



ARBEITSBERICHT NAB 24-26

Model Supported Assessment of the
Containment-Providing Rock Zone in
Support of the Site Selection

Oktober 2024

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

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KEYWORDS

Safety assessment, site comparison, safety scenario development, analysis of radiological consequences, performance assessment, demonstration of safety, post-closure safety case, general licence application

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Nagra Arbeitsberichte ("Working Reports") present the results of work in progress that have not necessarily been subject to a comprehensive review. They are intended to provide rapid dissemination of current information.

The report "Model Supported Assessment of the Containment-Providing Rock Zone in Support of the Site Selection" has been elaborated by a project team consisting of P. Marschall¹, A. Papafotiou¹, Y. Schaub¹, C. Li², M. Hayek², U. Lengler², K. Luu²

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Abstract

The primary aim of the present report has been to provide a traceable documentation of the model-based assessments, supporting the safety-related site comparison in the context of SGT-Stage 3. The focus was on (i) the vertical and lateral delimitation of the containment-providing rock zone (CRZ) and (ii) the indicator-based assessment of the barrier performance of the CRZ for a HLW and L/ILW repository project in the 3 siting regions.

The “thickness of the Opalinus Clay” is a delimitation indicator for the vertical extent of the CRZ, which is required to assess the efficiency of the CRZ as a transport barrier for radionuclides. Based on a dimensionless representation of advective-diffusive transport processes in the host rock, a minimum thickness of the undamaged rock mass above and below the emplacement of 20 – 35 m was estimated for the HLW repository to provide acceptable performance as a transport barrier for dissolved radionuclides. For the L/ILW repository with a diameter of approximately 10 m, a minimum thickness of the intact host rock package above and below the caverns of 20 m is estimated to ensure the confinement of the waste and the mechanical and chemical integrity of the repository system as a whole.

The delimitation indicator for lateral delimitation of the CRZ is called “distance to steeply dipping faults”. The corresponding performance target $L_{\min, \text{fault}} = 200$ m has been specified as a minimum distance of the HLW and L/ILW disposal areas from fault systems of hydraulic significance. Model-based assessments confirm that the lateral release to a steeply dipping fault is not relevant, when the respect distance of 200 m is maintained.

Another delimitation indicator used for lateral delimitation of the prospected protection zone is called “minimum lateral distance between the prospected protection zone and the next injection / pumping well”. The corresponding performance target $L_{\min, \text{well}} = 50$ m has been specified as a minimum distance of prospected repository zone from any deep boreholes. Model-based assessments confirm that the lateral release into a deep borehole is not relevant, when the respect distance of 50 m is maintained.

A complementary workflow was pursued for setting out favourable repository areas and for delineation of the corresponding repository footprints in the three siting regions. The screening process was aimed at mapping lateral variations of barrier performance of the host rock. Significant lateral variations in barrier performance of the host rock could not be identified; it can be concluded, that the entire prospected protection zone is equally well suited to host the repository.

Model-supported assessments have been performed to identify safety-relevant differences between the site-specific repository projects. The indicator-based evaluations concentrated on the SGT criteria 2.3 (“repository induced influences”) and the three criteria in criteria group 3 (“reliability of findings”).

The effects of the excavation damaged zone (EDZ) were evaluated by numerical calculations of the vertical extent of the EDZ above / below the emplacement rooms, both for the HLW and the L/ILW repository projects. The analyses revealed that none of the repository projects is detrimentally affected by a safety-relevant loss of barrier function of the CRZ, caused by the vertical extent of the EDZ.

Thermally induced overpressures in the host rock around the HLW drifts have a significant power to distinguish between the three HLW repositories. The HLW-NL and HLW-ZNO repository configurations are characterized by significantly higher safety margins with regard to thermally induced shear failure than the HLW-JO project. A similar picture emerges when taking into account the parametric and conceptual uncertainties addressed in criteria group 3. The reason for the less favorable performance of the HLW-JO configuration is the lower repository depth at the JO site.

Gas induced overpressures develop both, in the HLW and the L/ILW repository structures. The gas impacts have a significant power to distinguish between the three repository sites. The repository projects at the NL site perform best due to the greatest repository depth, the configurations in ZNO performs also well, whereas low safety margins are seen for the JO projects due to the lowest repository depth.

Finally, model-based assessments were performed to evaluate the impact of parametric, conceptual and scenario uncertainties on the efficiency of the host rock and the CRZ in the three siting regions as a transport barrier for dissolved radionuclides. Tracer flux of a conservative tracer was used as a performance indicator which can be calculated with numerical modelling tools. Probabilistic simulations confirmed an excellent barrier performance of the CRZ for all repository configurations at all sites, indicating that the power to distinguish between the three repository sites is low.

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List of Acronyms

ATW	Alpha-toxic waste
BDCF	Biosphere dose conversion factor
CRZ	Containment-providing rock zone
EDZ	Excavation damaged zone
ENSI	Swiss Federal Nuclear Safety Inspectorate (<i>Eidgenössisches Nuklearsicherheitsinspektorat</i>)
FEP	Features, events and processes
FHA	Future human actions
HLW	High-level waste (spent fuel assemblies and high-level waste from reprocessing)
JO	Jura Ost (siting region)
KEG	Nuclear Energy Act (<i>Kernenergiegesetz</i>)
KEV	Nuclear Energy Ordinance (<i>Kernenergieverordnung</i>)
L/ILW	Low- and intermediate-level waste
MIRAM	Model Inventory for Radioactive Materials
MOX	Mixed oxide fuel
NAB	Nagra work report
NEA	Nuclear Energy Agency of the Organisation for Economic Co-operation and Development (OECD)
NL	Nördlich Lägern (siting region)
NTB	Nagra technical report
PDF	Probability density function
QA	Quality assurance
QC	Quality control
RBG	General licence application (<i>Rahmenbewilligungsgesuch</i>)
RD&D	Research, development & demonstration
RIE	Repository-induced effects
RP-HLW	Vitrified HLW from reprocessing
SF	Spent fuel
SGT	Sectoral Plan for Deep Geological Repositories (<i>Sachplan Geologische Tiefenlager</i>)
THM-C	Thermo-hydro-mechanical and chemical (evolution)
ZNO	Zürich Nordost (siting region)

1 Introduction

1.1 Context

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 (2002).

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 2023, ENSI 2020) 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 for both repository types 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*"; (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 (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 2024f).
- 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*.

The present report (bordered in red in Fig. 1-1) documents the model-supported analyses carried out both for the delimitation of the CRZ and the qualitative assessment of the CRZ in the three siting regions.

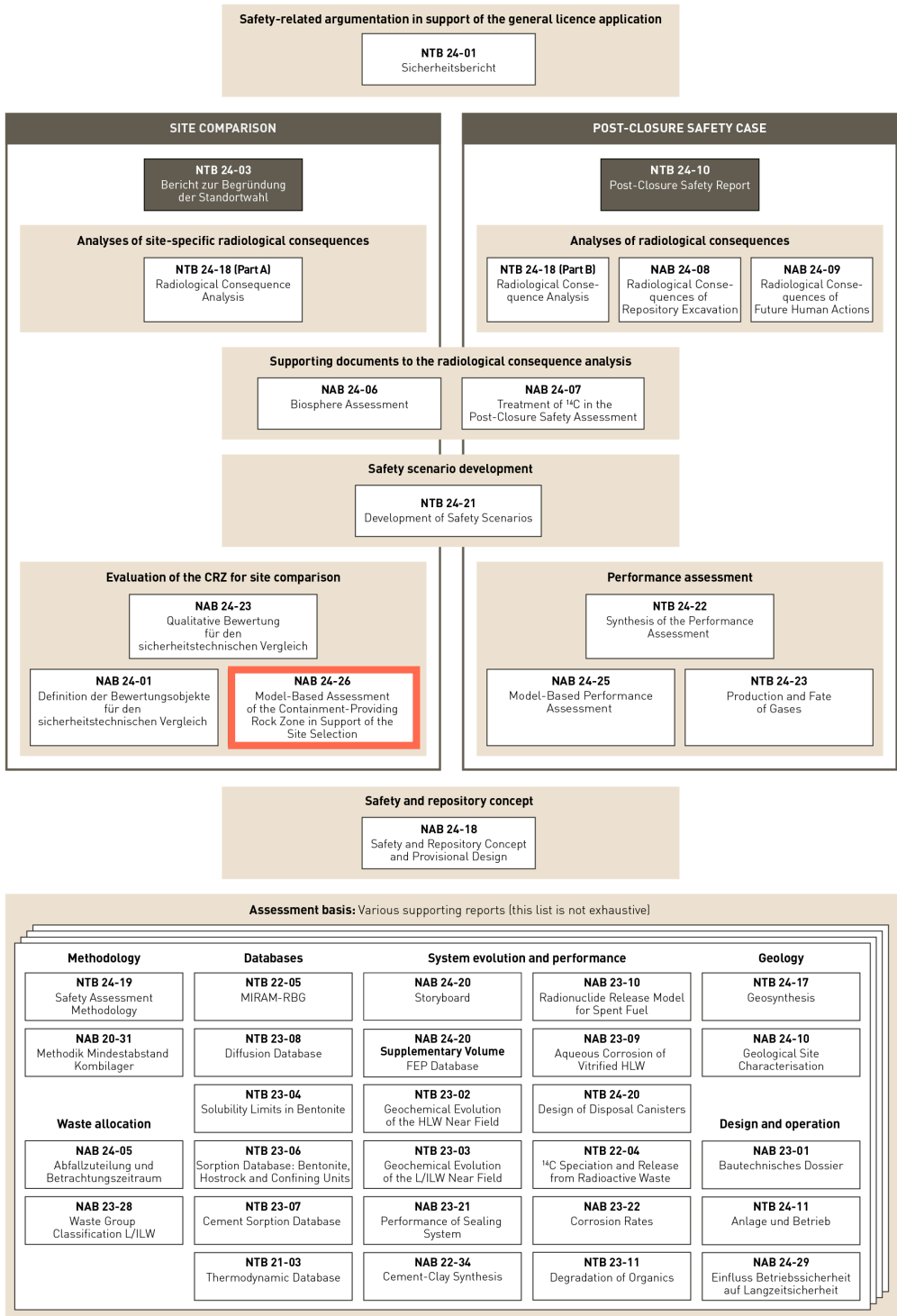


Fig. 1-1: Structure of reports covering post-closure safety aspects of the site comparison and the post-closure safety case

1.2 Scope of the present report

ENSI has set out the regulatory requirements for the site selection process in ENSI 33/649 (ENSI 2018), containing the guidelines and specifications for the safety-related comparison of the siting areas to be examined further in Stage 3. A stepwise workflow was requested, comprising among other aspects the delimitation of the Containment Providing Rock Zone (CRZ) and the qualitative assessment of the CRZ. This report documents the model-supported analyses carried out both for the delimitation of the CRZ and the qualitative assessment of the CRZ in the three siting regions. The objectives of the report are the following:

- traceable documentation of the model-supported assessment workflow in the context of Nagra's general performance assessment methodology;
- specification of the quantitative indicators which are needed for the delineation of the CRZ and for the assessment of barrier performance;
- indicator-based delimitation of the CRZ, representing the favourable areas for the HLW- and L/ILW repository in the three siting regions. Quantitative performance targets are provided for lateral and vertical delineation of the CRZ;
- indicator-based assessment of the barrier performance of the CRZ, representing the favourable areas for the HLW- and L/ILW repository in the three siting regions. Model-based assessments are performed for SGT criteria 2.3 ("repository induced influences") and for criteria group 3 ("reliability of findings") and the
- documentation of the model-supported analyses, contributing to the qualitative assessments of the CRZ.

