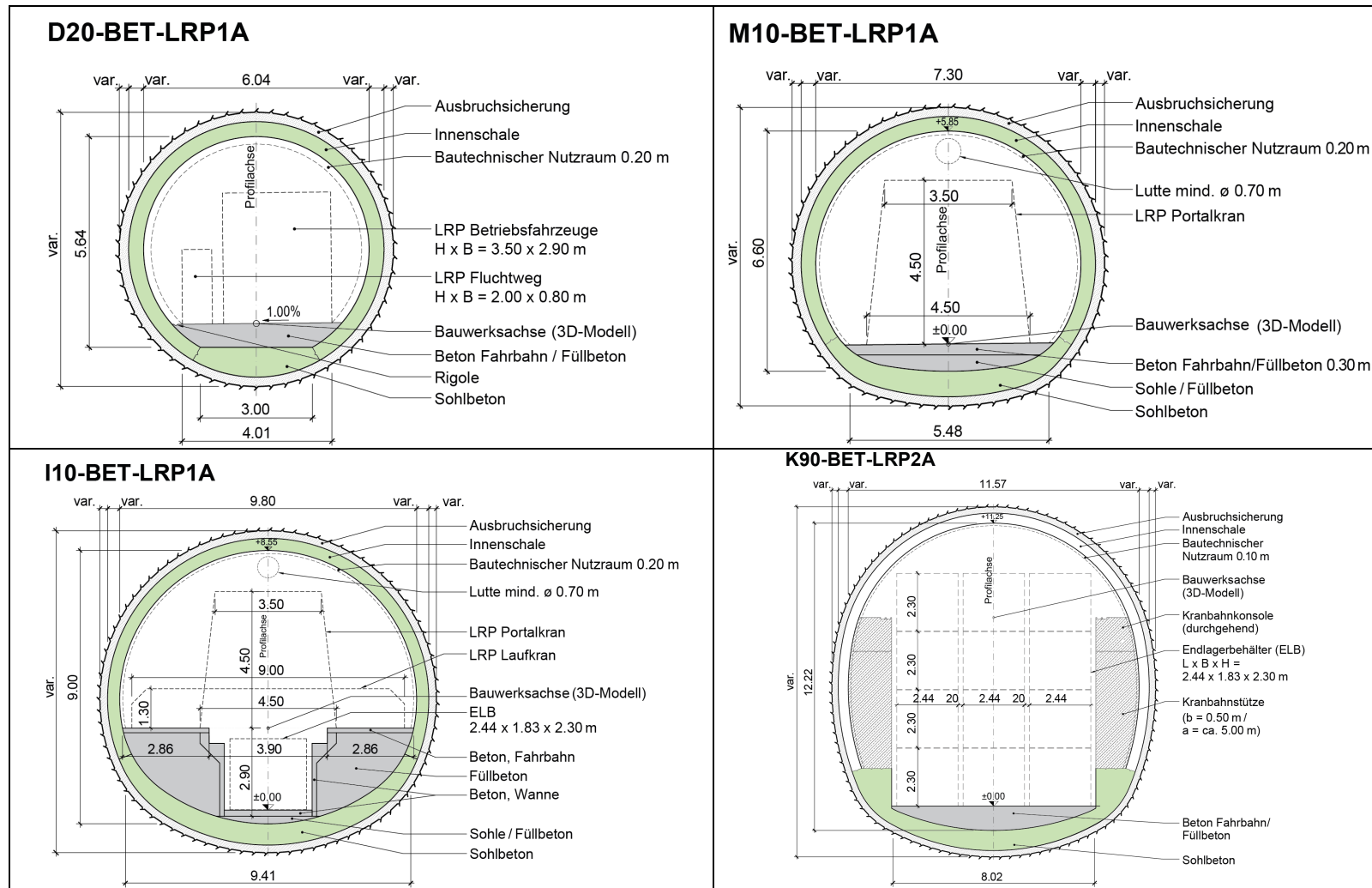


Fig. A-2: Cross-sections of tunnels in the L/ILW disposal area

D20: branching tunnel; M10: unloading area; I10: waste transfer area; K90: emplacement cavern. Adapted from Nagra (2023a).

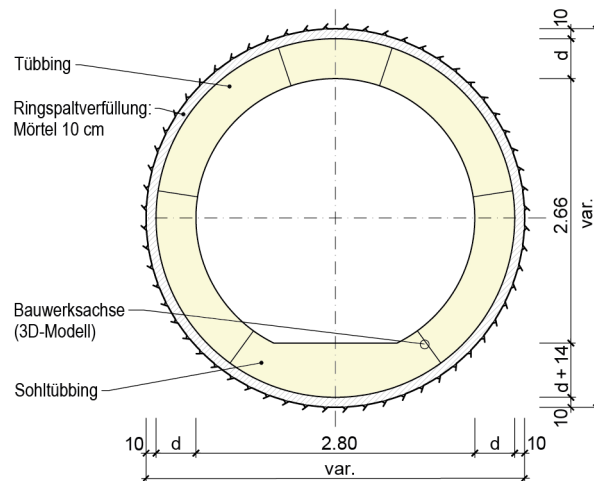


Fig. A-3: Cross-section of an HLW emplacement drift
Adapted from Nagra (2023a).

A.2 Waste

The L/ILW container LC-86H is schematically illustrated in Fig. A-4. The container dimensions are provided in the same figure.

The disposal canisters used for SF and RP-HLW are shown in Fig. A-5.

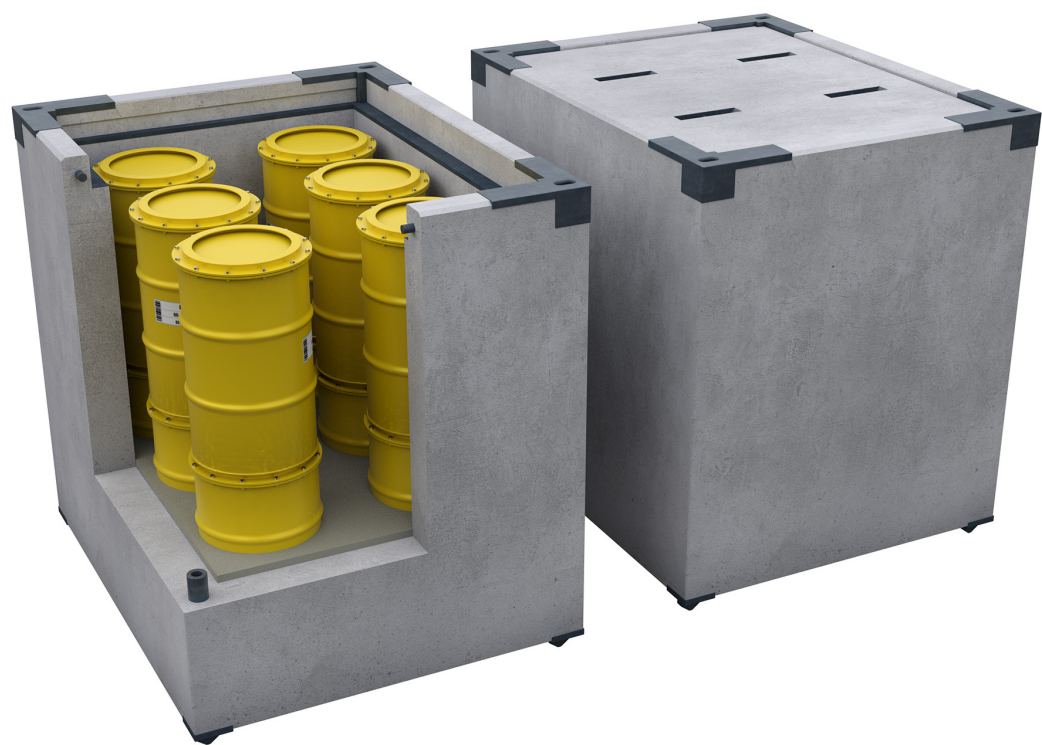


Fig. A-4: Schematic illustration of the LC-86H disposal container filled with 200 L waste packages
Dimensions (L×B×H): 2.44×1.98×2.30 m.