The quantitative results of the model-based assessments are forming the input for the Qualitative assessment for the safety-related comparison of sites in the context of SGT-Stage 3 which is documented in Nagra (2024h).

1.3 Structure of the present report

The remaining chapters of this report are structured as follows:

- Chapter 2 describes the regulatory background.
- Chapter 3 gives an account of the methodology for site comparison.
- Chapter 4 presents the model-based contribution to delimitation of the CRZ.
- Chapter 5 presents the model-supported analyses needed for the site selection process.
- Chapter 6 contains the conclusions and a discussion of uncertainties.

2 Regulatory background

2.1 Overview

(Nagra 2024j) gives an extensive overview of the legal and regulatory requirements with respect to safety, as well as institutional decisions and strategic choices made in Switzerland. (Nagra 2024j) also describes the Nagra safety concept and safety-related design requirements in detail. A high-level description of the methodology used in the post-closure safety assessment is presented in Nagra (2024k), including the regulatory framework and the methodology adopted in site comparison. A comprehensive discussion of aspects specific to the final stage in the site selection process is provided in Nagra (2025a). In the following sections, we summarise aspects related to the safety argumentation for the site comparison.

2.2 Comparison of siting regions

The comparison of the siting regions is conducted within the framework of a safety-based optimisation in line with the safety criteria defined in the Sectoral Plan BFE (2008) and the ENSI requirements specified and supplemented for Stage 3 of the Sectoral Plan in ENSI 33/649 (ENSI 2018). Chapter 4 of the latter includes safety-related requirements for the site comparison and describes the procedure to be followed for the comparative overall evaluation of the potential siting regions leading to the siting proposal, as shown in Fig. 2-1.

The procedure begins with the waste allocation to the two repository types; since the requirements for a repository site also depend on the inventory to be disposed of, the waste allocation must be used consistently for both the site comparison and the safety assessment for the proposed siting region. Thereafter, the next step is to select the location for a potential HLW repository. Finally, a location for the L/ILW repository is selected, which can include the possibility of co-disposal of L/ILW with HLW at the same site.

As also set out in Chapter 4 of ENSI 33/649 (ENSI 2018), the proposed site or sites for the potential HLW repository, L/ILW repository or combined repository are chosen using an approach consisting of the following sub-steps:

1. Delimitation of the containment-providing rock zone (CRZ):

The CRZ is defined by ENSI 33/649 (ENSI 2018) as the spatial area in the geological subsurface that, in conjunction with engineered barriers, ensures the containment and retention of the radioactive substances contained in the waste during the expected evolution of the deep geological repository for the period under consideration. The CRZ includes the host rock as well as over- and underlying confining geological units that support barrier performance (Fig. 2-2). Nagra must propose at least one CRZ for the site comparison per siting region and per repository type and justify how spatially effective elements have been included in its delimitation.

2. Concept, design and planning of the deep geological repositories (i.e., establishment of site-specific repository projects):

For the CRZs used in the site comparison, site-specific facility designs must be developed that adequately address the aspects of construction, operation, retrieval without undue effort, closure, and post-closure safety.

3. Site-specific, quantitative safety analyses for the site comparison:

Safety analysis is understood here as a systematic quantitative investigation with the aim of showing compliance with the protection criteria and the fulfilment of the specified safety requirements.

4. Qualitative evaluation of the CRZ:

The qualitative evaluation of the CRZ is based on 13 criteria for safety and engineering feasibility included in the Sectoral Plan (Annex I of BFE (2008)); see Tab. 2-1 and Section 3.2.5. The criteria are divided into four groups and, for each of the criteria, the Sectoral Plan also specifies the various “*aspect(s) to be evaluated*” and their corresponding “*relevance for safety*”.

5. Overall comparative safety evaluation:

Finally, an overall comparative safety evaluation and selection of proposed siting region or regions are carried out, based on the geological situation in each siting region, the delineated CRZs of the siting regions, the site-specific repository projects, the safety analyses for the site comparison, and the qualitative assessment of the CRZs with respect to the 13 criteria.

Tab. 2-1: Criteria for the qualitative evaluation of the CRZ to be assessed from the viewpoint of safety and engineering feasibility according to SGT

Table translated from BFE (2008).

Criteria group	Criteria
1. Properties of the host rock and the effective containment zone	1.1 Spatial extent 1.2 Hydraulic barrier effect 1.3 Geochemical conditions 1.4 Release pathways
2. Long-term stability	2.1 Stability of the site and rock properties 2.2 Erosion 2.3 Repository-induced influences 2.4 Conflicts of use
3. Reliability of geological findings	3.1 Ease of characterisation of the rock 3.2 Explorability of spatial conditions 3.3 Predictability of long-term changes
4. Engineering suitability	4.1 Rock mechanical properties and conditions 4.2 Underground access and drainage

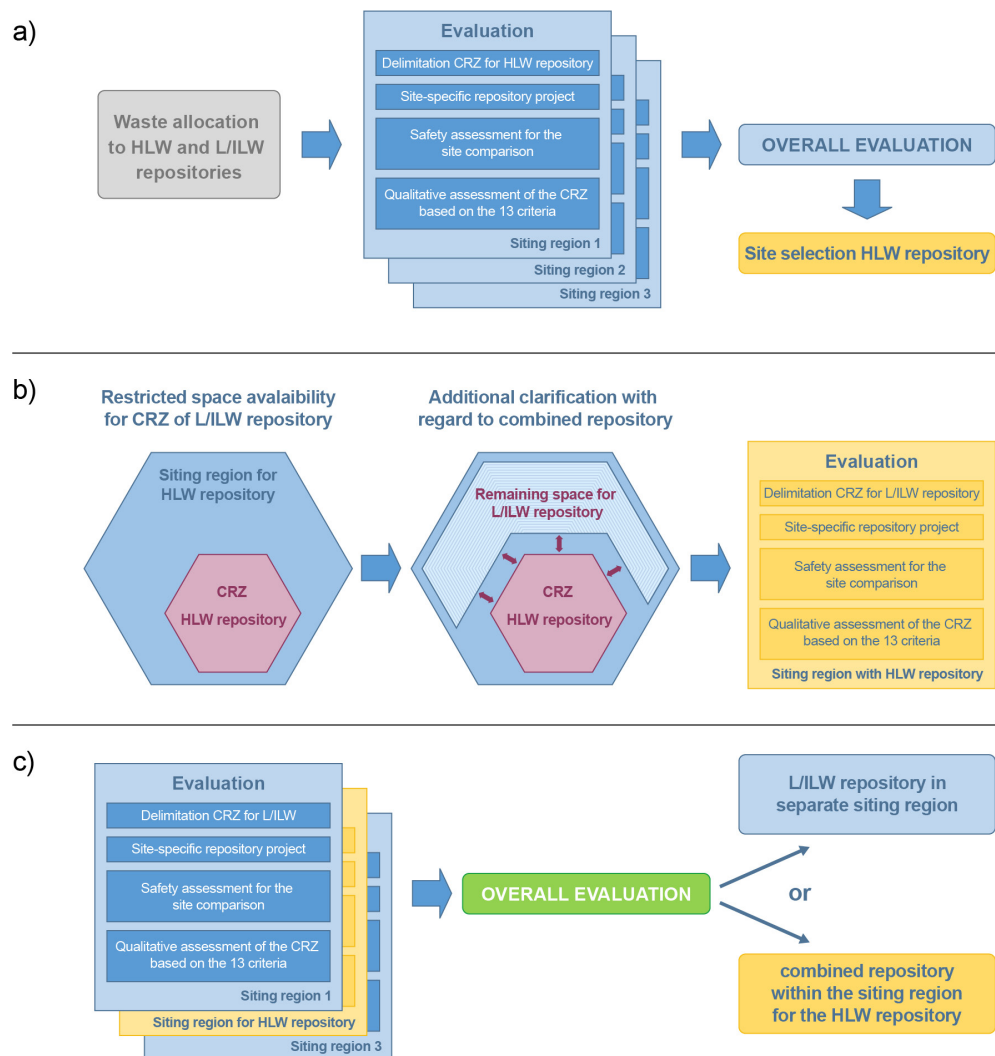


Fig. 2-1: Schematic illustration of the methodology for the site comparison in Stage 3 of the Sectoral Plan

Figure translated from ENSI 33/649 (ENSI 2018).

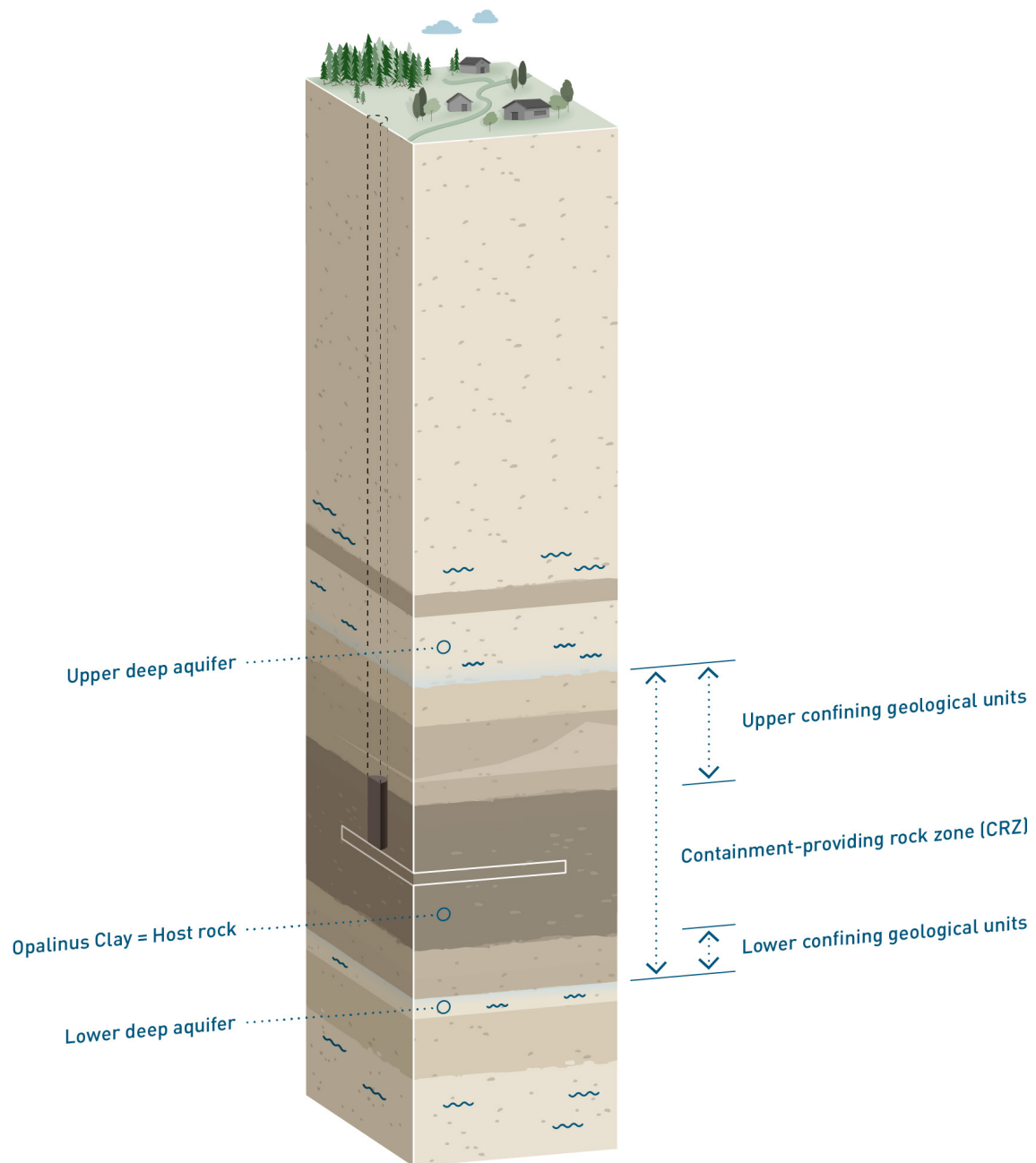


Fig. 2-2: Sketch of the location of the repository within the Opalinus Clay host rock, as well as the containment-providing rock zone (CRZ), which consists of the Opalinus Clay and its confining geological units, bounded above and below by deep aquifers

Figure is not to scale.

3 Methodology for site comparison (Nagra 2024k)

3.1 Main steps in site comparison

The high-level workflow for the comparison of the three siting regions, ZNO, JO and NL, and for the selection of a preferred siting region is illustrated in Fig. 3-1. The figure is organised to facilitate comparison with the steps of the safety assessment methodology (Nagra 2024k) and elaborated in the following sections of this chapter. The figure is also broadly consistent with the methodology set out in Chapter 4 of ENSI 33/649 (ENSI 2018) (see Fig. 2-1).

The methodology is described only briefly here, emphasising its consistency with the regulatory framework (Section 2.2). For a more detailed description of the methodology for site comparison and for the selection of the proposed siting region, see Nagra (2025a) and its supporting reports (Fig. 1-1).

The methodology begins with the allocation of waste to the HLW repository and to the L/ILW repository (or to the L/ILW section of a combined repository). Thereafter, the procedure involves:

- The comparison of siting regions with regard to HLW disposal, culminating in a decision on a preferred HLW siting region. This is represented in the vertical workflow on the left-hand side of Fig. 3-1 and is described further in Section 3.2.
- The comparison of siting regions with regard to L/ILW disposal, culminating in a decision on a preferred L/ILW siting region, including the possibility of co-disposal in the preferred HLW siting region. These are represented in the vertical workflow on the right-hand side of Fig. 3-1 and are described further in Sections 3.3 and 3.4, respectively.

3.2 Evaluation of siting regions for HLW disposal

The evaluation of each siting region for HLW disposal, i.e., the left-hand vertical workflow path in Fig. 3-1, involves the four substeps specified in Chapter 4 of ENSI 33/649 (see Section 2.2), the implementation of which is described in detail in Nagra (2024b), Nagra (2024h) and Nagra (2025a), and is summarised in the following paragraphs.

3.2.1 Delimitation of the CRZ

Siting area boundaries were defined in SGT Stage 1. For the site comparison in Stage 3 of the Sectoral Plan, preferred areas for waste disposal within these boundaries were identified in a multi-stage procedure. HLW disposal is assumed to take place within these areas, with the rock zone around the disposal areas that have similarly favourable properties constituting the CRZ. Laterally, the CRZ is dimensioned in such a way that it meets the spatial requirements for HLW disposal according to the current repository concept, with additional spatial reserves for optimisation. An indicator-based delineation approach has been followed to delimit the areas with sufficient distance to steeply dipping faults of hydraulic significance³, which could represent a lateral release path to the regional aquifer systems. A performance indicator “*distance to steeply dipping faults*” was defined together with the performance target “*minimum lateral distance to the next steeply dipping fault*”, required to establish the host rock as an efficient lateral diffusion-dominated transport barrier. The performance target for lateral delimitation of the host rock is described in Section 4.2.

³ Structural elements such as minor faults and other tectonic features were observed in the Opalinus Clay in all deep investigation boreholes. Packer testing of such faults did not reveal a distinct increase of the rock permeability. From a long-term safety perspective faults of hydraulic significance are characterized by transmissivities $>1 \times 10^{-11} \text{ m}^2/\text{s}$.

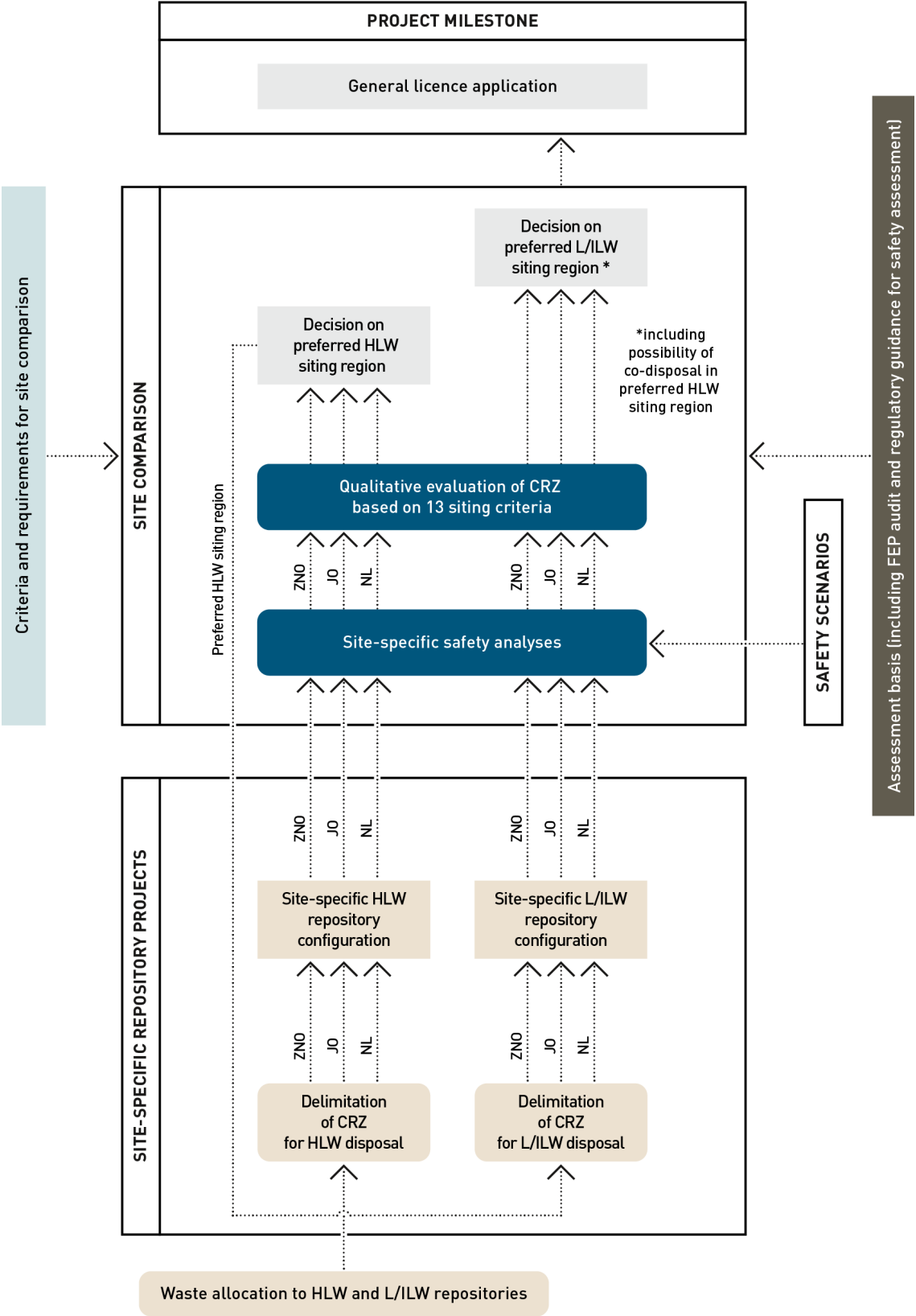


Fig. 3-1: Overview of the general approach for site comparison

Vertically, the CRZ includes the host rock as well as its barrier-effective confining units (Fig. 2-2), bounded above and below by aquifers. An indicator-based delineation approach has been developed to identify areas with suitable Opalinus Clay thickness, which is based on the delineation indicator “*Opalinus Clay thickness*” and the corresponding performance target “*minimum thickness of the Opalinus Clay*”, required to establish the host rock as an efficient diffusion-dominated transport barrier. The performance target for vertical delimitation of the host rock is described in Section 4.1.

3.2.2 Provisional site-specific repository projects

The HLW repository is then configured within the space available in the CRZ. The development of site-specific configurations for an HLW repository is part of the design development process, as described in general terms in Nagra (2024k). Provisional site-specific repository projects are established for the planning of the repository facilities and are needed specifically for the site-specific safety analyses and for the qualitative evaluation of the CRZ, as described in Sections 3.2.4 and 3.2.5, respectively. As well as the positioning of the emplacement drifts for HLW, this involves locating the other underground structures, including access structures and the logistics area, in accordance with relevant safety, structural and operational requirements. A complete description of the provisional repository projects for both HLW and L/ILW disposal can be found in the civil engineering dossier (Nagra 2023).