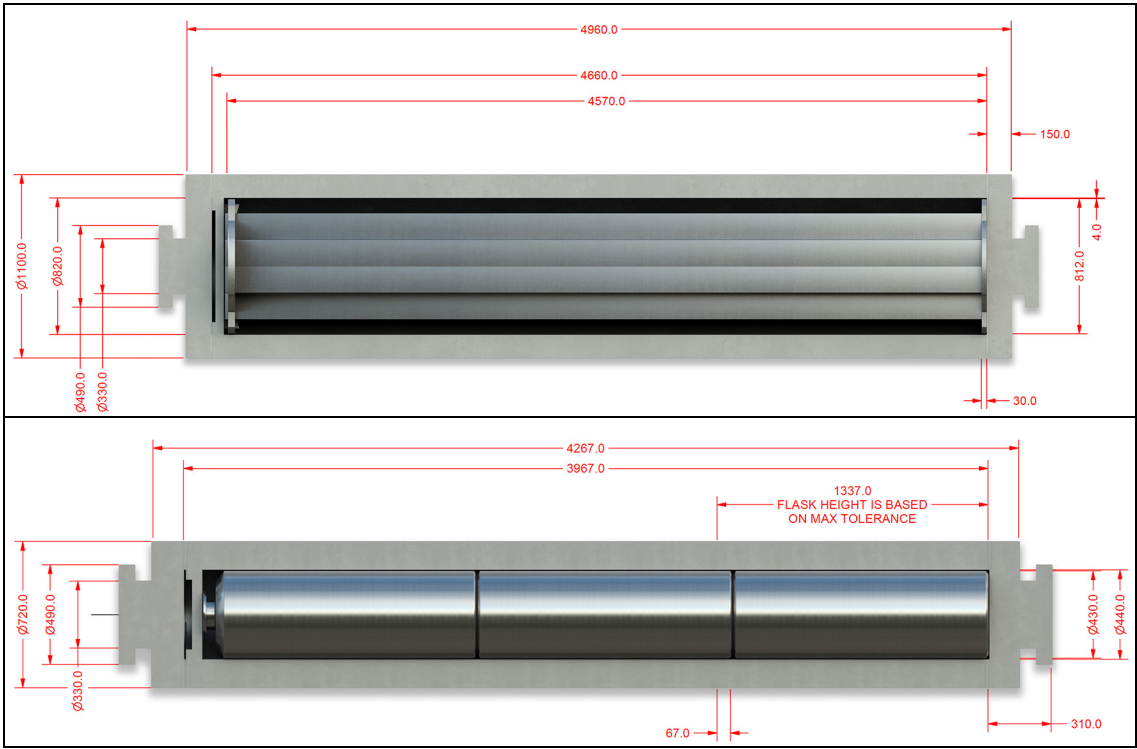


Fig. A-5: Schematic illustration and dimensions of disposal canisters used for SF (top) and RP-HLW (bottom)

A.3 Seals

The following figures illustrate the different seals implemented in the repository. The elements included in the seals with their respective lengths are shown in each figure. The tunnel diameters are only indicative.

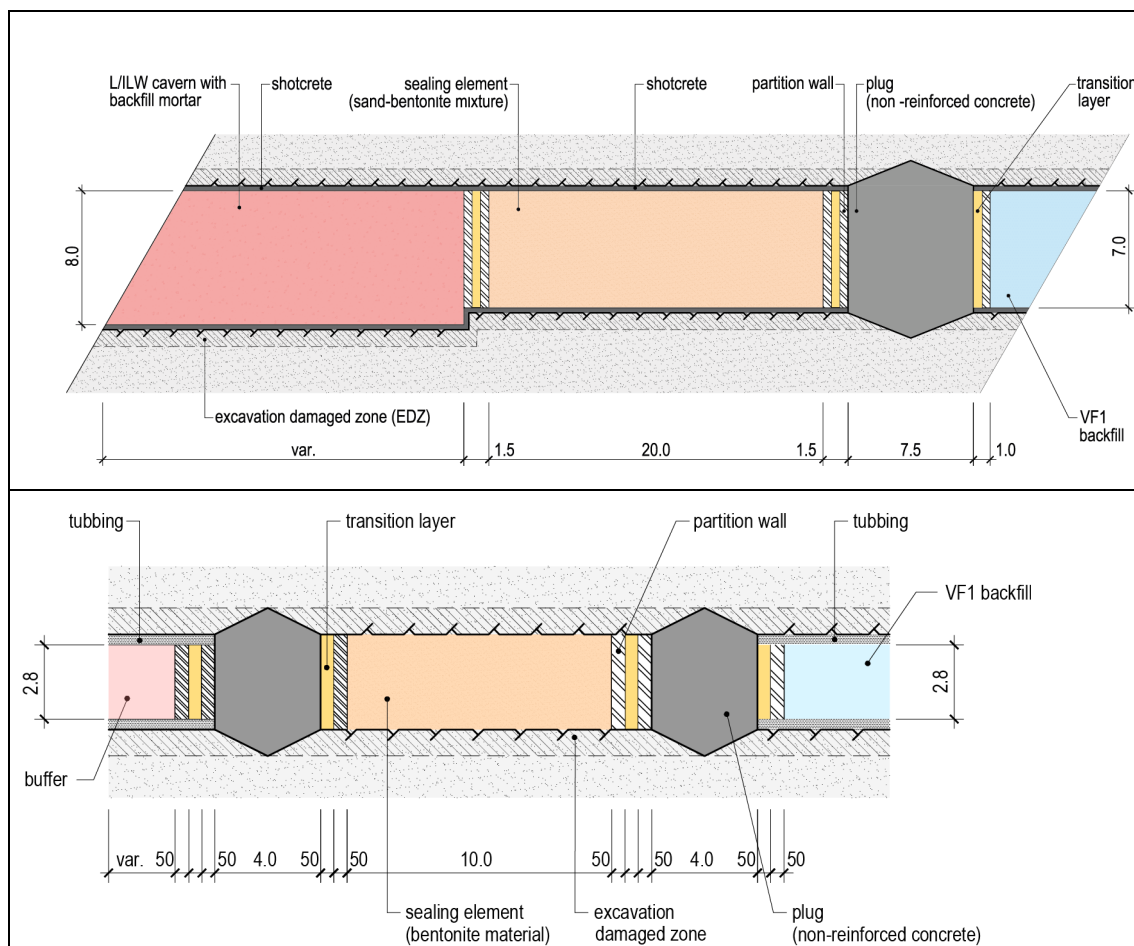


Fig. A-6: V1-L/ILW seal (top) and V1-HLW seal (bottom)

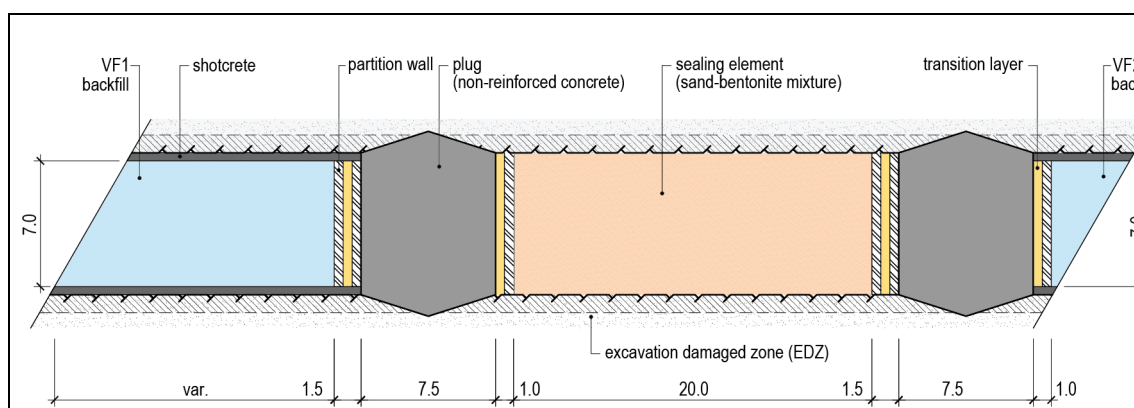


Fig. A-7: V2 seal

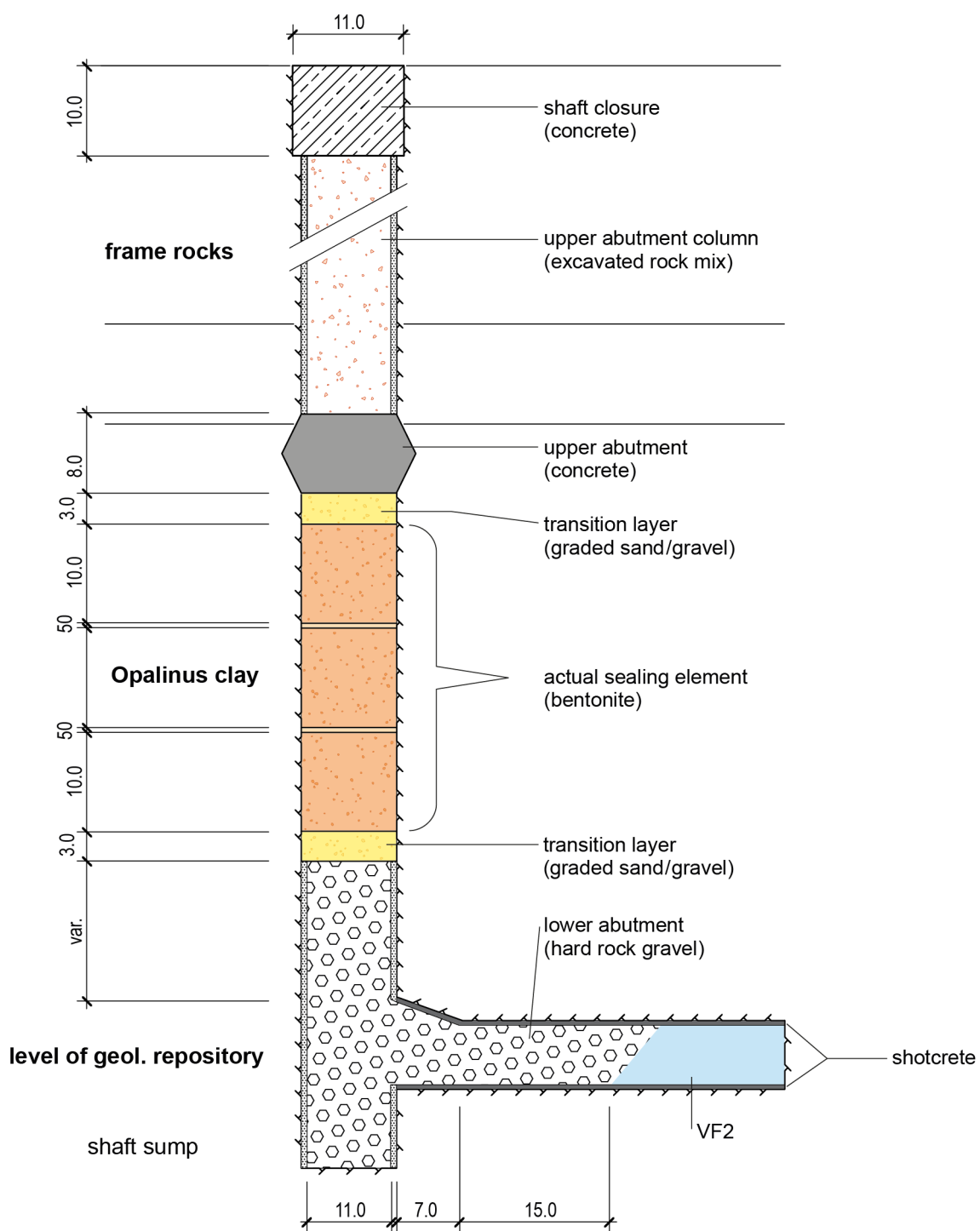


Fig. A-8: V3 seal

App. B Inventory of metals and associated corrosion groups

B.1 L/ILW, including waste form and containers

Tab. B-1: List of metals and alloys to be disposed of in L/ILW emplacement caverns, and associated corrosion groups⁴ as defined in Section 3.1.2 and their mass

Based on MIRAM RBG (Nagra 2023c).

Metals and alloys	Corrosion group	Mass (kg)
Steel	Iron and carbon steel	1.6×10^7
Cast iron	Iron and carbon steel	5.8×10^6
Steel III SIA 162	Iron and carbon steel	3.9×10^6
CrNi-steel	Stainless steel and Ni alloys	2.3×10^6
Steel 12.03	Iron and carbon steel	1.9×10^6
Aluminium Al	Aluminium	1.8×10^6
Lead Pb	Lead	1.8×10^6
Steel US A508	Stainless steel and Ni alloys	1.2×10^6
Steel 37	Iron and carbon steel	8.4×10^5
Iron Fe	Iron and carbon steel	8.2×10^5
Steel US 304	Stainless steel and Ni alloys	6.5×10^5
Stainless steel	Stainless steel and Ni alloys	3.8×10^5
Copper Cu	Copper	3.5×10^5
Steel 1.6751	Stainless steel and Ni alloys	3.3×10^5
Zircaloy-2	Zircaloy	2.4×10^5
Steel 1.4550	Stainless steel and Ni alloys	1.2×10^5
Steel 1.4571	Stainless steel and Ni alloys	1.2×10^5
Steel 1.4301	Stainless steel and Ni alloys	7.6×10^4
Zircaloy-4	Zircaloy	5.7×10^4
Nickel Ni	Stainless steel and Ni alloys	4.0×10^4
Steel 1.6958	Stainless steel and Ni alloys	2.3×10^4
Zinc Zn	Zinc	1.8×10^4
Steel 18.8	Stainless steel and Ni alloys	1.7×10^4
Inconel 600	Stainless steel and Ni alloys	1.4×10^4
Steel 1.4541	Stainless steel and Ni alloys	9.2×10^3
PbBi-Eutectic (PbBi55.5%)	Lead	7.4×10^3
Brass CuZn37%	Zinc	7.1×10^3
Silver Ag	-	6.9×10^3

⁴ “Unclassified” metals without an assigned corrosion group are metals that are either not expected to corrode under repository conditions or the amounts are negligible compared to the other groups.

Tab. B -1: Cont.

Metals and alloys	Corrosion group	Mass (kg)
Uranium U	-	6.8×10^3
Aluminium Al (Mg3%Si1%)	Aluminium	4.5×10^3
Mild/construction steel	Iron and carbon steel	3.5×10^3
Halfnium Hf	Zircaloy	3.4×10^3
Inconel 750	Stainless steel and Ni alloys	3.2×10^3
Aluminium Al (Mg0.5%Si0.5%)	Aluminium	2.9×10^3
Tungsten W	Zircaloy	2.0×10^3
Tungsten W (Ni6%Cu4%)	Zircaloy	9.9×10^2
Magnesium Mg	Magnesium	8.5×10^2
Tin Sn	-	6.9×10^2
Tantalum Ta	Zircaloy	6.1×10^2
Nickel Ni (Mo28%)	Stainless steel and Ni alloys	4.8×10^2
Titanium Ti	Zircaloy	3.3×10^2
Stellite	Stainless steel and Ni alloys	1.7×10^2
Gold Au	-	1.0×10^2
Beryllium Be	-	8.6×10^1
Thorium Th	-	6.2×10^1
Inconel 718	Stainless steel and Ni alloys	5.0×10^1
Cadmium Cd	-	4.8×10^1
Antimony Sb	-	9.3
Zirconium Zr	Zircaloy	1.5
Niobium Nb	-	1
Chromium Cr	Stainless steel and Ni alloys	< 1
Calcium Ca	-	< 1
Cobalt Co	-	< 1
Total		4.2×10^7

B.2 HLW, including waste form and containers

Tab. B-2: List of metals and alloys to be disposed of in HLW emplacement drifts, and associated corrosion groups as defined in Section 3.1.2 and their mass

Based on MIRAM RBG (Nagra 2023c).