3.2.3 Application of safety scenarios for site comparison

ENSI 33/649 (ENSI 2018) requires that the safety analysis for site comparison includes analyses of both reference and alternative safety scenarios. Given the similarity in the geological characteristics, the engineering design of the disposal system and the expected evolution of all three siting regions, the same reference safety scenario and alternative safety scenarios are applicable to all three siting regions. Site-specific differences, e.g., in the likelihood, rates or extent of some phenomena, are, however, accounted for. There is thus no need for dedicated site-specific performance assessments to support safety scenario development. However, analyses similar to those used in the performance assessment for the safety case are among those used to support the qualitative evaluation of the CRZ (see Section 3.2.5).

No FHA safety scenarios and no “what-if?” cases are analysed in the context of the site-specific safety analyses for the site comparison (Fig. 3-2).

Carrying out a more limited set of calculations in the site-specific safety analyses is in line with Section 5.2 of ENSI (2018), which states that the demonstration of the effectiveness and robustness of the engineered and geological barriers, the safety scenario analysis and the sensitivity analyses in the safety assessment in support of the general licence application are more detailed than those carried out within the safety analyses supporting site selection⁴. Furthermore, the consequences of FHA safety scenarios, as well as potential measures available to reduce these consequences, are not expected to be site-specific.

⁴ Die Sicherheitsanalyse des Standortvergleichs (siehe Kap. 4.4) für den gewählten Standort wird entsprechend vertieft und mit umfassenden Szenarien- und Risikoanalysen gemäss Richtlinie ENSI-G03 ergänzt. Insbesondere wird für die in Kap. 4.4 aufgeführten Punkte b) «Wirkung und Robustheit der technischen und natürlichen Barrieren», e) «Szenarienanalyse mit einer umfassenden FEP-Analyse» und h) «Sensitivitätsanalyse» ein höherer Detaillierungsgrad erwartet.

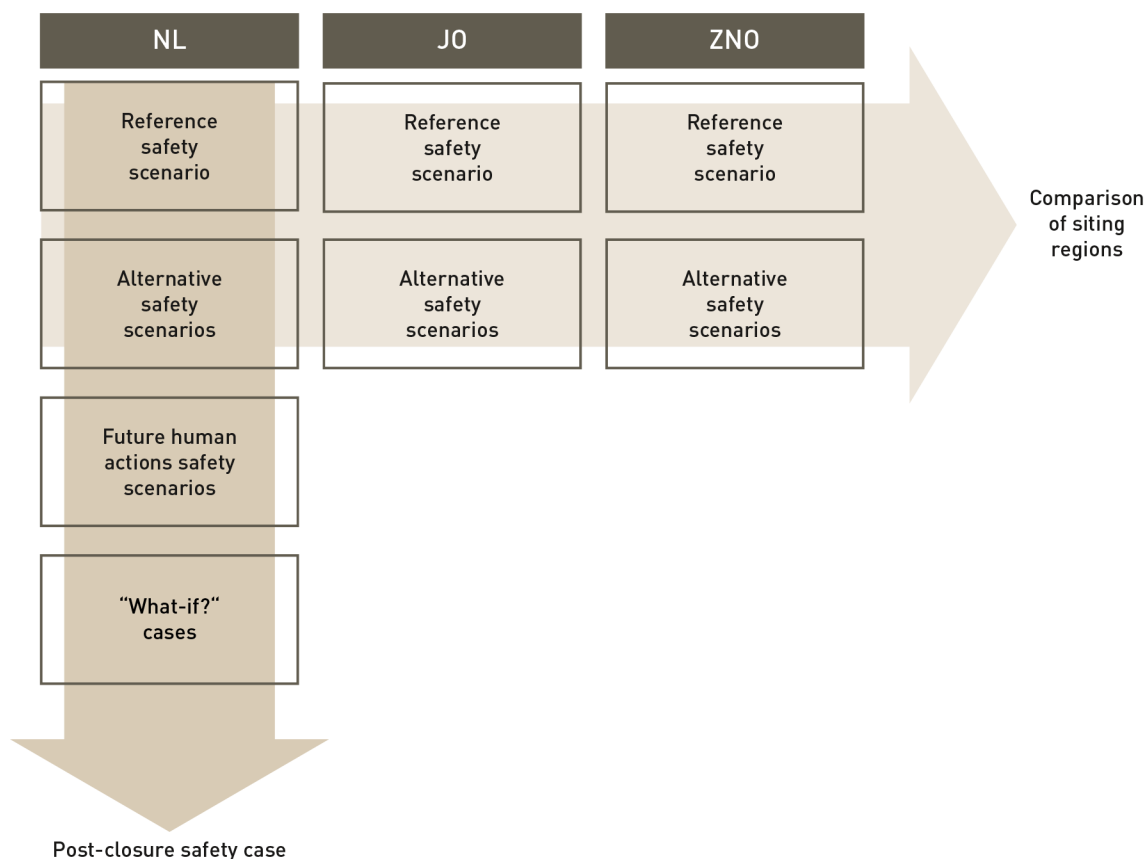


Fig. 3-2: Safety scenarios, variants and “what-if?” cases as input to the post-closure safety case and to the comparison of siting regions

3.2.4 Site-specific safety analyses

Each site-specific safety analysis consists of an evaluation of radionuclide release rates to the surface environment as a function of time in a defined set of safety scenarios. Furthermore, they also include the conversion of these release rates into either annual individual effective doses or annual individual risks, which are compared with regulatory protection criteria to assess the available safety margins. The modelling approach used in the site-specific safety analyses carried out for an HLW repository in each siting region is essentially the same as that used in the analysis of radiological consequences of releases from the HLW disposal section of a combined repository in Nagra’s proposed siting region (Nagra 2024i / Part B). However, the geosphere retention and transport model is tailored to the characteristics of each siting region. Uncertainty in models and data is again accounted for by a combination of conservative assumptions and calculation cases combined with probabilistic analyses, in line with regulatory guidance set out in ENSI 33/649⁵ (ENSI 2018).

⁵ *Wo Ungewissheiten bestehen, sind in der Sicherheitsanalyse die maximalen radiologischen Konsequenzen durch die Berechnung umhüllender Varianten oder durch konservative Annahmen abzuschätzen. Der Einfluss von Ungewissheiten auf die berechneten Ergebnisse ist systematisch aufzuzeigen, und die daraus gezogenen Schlüsse für die Langzeitsicherheit sind darzulegen.*

3.2.5 Qualitative evaluation of the CRZ

In the qualitative evaluation of the CRZ, as in earlier stages of the siting process, the 13 siting criteria presented in Tab. 2-1 are evaluated for each siting region using an indicator-based procedure. Some of the indicators are quantitative and can be evaluated using models. However, the establishment of a preferred siting region for HLW disposal based on these indicators is a qualitative process, as is the evaluation of the potential for a combined repository, which is why the process as a whole is referred to as qualitative.

Nagra (2024h) contains an overview of the indicators used in Stage 3 that correspond to each criterion, as well as their justifications and their comparison against evaluation scales. As noted in Section 2.2, the Sectoral Plan (BFE 2008) specifies, for each of the criteria, the various “*aspect(s) to be evaluated*” and their corresponding “*relevance for safety*”. These form the basis for the selection of the indicators and evaluation scales. Nagra has defined different *assessment perspectives* for each of the four criteria groups. The assessment perspectives are as follows:

- **Group 1** considers the performance of the CRZ based on its characteristics at the start of the time period under consideration (i.e., at the time of repository closure), assuming that these have not been impacted by the presence of the repository.
- **Group 2** is concerned with the expected evolution of the CRZ during the time period under consideration, due to the effects of geological and climatic long-term processes, repository-induced effects and human actions.
- **Group 3** addresses uncertainties originating from limitations to the level up to which it is possible to characterise and explore the geological barrier and to predict its long-term evolution based on site investigations.
- **Group 4** concentrates on the suitability of the CRZ and overlying strata at each site from an engineering perspective, both for expected conditions and for conditions that deviate negatively from the expected.

Like the performance assessment, the analysis of the siting criteria includes an analysis of the thermos-hydro-mechanical and chemical (THM-C) evolution of the disposal system, with an emphasis on their relevance to post-closure safety in a given siting region. Also, as in the performance assessment, the qualitative evaluation of these criteria is, in some cases, supported by quantitative modelling, and many of the same models and data are used in the analysis of these criteria and in the performance assessment part of the safety assessment.

Finally, in the qualitative evaluation of the CRZ, the results of the evaluation carried out for individual criteria are aggregated in a multi-criteria analysis, as described in Nagra (2024h).

3.2.6 Establishment of preferred siting region for HLW disposal

A safety-based comparison of the siting options available for HLW disposal based on the steps summarised in Sections 3.2.1 to 3.2.4, and an evaluation of the characteristics that were decisive for the selection of the proposed site for this repository type, is provided in Nagra (2025a).

3.3 Evaluation of siting regions for L/ILW disposal

The evaluation of each siting region with respect to L/ILW disposal involves the same steps as described above for HLW disposal. The demarcation of favourable siting regions and the development of site-specific repository configurations for an L/ILW repository consider the possibility of co-disposal of L/ILW in the proposed siting region for the HLW repository. As a specific example of the iterative nature of the development of repository configurations, analyses were carried out to formulate requirements on the minimum distance between the HLW and L/ILW repository sections of the combined repository (Nagra 2021). As in the case of the HLW repository, the modelling approach used in the site-specific consequence analyses carried out for an L/ILW repository in each siting region is similar to that used in the analysis of radiological consequences carried out as part of the safety assessment for the L/ILW repository section of a combined repository in Nagra's proposed siting region, i.e., the approach described in detail in the context of safety assessment. The qualitative evaluation of the CRZ is again based on the 13 siting criteria presented in Tab. 2-1, including repository induced effects (EDZ, gas).

3.4 Evaluation of co-disposal of HLW and L/ILW in a combined repository

When evaluating the potential for a combined repository in the same siting region, safety-related, ecological, spatial planning and economic factors are taken into account, as described in Nagra (2025a).

4 Model based contributions to the delimitation of the CRZ

The CRZ is the part of the geological barriers which, with the expected evolution of the repository for the period under consideration, ensures the effective containment and retention of the radioactive substances contained in the waste (BFE (2008)). The sectoral plan requires that the CRZ is to be delimited laterally and vertically at a suitable depth.