Metals disposed of in HLW	Corrosion group	Mass (kg)
Steel	Iron and carbon steel	4.1×10^7
Zircaloy-2	Zircaloy	6.5×10^5
Zircaloy-4	Zircaloy	4.3×10^5
Stainless steel	Stainless steel and Ni alloys	2.1×10^5
CrNi-steel	Stainless steel and Ni alloys	5.9×10^4
Inconel	Stainless steel and Ni alloys	1.6×10^4
Aluminium (Mg3%Si1%)	Aluminium	2.7×10^3
Lead	Lead	1.4×10^2
Aluminium	Aluminium	6.4×10^1
Copper	Copper	2.1×10^1
Brass (CuZn37%)	Zinc	2.1×10^1
Total		4.3×10^7

B.3 Construction materials

In the emplacement drifts, steel lining, fibres, anchors, ribs and reinforced steel for cast-in-place concrete will be used:

- Steel lining consists of a stainless steel plate with a thickness of 10 mm and a density of 7,850 kg/m³.
- Steel fibres used for concrete reinforcement will be made of carbon steel with a diameter of 0.7 mm and a length of 35 mm.
- Reinforced steel for cast-in-place concrete is foreseen to be in carbon steel structures made of steel rods with diameters of 14 mm.
- Steel anchors, made of carbon steel rods, are expected to have a diameter of 25 mm. The length of each steel anchor may vary between 3 and 6 m, depending on the tunnel profile and the anchoring pattern.
- Steel ribs, also in carbon steel, have two different Toussaint-Heintzmann (TH) profiles (i.e., TH36 or TH44).

Fig. B-1 shows cross-section of a TH profile. Tab. B-3 reports the associated dimensions of the TH36 and TH44 profiles.

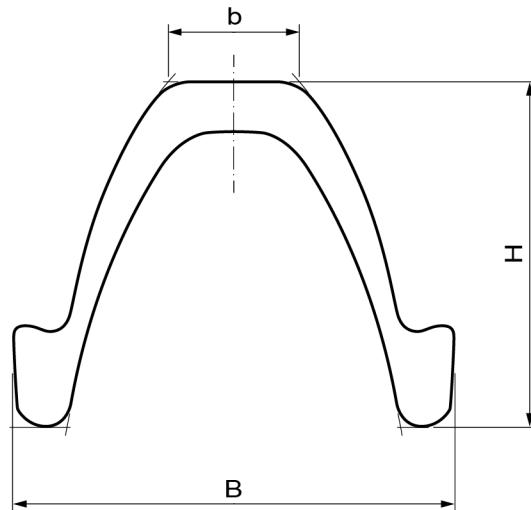


Fig. B-1: Cross-section of steel rib with TH profile

Tab. B-3: Section measurement of steel ribs foreseen in the provisional repository design

Steel rib profile	TH36	TH44
H [mm]	138	148
B [mm]	171	172
b [mm]	51	50
Surface [cm ²]	46	56
Perimeter [m]	0.702	0.753
Weight [kg/m]	35.9	44

The shape of the steel ribs is approximated with plates as input to the gas generation tool with thicknesses of 14 and 16 mm for rib profiles of TH36 and TH44, respectively.

In the current repository concept, the total amount of metals used as building materials is defined per the modules listed in Tab. B-4. Two anchoring patterns are currently used in the provisional engineering design. Pattern 1 refers to the minimum amounts of anchors required and Pattern 2 to the maximum amount. The pattern to be implemented will be selected at the time of tunnel construction according to the properties of the bedrock.

Tab. B-4: Amount of steel components foreseen for different parts of the combined repository at the Haberstal site

Repository module		Length [m]	Weight of the total required steel [kg]	
Code	Description		Assuming anchoring pattern 1 (min.)	Assuming anchoring pattern 2 (max.)
A	Underground access	2,456	7,274,465	7,274,465
B	Central area	3,255	7,722,332	7,981,022
C	Facilities for EUU	1,391	3,552,026	3,674,601
D	Access to L/ILW repository section	5,012	12,256,832	12,654,131
E	Access to HLW repository section	10,648	26,232,868	27,122,288
F	Main L/ILW repository	1,640	7,435,975	7,686,010
G	Main HLW repository	18,197	8,781,034	8,781,034
H	L/ILW pilot repository (incl. access to pilot repository and observation drift)	267	847,233	875,598
I	HLW pilot repository (incl. access to pilot repository and observation drift)	878	958,497	987,621
Total			75,061,262	77,036,769

It should be noted that the amount of reported steel for anchoring includes the weight of a base plate for each anchor. It is assumed to be 10% of the weight of the anchor. The base plate was not dissociated from the anchor in the calculation of gas generation by corrosion.

Tab. B-5 summarises the model input parameters defined for metals used as building materials and Tab. B-6 the amounts of metals used as building materials per tunnel profiles.

Tab. B-5: Shape, dimension, and corrosion class of the steel structures in the combined repository as input to the gas generation tool

	Material	Corrosion class	Shape model	Diameter	Length	Thickness
				[mm]	[mm]	[mm]
Fibres	carbon steel	$\text{pH} \geq 10.5$	cylinder	0.7	35	-
Reinforced steel	carbon steel	$\text{pH} \geq 10.5$	rod	14	-	-
Anchors	carbon steel	$\text{pH} < 10.5$	cylinder	25	variable	-
Rib TH36	carbon steel	$\text{pH} \geq 10.5$	plate	-	-	14
Rib TH44				-	-	16

Tab. B-6: Tunnel profile types based on amount of steel structures per tunnel length for the gas generation tool

Profile type	Steel fibres	Anchors				Ribs		Reinforced steel for cast-in-place concrete		
		Pat-tern 1 (min)	Ref.	Pat-tern 2 (max)	Anchor length[m]	TH44	TH36	Bew. Gewölbebeton	Bew. Sohlenbeton	Bew. Tübbingbeton
	Weight [kg/m] ⁵	Weight [kg/m]	Weight [kg/m]	Weight [kg/m]		Weight [kg/m]	Weight [kg/m]	Weight [kg/m]	Weight [kg/m]	Weight [kg/m]
D10	209.23	76.23	114.345	152.46	3	-	918.06	938.62	211.28	-
D20-1	227.33	76.23	114.345	152.46	3	-	997.45	1020.11	232.43	-
D20-2	224.50	76.23	114.345	152.46	3	-	985.05	1020.11	232.43	-
D20-3	221.67	76.23	114.345	152.46	3	-	972.64	918.02	212.01	-
D20-4	224.50	76.23	114.345	152.46	3	-	985.05	918.02	212.01	-
E10	238.92	279.51	355.74	431.97	6	1148.00	-	987.28	230.87	-
F10	-	-	-	-		-	-	-	-	482.55
I10	330.81	279.51	355.74	431.97	6	1642.17	-	1420.77	358.95	-
K90	393.58	279.51	355.74	431.97	6	2116.58	-	1356.81	387.65	-
M10	260.12	279.51	355.74	431.97	6	1262.04	-	1088.54	259.21	-
R10	276.52	279.51	355.74	431.97	6	1350.23	-	1166.34	282.62	-
T10	235.24	279.51	355.74	431.97	6	1128.23	-	969.66	226.03	-
U10	279.35	279.51	355.74	431.97	6	1365.44	-	1179.71	285.53	-
W10	249.10	279.51	355.74	431.97	6	1210.34	-	1042.73	246.27	-
Y10	172.47	76.23	114.345	152.46	3	-	756.78	902.82	-	-

⁵ Amount of steel [kg] per length of tunnel [m].

App. C Inventory, degradation reactions and gas generation rates from organic materials

Tab. C-1: List of L/ILW organics, chemical formulae and mass based on the inventory of the waste package types

Based on MIRAM-RBG.

Organic materials	Formulae	Group	Total mass (kg)
Cationic IERs (polystyrene / sulphonate groups)	$C_8H_7SO_3Na$	O2	6.2×10^5
PVC	C_2H_3Cl	O2	5.9×10^5
Anionic IERs (polystyrene / quaternary amino groups)	$C_{11}H_{16}NCl$	O2	4.0×10^5
Bitumen	$C_{160}H_{200}ONS_2$	O2	3.5×10^5
Polystyrene (including styrene and polystyrene/divinylbenzol)	$(C_8H_8)_n$	O2	1.1×10^5
Plastic	C_2H_4	O2	9.1×10^4
Cellulose (including cotton)	$C_6H_{10}O_5$	O1a	6.8×10^4
Plexiglas	$C_5H_8O_2$	O2	3.4×10^4
Polyethylene	$(C_2H_4)_n$	O2	3.0×10^4
Polyester	$C_{15}H_{16}O_2$	O1a	2.8×10^4
Diethanolamine	$C_4H_{11}NO_2$	O1b	2.7×10^4
Polycarboxylate	$C_3H_3O_2Na$	O2	2.4×10^4
Rubber	C_4H_4	O2	2.3×10^4
Urea	CH_4N_2O	O1b	1.8×10^4
Ethylenediaminetetraacetic acid	$C_{10}H_{14}N_2O_8Na_2$	O1b	1.4×10^4
Polypropylene	$(C_3H_6)_n$	O2	1.4×10^4
Gluconic acid	$C_6H_{12}O_7$	O1b	1.3×10^4
Epoxy phenolic	$C_{18}H_{20}O_3$	O2	8.4×10^3
Formaldehyde	CH_2O	O1b	8.3×10^3
Polyacrylamide	C_3H_5NO	O2	8.1×10^3
Tartaric acid	$C_4H_6O_6$	O1b	6.3×10^3
Na-dimethyldithiocarbamate	$C_3H_6NS_2Na$	O1b	5.9×10^3
Laurylamine PE glycol ether	$C_{22}H_{49}O_6N$	O1b	5.5×10^3
Surfactant	??	O1b	3.1×10^3
Methanol	CH_3OH	O1b	2.9×10^3
Naphthalene sulphonate	$C_{10}H_7SO_3Na$	O2	2.7×10^3

Tab. C-1: Cont.

Organic materials	Formulae	Group	Total mass (kg)
Ethylene glycol	C ₂ H ₆ O ₂	O1b	2.3×10 ³
Melamine resin	C ₃ H ₆ N ₆	O2	1.4×10 ³
Tributyl phosphate	C ₁₂ H ₂₇ O ₄ P	O1b	1.2×10 ³
Palmitic acid	C ₁₆ H ₃₂ O ₂	O1b	1.1×10 ³
Butyl diglycol	C ₈ H ₁₈ O ₃	O1b	6.4×10 ²
Benzyl alcohol	C ₇ H ₈ O	O1b	6.4×10 ²
Distearyl dimethyl ammonium Cl	C ₃₈ H ₈₀ ClN	O1b	4.0×10 ²
Nylon	C ₁₂ H ₂₂ N ₂ O ₂	O2	3.7×10 ²
Diethylene glycol	C ₄ H ₁₀ O ₃	O1b	3.1×10 ²
Sodium citrate	C ₆ H ₅ O ₇ Na ₃	O1b	3.0×10 ²
Melamine / formaldehyde sulphonate	C ₉ H ₁₇ O ₈ N ₆ SNa	O1a	3.0×10 ²
Lignin sulphonate	C ₁₁ H ₁₄ O ₇ SNa	O2	1.8×10 ²
Oil	C ₈ H ₁₆	O1b	9.5×10 ¹
Isopropanol	C ₃ H ₈ O	O1b	8.6×10 ¹
Hexamethylenetetramine	C ₆ H ₁₂ N ₄	O1b	5.6×10 ¹
Detergents	C ₂₃ H ₃₉ O ₃ SNa	O1b	2.9×10 ¹
Nitrilotriacetic acid	C ₆ H ₆ NO ₆ Na ₃	O1b	2.2
Total mass			2.5×10⁶

Tab. C-2: Degradation reactions of the L/ILW organics and associated gas generation rates

Degradation reactions are extracted from Cloet et al. (2014) and the gas generation rates from Guillemot et al. (2023).

Materials	Chemical formulae	Degradation reaction	Group	Gas generation rates (mol gas/kg a ⁻¹)		
				upper bound	reference	lower bound
Cationic IERs (polystyrene / sulphonate groups)	C ₈ H ₇ SO ₃ Na	C ₈ H ₇ SO ₃ Na + 5 H ₂ O + H ⁺ = 4 CO ₂ + 4 CH ₄ + H ₂ S + Na ⁺	O2	0.05	0.005	1×10 ⁻⁶
PVC	C ₂ H ₃ Cl	4 C ₂ H ₃ Cl + 6 H ₂ O = 3 CO ₂ + 5 CH ₄ + 4 HCl	O2	0.05	0.005	1×10 ⁻⁶
Bitumen	C ₁₆₀ H ₂₀₀ ONS ₂	8 C ₁₆₀ H ₂₀₀ ONS ₂ + 890 H ₂ O = 449 CO ₂ + 831 CH ₄ + 8 NH ₃ + 16 H ₂ S	O2	0.05	0.005	1×10 ⁻⁶
Anionic IERs (polystyrene / quaternary amino groups)	C ₁₁ H ₁₆ NCl	C ₁₁ H ₁₆ NCl + 7 H ₂ O + OH ⁻ = 4 CO ₂ + 7 CH ₄ + Cl ⁻ + NH ₃	O2	0.05	0.005	1×10 ⁻⁶
Polystyrene (including styrene and polystyrene/divinylbenzene)	(C ₈ H ₈) _n	C ₈ H ₈ + 6 H ₂ O = 3 CO ₂ + 5 CH ₄	O2	0.05	0.005	1×10 ⁻⁶
Plastic	C ₂ H ₄	2 C ₂ H ₄ + 2 H ₂ O = CO ₂ + 3 CH ₄	O2	0.05	0.005	1×10 ⁻⁶
Cellulose (including cotton)	C ₆ H ₁₀ O ₅	C ₆ H ₁₀ O ₅ + H ₂ O = 3 CO ₂ + 3 CH ₄	O1a	0.7	0.02	0.0003
Plexiglas	C ₅ H ₈ O ₂	C ₅ H ₈ O ₂ + 2 H ₂ O = 2 CO ₂ + 3 CH ₄	O2	0.05	0.005	1×10 ⁻⁶
Polyethylene	(C ₂ H ₄) _n	2 C ₂ H ₄ + 2 H ₂ O = CO ₂ + 3 CH ₄	O2	0.05	0.005	1×10 ⁻⁶
Polyester	C ₁₅ H ₁₆ O ₂	C ₁₅ H ₁₆ O ₂ + 10 H ₂ O = 6 CO ₂ + 9 CH ₄	O1a	0.7	0.02	0.0003
Diethanolamine	C ₄ H ₁₁ NO ₂	2 C ₄ H ₁₁ NO ₂ + 2 H ₂ O = 3 CO ₂ + 5 CH ₄ + 2 NH ₃	O1b	0.7	0.07	0.0003
Polycarboxylate	C ₃ H ₃ O ₂ Na	2 C ₃ H ₃ O ₂ Na + 2 H ₂ O + 2 H ⁺ = 3 CO ₂ + 3 CH ₄ + 2 Na ⁺	O2	0.05	0.005	1×10 ⁻⁶
Rubber	C ₄ H ₄	2 C ₄ H ₄ + 6 H ₂ O = 3 CO ₂ + 5 CH ₄	O2	0.05	0.005	1×10 ⁻⁶

Tab. C-2: Cont.