The workflow for the safety-related comparison of the repository projects foresees, in a first step, the identification of favourable areas in the three siting regions, followed by the vertical and lateral delimitation of the CRZ for the site-specific repository projects (Fig. 3-1). An indicator-based approach, founded on reliable performance targets and evaluation scales, ensures a traceable demarcation of the favourable areas and, within these areas, the vertical and lateral delimitation of the CRZ. It is the emphasis of this chapter to provide model-supported justification of the performance targets and evaluation scales used in the context of the delimitation process:

- estimation of the minimum thickness of the Opalinus Clay, required to act as an efficient transport barrier for radionuclides (Section 4.1);
- reasoning for the minimum lateral distance between the disposal field to the next steeply dipping fault (Section 4.2);
- reasoning for the minimum lateral distance between the prospected protection zone and the next injection / pumping well (Section 4.3);
- confirmation of the selected repository footprint in the siting region by indicator-based assessments of barrier efficiency of the host rock (Section 4.4).

4.1 Minimum thickness of the host rock

In the Swiss disposal concept the Opalinus Clay has been selected as the host rock formation both for the HLW and the L/ILW repository. Favourable features of the host rock were formulated in (ENSI 2018) with a view on the site selection process. These are:

- diffusion-dominated transport of dissolved radionuclides in the porewater of the host rock;
- distinct self-sealing and
- retention capacity of the clay-rich zones in the CRZ.

The indicator-based delimitation approach described in Chapter 3 evaluates the barrier performance of the Opalinus Clay with the delimitation indicator “*Opalinus Clay thickness*” and the corresponding performance target “*minimum thickness of the Opalinus Clay*”, required to establish the host rock as an efficient diffusion-dominated transport barrier. The minimum thickness of the Opalinus Clay is not only required for the vertical delimitation of the CRZ but also for the assessment of the EDZ in Section 5.1.1.

Different performance targets “*minimum thickness of the Opalinus Clay*” are required for HLW repository and the L/ILW repository due to different radionuclide inventories. For the HLW repository, the derivation of the “*minimum thickness of the Opalinus Clay*” is based on simple back-of-the-envelope calculations with a generic transport model, aimed at bracketing the minimum thickness of the Opalinus Clay formation for a wide range of diffusion coefficients and vertical Darcy fluxes, respectively. The modelling approach and the results of the corresponding simulations are detailed in App. A. For the L/ILW repository, the specification of a minimum thickness of the Opalinus Clay is based on pragmatic considerations. The following paragraphs discuss the results of the model-based assessments and provide the corresponding parameter values for the HLW and L/ILW repository.

4.1.1 Minimum thickness of the host rock required for the HLW repository

The tracer flux of a dissolved, non-sorbing radionuclide, released from the HLW nearfield through the host rock into the Upper/Lower Confining Units (UCU/LCU) is a performance indicator used in the context of the site selection for several purposes (see App. A and App. E). For the HLW repository, the dose relevant radionuclide is ^{129}I . The following section sets out the corresponding performance target “*Minimum thickness of the Opalinus Clay* – $L_{\min, \text{HLW}}$ ” for the HLW repository, deduced from the NTF indicator with the effective diffusion coefficient of the dose relevant radionuclide ^{129}I . The workflow is based on a dimensionless representation of diffusion-dominated tracer transport and advective-diffusive transport at Peclet numbers < 30 . Details of the modelling approach are given in App. A.

In this context the Peclet number Pe defined as:

$$Pe = \frac{L \cdot u}{D_L} = \frac{L \cdot v_f}{n \cdot D_L} \quad (4-1)$$

where L represents the length of transport path, D_L is the longitudinal dispersion coefficient, u is the particle velocity, n is porosity and v_f is the Darcy velocity. Due to the ultra-low Darcy velocity of porewater flow in Opalinus Clay, it is assumed here that $D_L \approx D_{eff}$, representing the effective diffusion coefficient of the Opalinus Clay. The numerical analyses in App. A reveal that the minimum thickness of the host rock depends not only on the flow and transport properties of the host rock (i.e., $D_{eff, \text{OPA}}$ and $K_{v, \text{OPA}}$), but also on the vertical component of the hydraulic gradient across the Opalinus Clay. Based on the recent site investigations in the three candidate sites (Nagra 2024c), the relevant parameters can be bracketed in the ranges given in Tab. 4-1.

Tab. 4-1: Relevant transport parameters of the Opalinus Clay formation in the three candidate siting regions

Deduced from Nagra (2024c).

The parameters are needed for estimating the minimum thickness required to establish the host rock as an efficient diffusion-dominated transport barrier. The diffusion coefficient corresponds to ^{129}I .

Parameter	Min	Best estimate	Max
$D_{eff, \text{OPA}} [\text{m}^2/\text{s}] - ^{129}\text{I}$	1.22×10^{-12}	2.65×10^{-12}	5.48×10^{-12}
$K_{v, \text{OPA}} [\text{m/s}]$	2×10^{-15}	1×10^{-14}	1×10^{-13}
Vertical hydraulic gradient $i_v [-]$	0	0.01	1*
$n [-]$	0.11	0.12	0.14

* Hypothetical upper bound, required for PA/SA calculations

The evaluation scales for the performance indicators NTF, the corresponding climate scenarios and the corresponding quality levels are detailed in App. A. The model-supported derivation of the performance target “*Minimum thickness of the Opalinus Clay*”, $L_{\min, \text{HLW}}$, is specified such that the host rock provides barrier performance at the quality level “unfavourable” but still below the performance limit ($II = 1$). Furthermore, it is assumed that the present-day climate scenario (expressed in terms of the corresponding biosphere dose conversion factor) applies and the total inventory of the ^{129}I is released instantaneously (conservative assumption).

A graphical representation of the dependence of $L_{\min,HLW}$ on the effective diffusion coefficient D_{eff} for Peclet numbers up to 50 is given in Fig. 4-1. The diagram allows to determine $L_{\min,HLW}$ for the HLW repository configuration for a given Peclet number and effective diffusion coefficient of the host rock. According to Tab. 4-1, the effective diffusion coefficient of ^{129}I ranges between 1.2×10^{-12} and $5.5 \times 10^{-12} \text{ m}^2/\text{s}$, the upper bound of the Peclet number could reach a value between 10 and 20, assuming a high hydraulic gradient combined with an upper bound hydraulic conductivity and a low diffusion coefficient. The graph in Fig. 4-1 allows to infer the minimum thickness of the Opalinus Clay, required to perform as a transport barrier for dissolved radionuclides, remaining within the regulatory dose limits. With the aforementioned upper bounds of Peclet number and diffusion coefficient a minimum thickness above and below the emplacement tunnels within the Opalinus Clay of 20 - 35 m is deemed a sensible value. A favourable barrier performance is ensured, if the total thickness of the Opalinus Clay is at least 100 m; very favourable conditions exist from 110 m thickness. This applies to the HLW and the L/ILW repository.

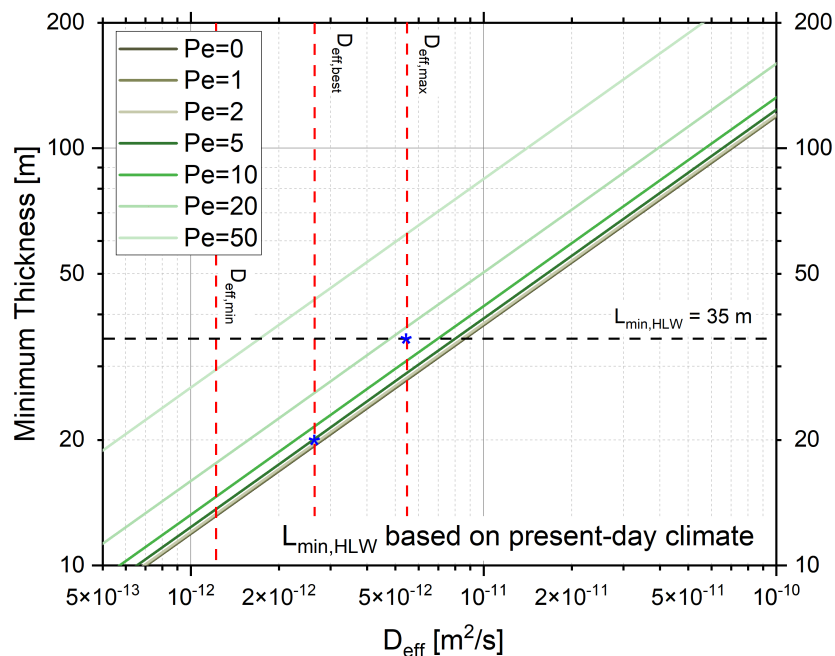


Fig. 4-1: Minimum thickness of the Opalinus Clay, derived from performance indicator II_{HLW} at performance level “unfavourable” using the present-day climate scenario

For the HLW repository a minimum thickness above and below the emplacement tunnels within the Opalinus Clay of 35 m is derived, based on the upper bound diffusion coefficient $D_{\text{eff,max}} = 5.5 \times 10^{-12} \text{ m}^2/\text{s}$ and a Peclet number between 10 and 20 as constraints (blue star). A minimum thickness of 20 m is derived, based on the best estimate diffusion coefficient $D_{\text{eff,best}} = 2.65 \times 10^{-12} \text{ m}^2/\text{s}$ and a Peclet number <5 as constraints (blue star).

4.1.2 Minimum thickness of the host rock required for the L/ILW repository

A similar approach was developed to determine the minimum thickness of the Opalinus Clay for the L/ILW repository. The dose relevant radionuclide was ^{36}Cl . The calculations indicated a required minimum thickness of less than 10 m. Even if such a thickness of the host rock were sufficient to act as a transport barrier for dissolved radionuclides, the safety function of the mechanical protection of the EBS would not be guaranteed. From a PA perspective, the determination of the minimum thickness of the host rock must take into account other aspects in addition to the function as a transport barrier. Based on the diameter of the L/ILW caverns of approximately 10 m, a minimum thickness of the intact host rock⁶ package above and below the caverns of 20 m appears to be justified to ensure the confinement of the waste and the mechanical and chemical integrity of the repository system as a whole.