Materials	Chemical formulae	Degradation reaction	Group	Gas generation rates (mol gas/kg a ⁻¹)		
				upper bound	reference	lower bound
Urea	CH ₄ N ₂ O	CH ₄ N ₂ O + H ₂ O = CO ₂ + 2 NH ₃	O1b	0.7	0.07	0.0003
Ethylenediaminetetraacetic acid	C ₁₀ H ₁₄ N ₂ O ₈ Na ₂	4 C ₁₀ H ₁₄ N ₂ O ₈ Na ₂ + 14 H ₂ O + 8 H ⁺ = 23 CO ₂ + 17 CH ₄ + 8 NH ₃ + 8 Na ⁺	O1b	0.7	0.07	0.0003
Polypropylene	(C ₃ H ₆) _n	4 C ₃ H ₆ + 6 H ₂ O = 3 CO ₂ + 9 CH ₄	O2	0.05	0.005	1×10 ⁻⁶
Gluconic acid	C ₆ H ₁₂ O ₇	4 C ₆ H ₁₂ O ₇ = 13 CO ₂ + 11 CH ₄ + 2 H ₂ O	O1b	0.7	0.07	0.0003
Epoxy phenolic	C ₁₈ H ₂₀ O ₃	4 C ₁₈ H ₂₀ O ₃ + 46 H ₂ O = 29 CO ₂ + 43 CH ₄	O2	0.05	0.005	1×10 ⁻⁶
Formaldehyde	CH ₂ O	2 CH ₂ O = CO ₂ + CH ₄	O1b	0.7	0.07	0.0003
Polyacrylamide	C ₃ H ₅ NO	2 C ₃ H ₅ NO + 4 H ₂ O = 3 CO ₂ + 3 CH ₄ + 2 NH ₃	O2	0.05	0.005	1×10 ⁻⁶
Tartaric acid	C ₄ H ₆ O ₆	4 C ₄ H ₆ O ₆ = 11 CO ₂ + 5 CH ₄ + 2 H ₂ O	O1b	0.7	0.07	0.0003
Na-dimethyldithiocarbamate	C ₃ H ₆ NS ₂ Na	2 C ₃ H ₆ NS ₂ Na + 6 H ₂ O + 2 H ⁺ = 3 CO ₂ + 3 CH ₄ + 2 NH ₃ + 4 H ₂ S + 2 Na ⁺	O1b	0.7	0.07	0.0003
Laurylamine PE glycol ether	C ₂₂ H ₄₉ O ₆ N	4 C ₂₂ H ₄₉ O ₆ N + 30 H ₂ O = 27 CO ₂ + 61 CH ₄ + 4 NH ₃	O1b	0.7	0.07	0.0003
Surfactants	C ₄ H ₁₁ NO ₂	2 C ₄ H ₁₁ NO ₂ + 2 H ₂ O = 3 CO ₂ + 5 CH ₄ + 2 NH ₃	O1b	0.7	0.07	0.0003
Methanol	CH ₃ OH	4 CH ₃ OH = CO ₂ + 3 CH ₄ + 2 H ₂ O	O1b	0.7	0.07	0.0003
Naphthalenesulphonate	C ₁₀ H ₇ SO ₃ Na	C ₁₀ H ₇ SO ₃ Na + 7 H ₂ O + H ⁺ = 5 CO ₂ + 5 CH ₄ + H ₂ S + Na ⁺	O2	0.05	0.005	1×10 ⁻⁶
Ethylene glycol	C ₂ H ₆ O ₂	4 C ₂ H ₆ O ₂ = 3 CO ₂ + 5 CH ₄ + 2 H ₂ O	O1b	0.7	0.07	0.0003
Melamine resin	C ₃ H ₆ N ₆	C ₃ H ₆ N ₆ + 6 H ₂ O = 3 CO ₂ + 6 NH ₃	O2	0.05	0.005	1×10 ⁻⁶
Tributyl phosphate	C ₁₂ H ₂₇ O ₄ P	C ₁₂ H ₂₇ O ₄ P + 6 H ₂ O = 3 CO ₂ + 9 CH ₄ + H ₃ PO ₄	O1b	0.7	0.07	0.0003
Palmitic acid	C ₁₆ H ₃₂ O ₂	2 C ₁₆ H ₃₂ O ₂ + 14 H ₂ O = 9 CO ₂ + 23 CH ₄	O1b	0.7	0.07	0.0003
Butyl diglycol	C ₈ H ₁₈ O ₃	2 C ₈ H ₁₈ O ₃ + 4 H ₂ O = 5 CO ₂ + 11 CH ₄	O1b	0.7	0.07	0.0003
Benzyl alcohol	C ₇ H ₈ O	4 C ₇ H ₈ O + 18 H ₂ O = 11 CO ₂ + 17 CH ₄	O1b	0.7	0.07	0.0003

Tab. C-2: Cont.

Materials	Chemical formulae	Degradation reaction	Group	Gas generation rates (mol gas/kg a ⁻¹)		
Distearyl dimethyl ammonium Cl	C ₃₈ H ₈₀ ClN	2 C ₃₈ H ₈₀ ClN + 36 H ₂ O + 2 OH ⁻ = 19 CO ₂ + 57 CH ₄ + 2 NH ₃ + 2 Cl ⁻	O1b	0.7	0.07	0.0003
Nylon	C ₁₂ H ₂₂ N ₂ O ₂	2 C ₁₂ H ₂₂ N ₂ O ₂ + 14 H ₂ O = 9 CO ₂ + 15 CH ₄ + 4 NH ₃	O2	0.05	0.005	1×10 ⁻⁶
Diethylene glycol	C ₄ H ₁₀ O ₃	2 C ₄ H ₁₀ O ₃ + H ₂ O = 3 CO ₂ + 5 CH ₄	O1b	0.7	0.07	0.0003
Sodium citrate	C ₆ H ₅ O ₇ Na ₃	4 C ₆ H ₅ O ₇ Na ₃ + 2 H ₂ O + 12 H ⁺ = 15 CO ₂ + 9 CH ₄ + 12 Na ⁺	O1b	0.7	0.07	0.0003
Melamine / Formaldehyde-Sulfonate	C ₉ H ₁₇ O ₈ N ₆ SNa	4 C ₉ H ₁₇ O ₈ N ₆ SNa + 22 H ₂ O + 4 H ⁺ = 27 CO ₂ + 9 CH ₄ + 24 NH ₃ + 4 H ₂ S + 4 Na ⁺	O1a	0.7	0.02	0.0003
Lignin sulfonate	C ₁₁ H ₁₄ O ₇ SNa	8 C ₁₁ H ₁₄ O ₇ SNa + 34 H ₂ O + 8 H ⁺ = 45 CO ₂ + 8 Na ⁺ + 8 H ₂ S + 43 CH ₄	O2	0.05	0.005	1×10 ⁻⁶
Oil	C ₈ H ₁₆	C ₈ H ₁₆ + 4 H ₂ O = 2 CO ₂ + 6 CH ₄	O1b	0.7	0.07	0.0003
Isopropanol	C ₃ H ₈ O	4 C ₃ H ₈ O + 2 H ₂ O = 3 CO ₂ + 9 CH ₄	O1b	0.7	0.07	0.0003
Hexamethylenetetramine	C ₆ H ₁₂ N ₄	C ₆ H ₁₂ N ₄ + 6 H ₂ O = 3 CO ₂ + 3 CH ₄ + 4 NH ₃	O1b	0.7	0.07	0.0003
Detergents	C ₂₃ H ₃₉ O ₃ SNa	2 C ₂₃ H ₃₉ O ₃ SNa + 24 H ₂ O + 2 H ⁺ = 15 CO ₂ + 31 CH ₄ + 2 H ₂ S + 2 Na ⁺	O1b	0.7	0.07	0.0003
Nitrilotriacetic acid	C ₆ H ₆ NO ₆ Na ₃	4 C ₆ H ₆ NO ₆ Na ₃ + 6 H ₂ O + 12 H ⁺ = 15 CO ₂ + 9 CH ₄ + 4 NH ₃ + 12 Na ⁺	O1b	0.7	0.07	0.0003
Prussian blue*	Fe ₄ [Fe(CN) ₆] ₃	2 Fe ₄ [Fe(CN) ₆] ₃ + 90 H ₂ O = 6 Fe(OH) ₂ + 4 Fe(OH) ₃ + 27 CO ₂ + 9 CH ₄ + 36 NH ₃	O1a	0.7	0.02	0.0003

App. D Mathematical formulations of gas transport

D.1 Transport of gas dissolved in porewater

Darcy's law represents the general basis for the quantitative descriptions of groundwater flow. It denotes the linear correlation between the specific discharge (Darcy velocity) through a representative elementary volume and the hydraulic gradient. The proportionality constant for the relationship is provided by the hydraulic conductivity.

Diffusion in a porous medium in its simplest form can be described by Fick's first law (Domineco & Schwartz 1990):

$$J = -D_d \text{grad}(C)$$

with J being the diffusive flux [mol/L²T]; D_d the effective diffusion coefficient [L²/T] and C the concentration [mol/L³] of a species. The effective diffusion coefficient depends on the molecular diffusion of a species in free solution and the porous medium structure, which is typically expressed in terms of the porosity and the tortuosity (see Greenkorn & Kessler 1972; Millington & Quirk 1961).

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

$$K_H = \frac{(gas)_{aq}}{P_{gas}}$$

where K_H is the Henry's law constant [mol Pa⁻¹], P_{gas} is the partial pressure of the gas in the gas phase [Pa] and $(gas)_{aq}$ is the molar concentration of the gas in the aqueous phase.

D.2 Visco-capillary two-phase flow

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

$$v_\beta = -\mathbf{k} \cdot \frac{k_{r\beta} \cdot \rho_\beta}{\mu_\beta} (\nabla p_\beta - \rho_\beta \cdot \mathbf{g})$$

where v_β is the Darcy velocity (volume flux) in phase β , k is the intrinsic permeability¹, $k_{r\beta}$ is the relative permeability (a function of saturation; see below) to phase β , μ_β is the viscosity, ρ_β is the density, and p_β is the fluid pressure of phase β . The coefficient $\mathbf{g}$ is the gravitational acceleration.

According to van Genuchten (1980), the parametric relationship between water saturation and capillary pressure is given as:

$$p_c = p_g - p_w = P_0 \cdot \left(S_e^{\frac{n}{1-n}} - 1 \right)^{\frac{1}{n}}$$

where p_c , p_g , and p_w represent the capillary pressure, gas pressure, and water pressure, respectively. P_0 , the inverse of van Genuchten's α parameter, is the capillary strength and n is a shape factor (pore size distribution index).

The porewater effective saturation, S_e , is the normalised volume of porewater, defined in terms of the porewater saturation, S_w and the liquid residual saturation, S_{wr} :

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

In practical terms, the functional relationship between capillary pressure and the saturation state of a porous medium is a measure of suction or, in other words, of the saturation state for any given pressure difference between the fluid phases. An example is shown in Fig. D-1, where *Material I* is assumed to have a lower capillary strength than *Material II*. At the boundary between the two materials, the pressure has to be continuous and correspond to value $P_{c,y}$. There are, however, two different saturation values on either side of the interface, $S_{w,I}$ and $S_{w,II}$. *Material I* has lower suction, and thus more gas is present in its pores (saturation $S_{w,I}$). *Material II* has higher suction and will maintain a higher liquid saturation ($S_{w,II}$).

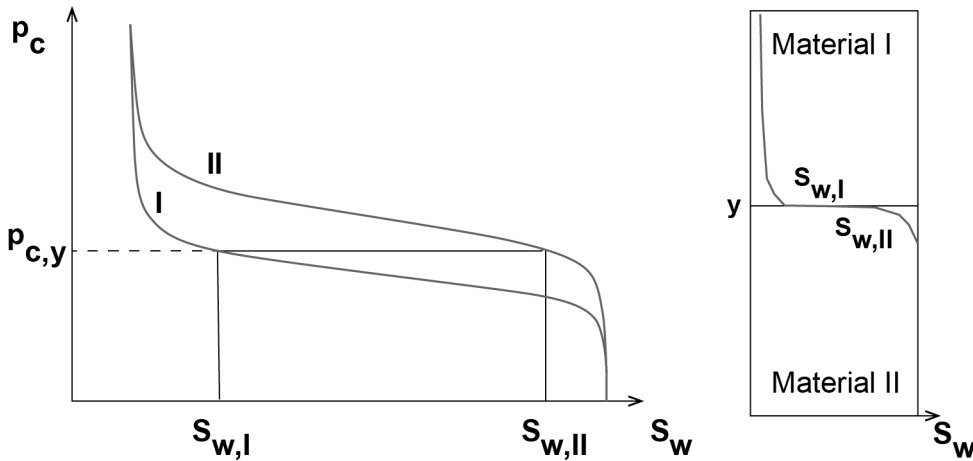


Fig. D-1: Capillary pressure and saturation difference at the boundary between two materials with different capillary strengths

Adapted from Papafotiou (2008).

The relative gas/water permeabilities $k_{r,g}$ and $k_{r,w}$ of a porous media can be described by the model given in Mualem (1976) (see also Helmig 1997):

$$k_{r,w} = S_e^\varepsilon \cdot \left[1 - \left(1 - S_e^{\frac{n}{n-1}} \right)^{\frac{n-1}{n}} \right]^2$$

$$k_{r,g} = (1 - S_{ekg})^\gamma \cdot \left(1 - S_{ekg}^{\frac{n}{n-1}} \right)^{2(1-1/n)}$$

where S_e and S_{ekg} are the effective saturations for water and gas, respectively, and ε and γ are empirical shape factors representing the pore connectivity of the medium. Typically, these are set to $\varepsilon = 1/2$ and $\gamma = 1/3$ (Luckner et al. 1989).

According to the Mualem approach, the definition of the effective saturation S_{ekg} for gas is defined using the residual gas saturation S_{gr} :

$$S_{ekg} = \frac{S_w}{1 - S_{gr}}$$

D.3 Pathway dilation

Alonso et al. (2006) developed a hybrid formulation for pathway dilation, expressing the effective permeability of the rock as the superposition of an intrinsic matrix permeability and a stress-dependent fracture transmissivity (embedded fracture approach). The approach was tested successfully for soft clays (bentonite) and for claystone. An even simpler approach has been introduced by Senger et al. (2008), which uses a pressure-dependent permeability multiplier to calculate an enhanced permeability:

$$k' = k \left[1 + (k_{factor} - 1) \frac{P - P_1}{P_2 - P_1} \right]$$

where k_{factor} is a scaling factor, P_1 is the characteristic pressure for the onset of dilation and P_2 is the maximum pressure corresponding to the maximum enhanced permeability. Accordingly, the capillary strength of the porous medium under dilatant conditions can be scaled through Leverett's function as:

$$P'_0 = P_0 \sqrt{\frac{k}{k'}}$$

Papafotiou & Senger (2014) performed analyses of gas-induced effects in a generic L/ILW repository, assuming an onset of dilation at 80% of the lithostatic stress at repository level and an enhancement factor of 10 between the onset (80%) and the lithostatic stress (100%). An important feature of this implementation is that permeability and capillary strength revert to their original values once pressure has dissipated.

App. E Additional data used in modelling

An overview of additional data used in gas modelling presented in this report is given in the following.

E.1 Heat source terms

Although they are not the focus of these report, thermal effects associated with the heat generated in the HLW repository are taken into account in the gas transport simulations presented in Chapter 5. The heat source term can be formulated in two ways depending on the intended use, as described in the following.

For repository-scale modelling (e.g., model described in Section 4.3.2.5) the heat source corresponds to the total inventory from MIRAM-RBG (Nagra 2023c). Accordingly, an average heat source of SF canisters can be derived from the total number of canisters as shown in Fig. E-1 (a, “Kombi”). Note that this average is obtained for the NPP operation time and emplacement schedule adopted in MIRAM-RBG (Nagra 2023c).

For component-scale modelling (e.g., model described in Section 4.3.2.2) the heat source corresponds to individual SF canisters (Nagra 2023c). Due to the different loadings and decays of the SF canisters, representative average heat rates are derived for PWR-MOX, PWR-UO₂, and BWR canisters separately, as shown in Fig. E-1a. For Case 11 presented in Section 5.3.11, so-called representative maximum heat rates are derived for the first 200 years after canister emplacement as shown in Fig. E-1b.