4.2 Minimum lateral distance to the next steeply dipping fault

The delimitation indicator for lateral delimitation of the CRZ is called “*distance to steeply dipping faults*”. It aims at identifying favourable areas in the siting regions with sufficient distance from steeply dipping fault systems. A target value of 200 m was specified as a minimum distance of the HLW and L/ILW disposal areas from any fault systems, that have been identified in the 3-D seismic surveys. Simple back-of-the-envelope calculations were carried out with a 2-D transport model of the HLW disposal field of the prospect repository at the Haberstal site in NL to confirm the barrier performance of the Opalinus Clay (Fig. 4-2) and to specify the upper limit dose rate expected to be released into the fault. Probabilistic assessments were carried out with the 2-D model set-up and the general assessment workflow, which is described in E.2. A vertical fault was implemented in the model at a distance of 200 m from the outermost HLW drift, which connects the Malm with the Keuper aquifer. A transmissivity of $1 \times 10^{-10} \text{ m}^2/\text{s}$ was assigned to the fault and pressure difference of 1 MPa was applied between Keuper and Malm aquifer to ensure a significant vertical Darcy flow through the fault. The release of a conservative tracer from the HLW nearfield through the Opalinus Clay to the regional aquifer systems and the lateral fault was modelled with a set of 100 Monte Carlo simulations.

⁶ The intact host rock is the undamaged rock zone beyond the EDZ which surrounds the drifts and caverns of the deep geological repository. The term «intact» expresses that its geomechanical and hydraulic properties are representative for the undamaged rock within the range of expected rock properties as specified in (Nagra 2024f). This does not exclude the presence of lithological features or structural discontinuities in the rock mass.

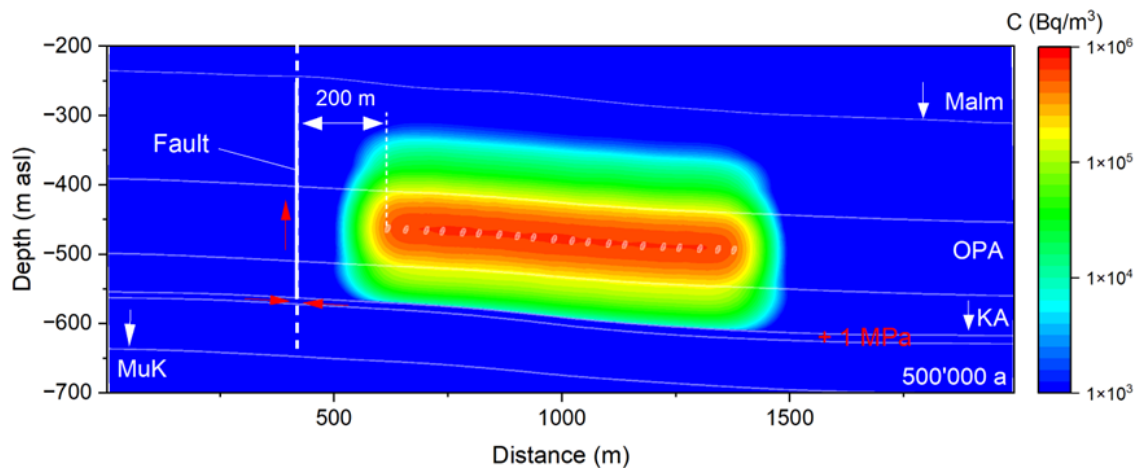


Fig. 4-2: Delimitation indicator “distance to steeply dipping faults”

A performance target value of 200 m is specified as a minimum distance of the HLW and L/ILW disposal areas from any fault systems, that have been identified in the 3-D seismic surveys.

The results of the Monte Carlo simulations are presented in Fig. 4-3. The transients of total tracer flux into the regional aquifer systems (sum of fluxes to Malm and Keuper aquifer) and lateral flux into the vertical fault are displayed in Fig. 4-3a. The maximum dose rates of the lateral releases to the fault, are more than 4 orders of magnitude below the regulatory dose limit and one order of magnitude lower than the releases into the regional aquifer systems. It is evident, that the release into the fault is not the dominating transport path, even when unfavourable hydraulic conditions are assumed (1 MPa overpressure in the Keuper aquifer, combined with a fault transmissivity of $1 \times 10^{-10} \text{ m}^2/\text{s}$). The histograms of the normalised NTF performance index in Fig. 4-3b confirm the results from visual inspection of the tracer breakthroughs in a quantitative manner, indicating that the dose rates of lateral release are more than 4 orders of magnitude below the regulatory limit for more than 95% of the Monte Carlo simulations (95th percentile in the frequency distribution).

Complementary transport simulations were carried out with a fault distance of 100 m and the same boundary conditions as described above. The results of the probabilistic simulations are shown in Fig. 4-4, indicating an early first arrival of the tracer at the fault and slightly reduced safety margins. The analyses indicate favourable barrier performance of the CRZ for the respect distance of 100 m and very very favourable conditions for 200 m.

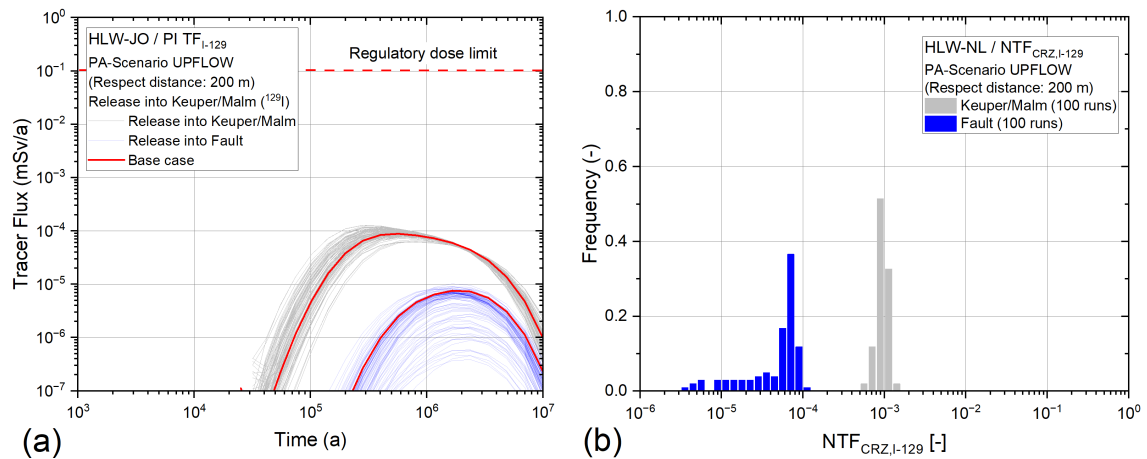


Fig. 4-3: Results of Monte Carlo simulations for substantiating the delimitation indicator “distance to steeply dipping faults”

(a) Tracer fluxes released into the Malm and Keuper aquifer and lateral release into the vertical fault at a distance of 200 m from the outermost HLW drift; (b) histogram of the NTF index, confirming that the dose rates of lateral release are more than 4 orders of magnitude below the regulatory limit for more than 95% of the Monte Carlo simulations (95th quantile of the frequency distribution).

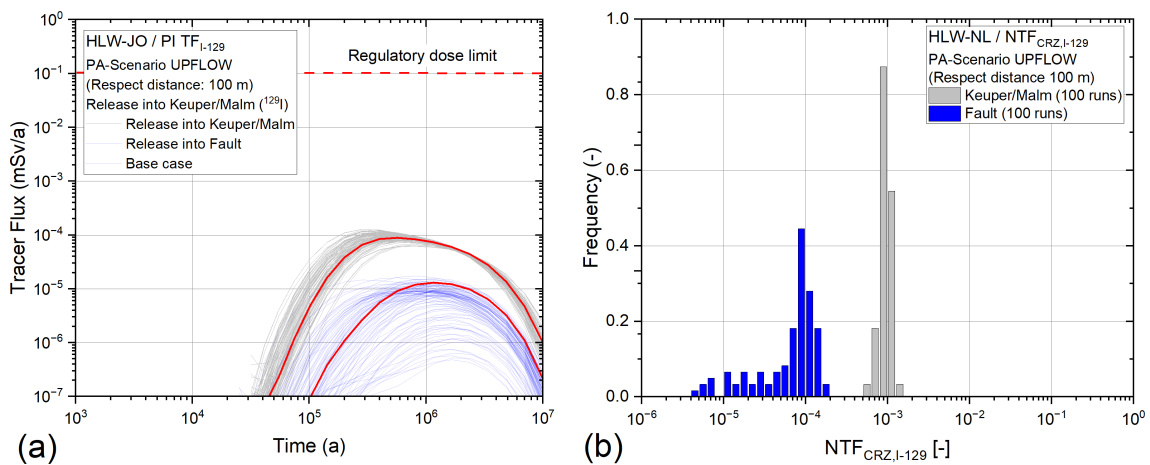


Fig. 4-4: Results of Monte Carlo simulations for substantiating the delimitation indicator

(a) Tracer fluxes released into the Malm and Keuper aquifer and lateral release into the vertical fault at a distance of 100 m from the outermost HLW drift; (b) histogram of the NTF index, confirming that the dose rates of lateral release are more than 4 orders of magnitude below the regulatory limit for more than 95% of the Monte Carlo simulations (95th quantile of the frequency distribution).

4.3 Minimum lateral distance between the prospected protection zone and the next injection / pumping well

Respect distances are not only required in the context of the site selection process (Nagra 2025a) but also for the delineation of the prospected repository zone as described in the safety report (Nagra 2025b). The delineation process foresees a prospected zone of the access structures and the repository zone (Fig. 4-5). A respect distance of 200 m from the potential repository zone must be met at the northern and southern rim and 50 m at the eastern and western rim of the prospected protection zone.

Recalling the modelling results presented in Section 4.2 it is conceivable that a deep injection or production well at the northern rim of the prospected protection zone with a lateral distance of 200 m would not affect repository safety in a detrimental manner. Therefore, the complementary modelling efforts concentrated on the effect of deep wells at a respect distance of 50 m. Two scenarios were investigated:

- *Abandoned well scenario:* It is assumed that a deep borehole is drilled down to the base of the Keuper aquifer, an aquifer system of regional extent, exhibiting artesian conditions at the borehole location (1 MPa above hydrostatic). The borehole is placed at a lateral distance of 50 m from the outermost drift of the HLW repository in the siting region NL (see Fig. B-1). At the end of its service life, the borehole is assumed to be insufficiently sealed. A permanent vertical flow of groundwater is established from the artesian Keuper aquifer to the hydrostatic Malm aquifer. The effect of this vertical flow in the abandoned well on the radionuclide release from the HLW repository is investigated by numerical modelling.
- *Geothermal well scenario:* It is assumed that in the distant future a geothermal well will be drilled to the aquifer systems below the Opalinus Clay (i.e., Keuper and Muschelkalk aquifer). Hydrostatic conditions prevail in both aquifers prior to the operational phase. The operating time of the geothermal well is 100 years and a pumping rate of 10 l/s is applied.