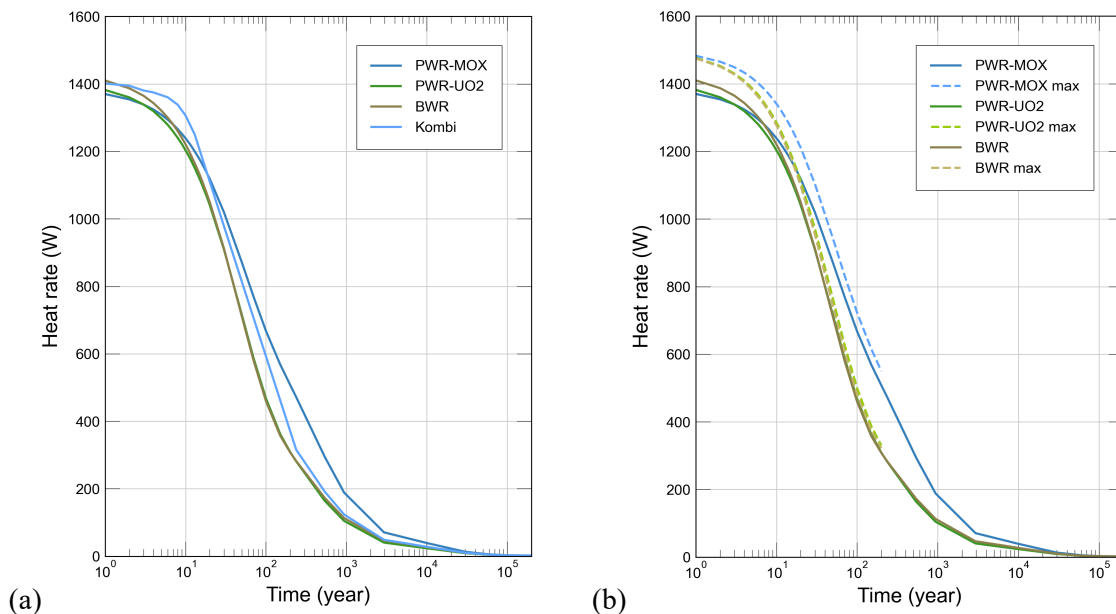


Fig. E-1: Heat source terms used in gas modelling presented in this report

- (a) comparison between average heat source purposed for repository-scale modelling (“Kombi”) to representative average heat rates for PWR-MOX, PWR-UO₂, and BWR purposed for component-scale modelling.
- (b) comparison between representative average and representative maximum heat rates purposed for component-scale modelling.

App. F Complementary results

Complementary outputs from the HLW nearfield model that are not used in the assessment of Chapter 5 are given here for completeness. As described in Section 4.4, pressure predictions with this model are in part overly conservative due to boundary effects and assumptions in the model conceptualisation. The pressure transients simulated in the Base Case are shown in Fig. F-1. Pressure transients simulated in Case 3 are shown in Fig. F-2. Pressure transients simulated in Case 11 are shown in Fig. F-3.

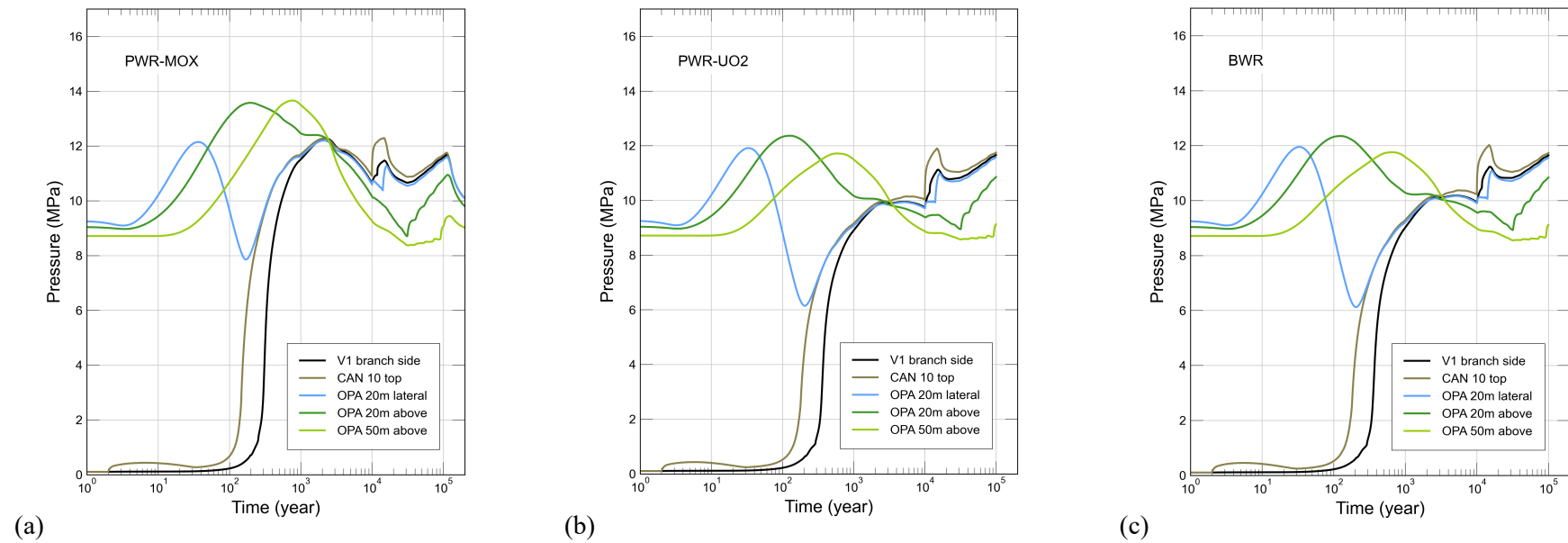


Fig. F-1: Base Case, HLW & V1 model

Transients of pressure assuming only canisters of type (a) PWR-MOX, (b) PWR-UO₂, (c) BWR, with representative average heat output.

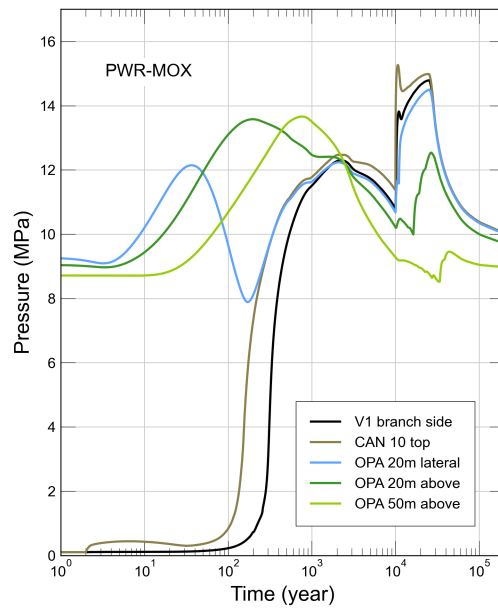


Fig. F-2: Case 3, HLW & V1 model

Transients of pressure assuming only canisters of type PWR-MOX with representative average heat output.

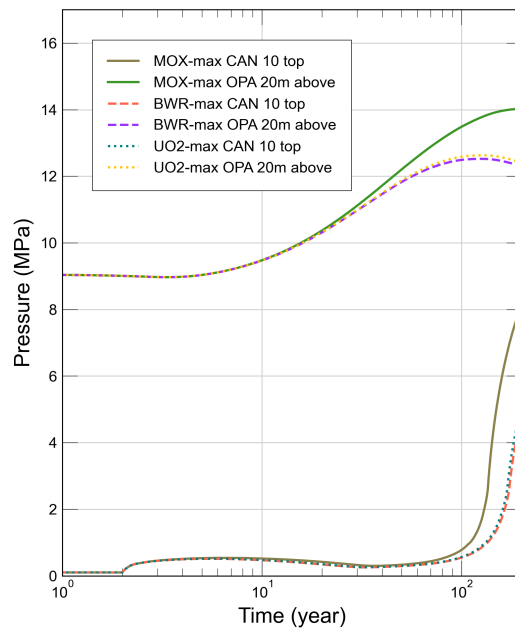


Fig. F-3: Case 11, HLW & V1 model

Transients of pressure assuming only canisters of type PWR-MOX / PWR-UO₂ / BWR with representative maximum heat output.