Modelling of the impact of a nearby well on repository performance at the system scale is carried out with a 3-D transport model (App. B). The model simulates advection and diffusion in a fully saturated porous medium. It accounts also for the for non-isothermal conditions in the repository near-field, including the natural heat flux from the basement to ground surface and the heat emitting wastes in the emplacement drifts. It is assumed that HLW canisters will breach 10,000 years after repository closure. At that time a conservative tracer, which represents the dose-relevant radionuclide ^{129}I , is released instantaneously from the HLW canisters. The prevailing transport mechanisms are diffusion and advection. Advective transport represents a superposition of a vertical flow component associated with the porewater overpressures in the Keuper aquifer and a radial flow component depending on the pressure conditions in the borehole.

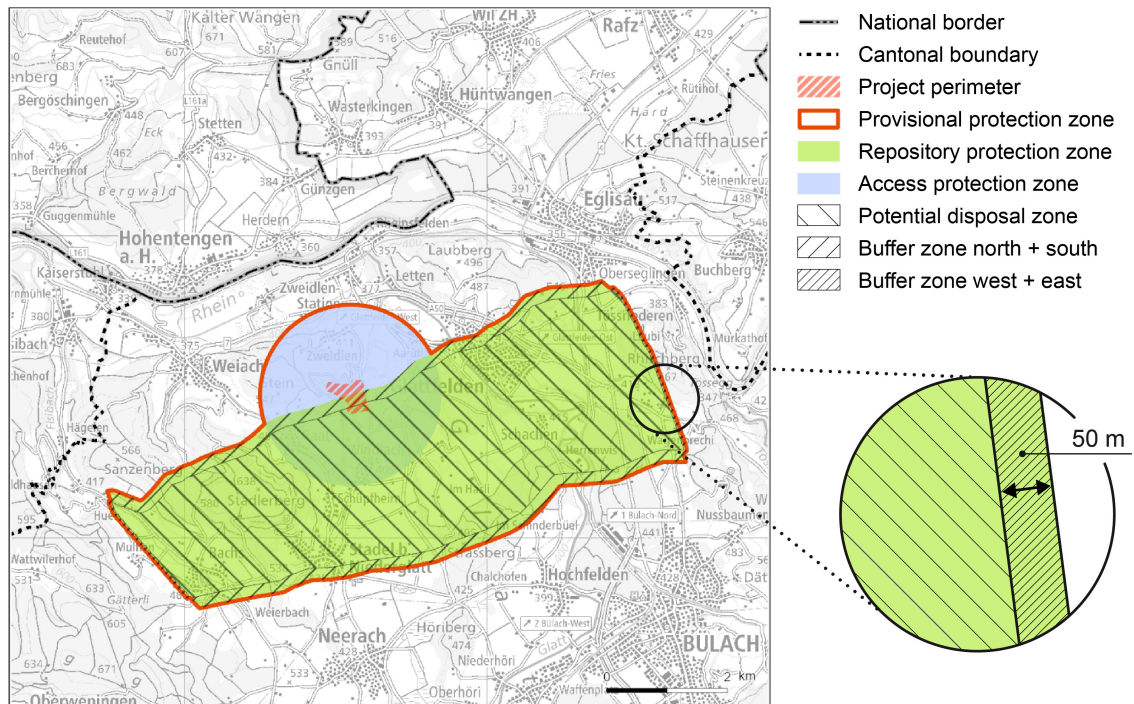


Fig. 4-5: Protection zone as defined in the safety report

Modified from Nagra (2025b)

A respect distance of 50 m has been specified at the western / eastern edge of the prospected protection zone.

4.3.1 Abandoned well scenario

The abandoned well scenario assumes a permanent vertical flow of groundwater (≈ 4.3 l/day at late times) from the artesian Keuper aquifer to the hydrostatic Malm aquifer, caused by insufficient sealing of the borehole at the end of its life service. The main effect of the vertical flow in the borehole is that the Opalinus Clay is “leached” in the vicinity of the borehole, which increases the diffusive tracer flux locally. The analysis of the abandoned well scenario follows closely the assessment workflow, which was used to substantiate the minimum distance to steeply dipping faults (Section 4.2). The transients of tracer fluxes to the regional aquifers and to the abandoned well are extracted from the modelling results, post processing follows the approach described in App. E.2.

The transients of the tracer releases to the regional aquifer systems (Malm and Keuper aquifer) together with the tracer flux from the Opalinus Clay into the abandoned well and from the well into the Malm are shown in Fig. 1-1. The results are comparable with the 2-D simulations in Section 4.1, indicating releases to the regional aquifer systems which are more than 3 orders of magnitude below the regulatory dose limit. The release path along the well is characterised by even lower dose rates more than 4 orders of magnitude below the regulatory dose limit. It can be concluded that the lateral release into a deep borehole is not relevant, when the respect distance of 50 m is maintained.

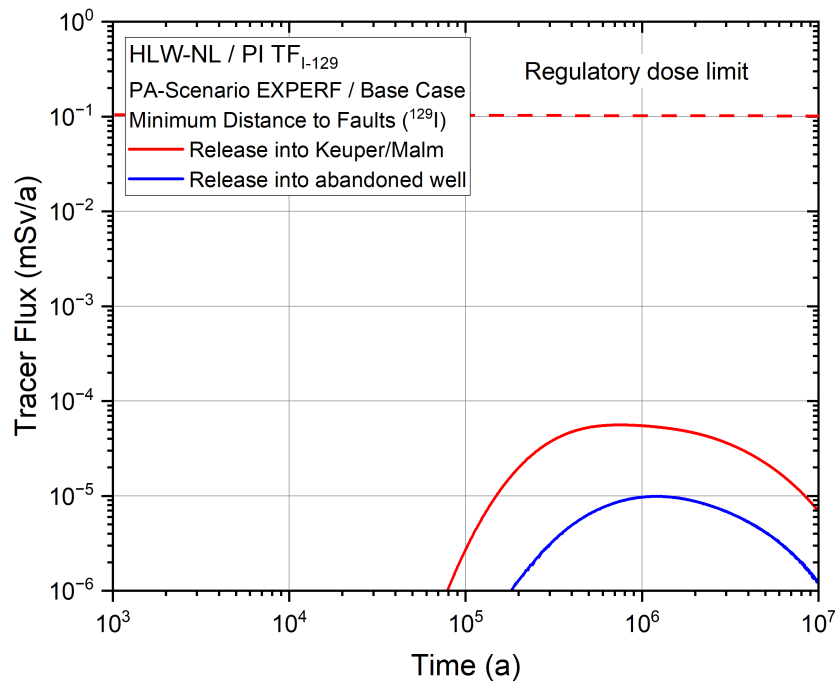


Fig. 4-6: Tracer fluxes released into the Malm and Keuper aquifer and lateral release to the “abandoned well” at a distance of 50 m from the outermost HLW drift

4.3.2 Geothermal well

The geothermal scenario is simulated for a point in time in distant future, namely 100,000 years. Pumping of groundwater from the Muschelkalk and Keuper aquifer collects the tracer, which is released from the CRZ into the Keuper and Malm aquifer. The transients of the tracer fluxes to the Keuper aquifer and the tracer fluxes from the Keuper and the Muschelkalk aquifers to the well are presented in Fig. 4-6 (converted to equivalent dose rates with the biosphere dose conversion factor, representing a present-day climate). After 100,000 years the tracer fluxes from the CRZ to the Keuper aquifer are still more than 5 orders below the regulatory dose limit. The tracer flux to the pumping well comes mainly from the Keuper aquifer, only a minor fraction originates from the Muschelkalk aquifer. The total dose rates to the well reach a maximum of $\approx 1 \times 10^{-6}$ mSv/year (5 orders of magnitude below the regulatory dose limit).

It does not seem particularly sensible to simulate concrete usages of deep groundwater systems in the distant future in great detail. Nevertheless, such calculations provide insight, how man-made perturbations of groundwater flow in the deep aquifers could affect the barrier performance of the repository system. For the geothermal well scenario, it can be ruled out that an geothermal application in the near future will compromise repository safety.

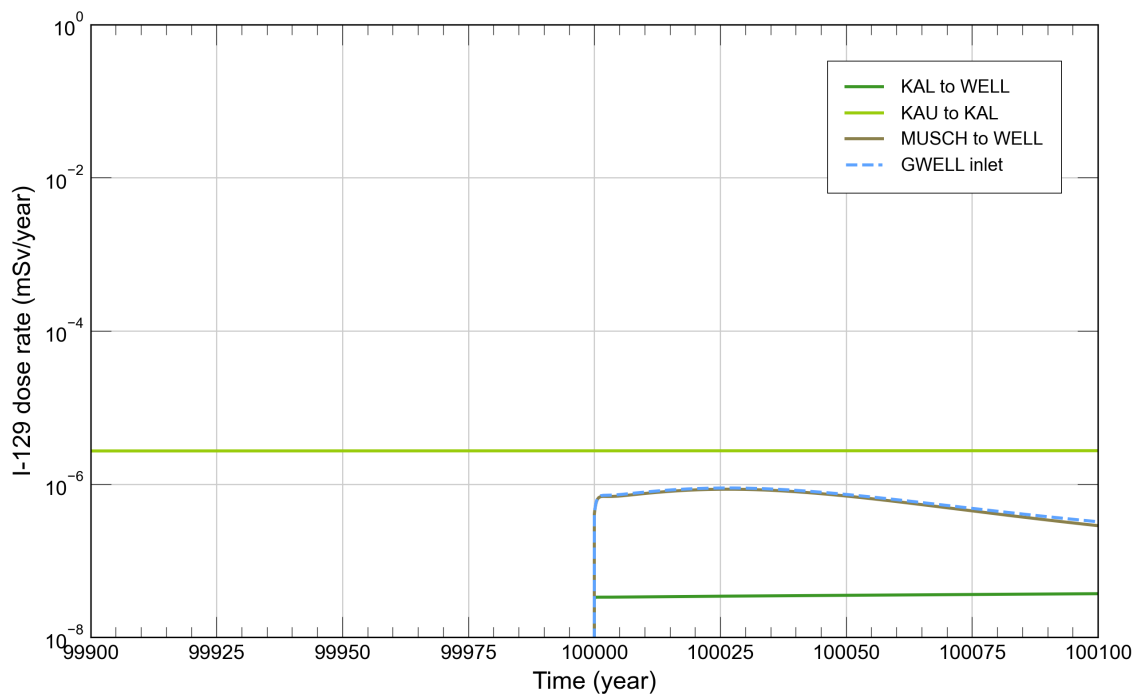


Fig. 4-7: Tracer fluxes of ^{129}I produced by the geothermal pumping well, which is located at a lateral distance of 50 m from the HLW repository

Start of pumping after 100,000 years. The dotted purple line (GWELL inlet) indicates the total tracer flux to the pumping well (KAU to KAL: tracer flux to the Keuper aquifer; KAL to AWELL: tracer flux from Keuper aquifer to the well; KAL to AWELL: tracer flux from Muschelkalk aquifer to the well).

4.4 Confirmation of the selected repository footprint in the siting regions

A complementary indicator-based workflow for lateral delimitation was pursued for setting out favourable repository areas and for delineation of the corresponding repository footprints in the three siting regions. From the perspective of long-term safety, the selected repository footprints have been confirmed by complementary transport simulations, aimed at mapping lateral variations of performance of the host rock in the siting areas as a transport barrier for dissolved species. The adopted methodology for lateral screening of the siting areas is introduced briefly in the following paragraph (Section 4.4.1) and reported in greater detail in App. C.1 The results of the screening process are presented in Sections 4.4.2 to 4.4.4.

4.4.1 Methodology

The screening process, aimed at mapping lateral variations of barrier performance of the host rock, was carried out for the site-specific repository projects using generic footprint areas with a square base of $0.5 \times 0.5 \text{ km}^2$. Vertically, the repository is assumed to be located in the centre of the Opalinus Clay. At repository level, a conservative, non-sorbing tracer is released with a constant source strength (i.e., as a step input function) for a period of 10 million years. Tracer simulations are carried out with 3-D models of the siting regions, assuming that diffusion is the prevailing transport process in the CRZ. The tracer flux at the host rock boundaries is extracted from the transport simulations as described in App. E.2 with the difference that it is determined at the top / base of the Opalinus Clay rather than at the boundaries of the CRZ (i.e., base Malm and top Keuper aquifer). The performance index NTF_{OPA} is derived by post processing as described in App. E.2. Tracer simulations were carried out at a total of 100 locations, equally distributed over the perimeters of the three siting areas JO, NL and ZNO (see App. C). The results are presented in the following sections.

4.4.2 Siting area JO

The performance index NTF_{OPA} was calculated at each of the 100 locations distributed over the perimeter of the siting area JO (Fig. C-1). Fig. 4-8 shows the contour map of NTF_{OPA} over the perimeter of the JO site together with the locations of the corresponding HLW project. The contour map does not indicate any preferred areas within the perimeter.

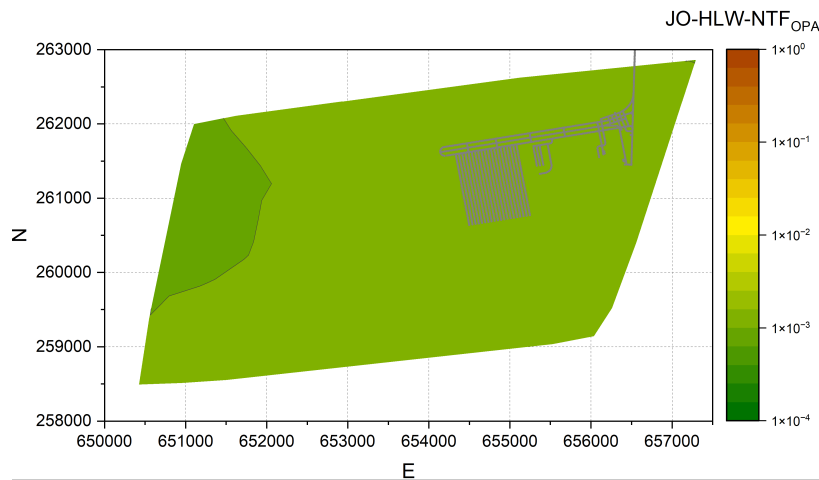


Fig. 4-8: Contour map of the NTF_{OPA} indicator over the perimeter of the JO site together with the location of the corresponding HLW project

The CRZ performs equally well as an excellent transport barrier over the entire perimeter of the JO site.

4.4.3 Siting area NL

The performance index NTF_{OPA} was calculated at each of the 100 locations distributed over the perimeter of the siting area JO (Fig. C-2). Fig. 4-9 shows the contour map of NTF_{OPA} over the perimeter of the NL site together with the location of the corresponding HLW repository section. The contour map does not indicate any preferred areas within the perimeter.

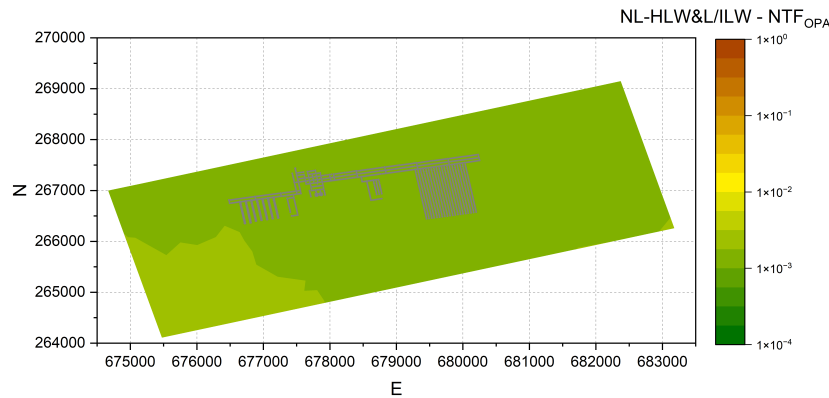


Fig. 4-9: Contour map of the NTF_{OPA} indicator over the perimeter of the NL site together with the location of the prospected repository project

The CRZ performs equally well as an excellent transport barrier over the entire perimeter of the NL site.

4.4.4 Siting area ZNO

The performance index NTF_{OPA} was calculated at each of the 100 locations distributed over the perimeter of the siting area ZNO (Fig. C-3). Fig. 4-10 shows the contour map of NTF_{OPA} over the perimeter of the JO site together with the locations of the corresponding HLW project. The contour map does not indicate any preferred areas within the perimeter.

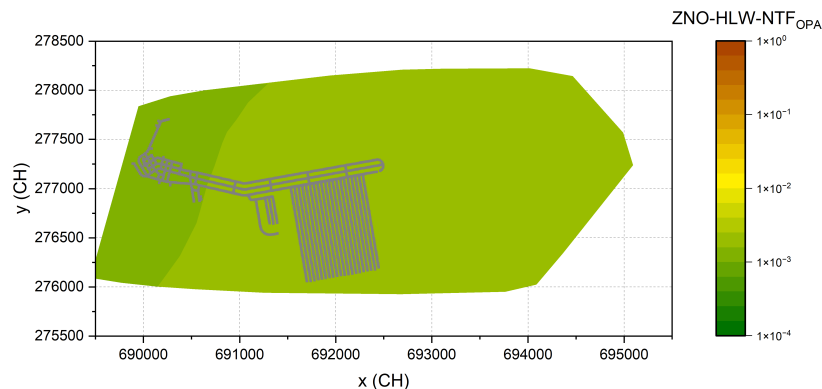


Fig. 4-10: Contour map of the NTF_{OPA} indicator over the perimeter of the ZNO site together with the location of the corresponding HLW project

The CRZ performs equally well as an excellent transport barrier over the entire perimeter of the ZNO site.

5 Model-supported analyses for the site selection process

The workflow for site selection and the execution of the indicator-based assessments is reported in Nagra (2024h). The performance indicators formulated in Nagra (2024h) for the assessment of the 13 SGT criteria are evaluating the performance of the CRZ with respect to the assessment aspect defined in BFE (2008).

For some criteria, the qualitative evaluation of the CRZ is supported by numerical modelling. This chapter documents all model-based assessments of the 13 SGT criteria, feeding in the

It is the emphasis of this chapter to report the model-based contributions for the assessment of the following SGT-criteria:

- Criterion 2.3 (“Repository-induced influences”);
- Criterion 3.1 (“Ease of characterisation of the rock”);
- Criterion 3.2 (“Explorability of spatial conditions”);
- Criterion 3.3 (“Predictability of long-term changes”).

5.1 Criterion 2.3 (“Repository-induced influences”)

The criterion “Repository-induced influences” (in this report “repository induced effects”, or RIE) was assigned to the criteria group “Long-term stability” (see Tab. 2-1). In the sectoral plan, the RIE criterion was divided in four assessment aspects (gas, heat, chemical interactions, EDZ). From a long-term safety perspective three of those aspects and the corresponding *performance indicators* were identified as potentially relevant for differentiating sites in terms of long-term safety, namely:

- the EDZ, which reduces the *length of release path in the intact host rock*;
- thermal effects in the vicinity of the HLW canisters, creating *thermally induced porewater overpressures in the host rock*; and
- gas pressure build-up in the backfilled repository structures, creating *gas induced porewater overpressures in the host rock*.

Known differences between the siting regions are the thickness of the host-rock formation, depth of the repository level, tectonic overprint and the ambient stress regime. The impact of such site-specific conditions on the three RIE aspects is evaluated as part of the site comparison. In contrast, chemical interactions are less suitable for differentiation. They are similar in all three siting regions, because the repository projects are located in the same host rock (Opalinus Clay).

5.1.1 The excavation damaged zone (EDZ)

The Opalinus Clay formation is the host rock for the HLW and L/ILW repository projects in the three siting regions. The thickness and the dip of the host-rock formation together with the repository depth below ground level and the ambient stress regime at repository level are known differences which may have an impact on the transport path length in the intact host rock. The evaluation of the assessment aspect *Effects of the EDZ* has to address these issues. Tectonic overprint is considered less important, because all repository projects were placed in areas displaying rather low deformation.

Quantitative performance indicator “*length of release path in the intact host rock*”

From a long-term safety perspective, the EDZ is a potential transport path for radionuclides. In the framework of SGT-Stage 2 radionuclide release calculations were conducted to estimate radionuclide transport along the backfilled underground structures. The analyses revealed that the release path along the EDZ is of low relevance due to the long transport distances. On the other hand, an extended EDZ reduces the effective thickness of intact host rock above and below the waste emplacement rooms and thus may reduce the radionuclide retention capacity of the geological barrier. Therefore, the effective “*length of release path in the intact host rock*” is used as a quantitative performance indicator for the evaluation of the performance of the host rock as a transport barrier. The corresponding dimensionless performance index RPL is defined in the following paragraphs.

A minimum thickness $M_{\min, \text{intact}}$ of the zone of intact host rock above/below the repository structures was introduced in Leupin et al. (2016b) and Leupin et al. (2016a) for both, the L/ILW repository and the SF/HLW repository (Fig. 5-1a), representing a performance target for the quantitative evaluation of the radionuclide retention capacity of the host rock.

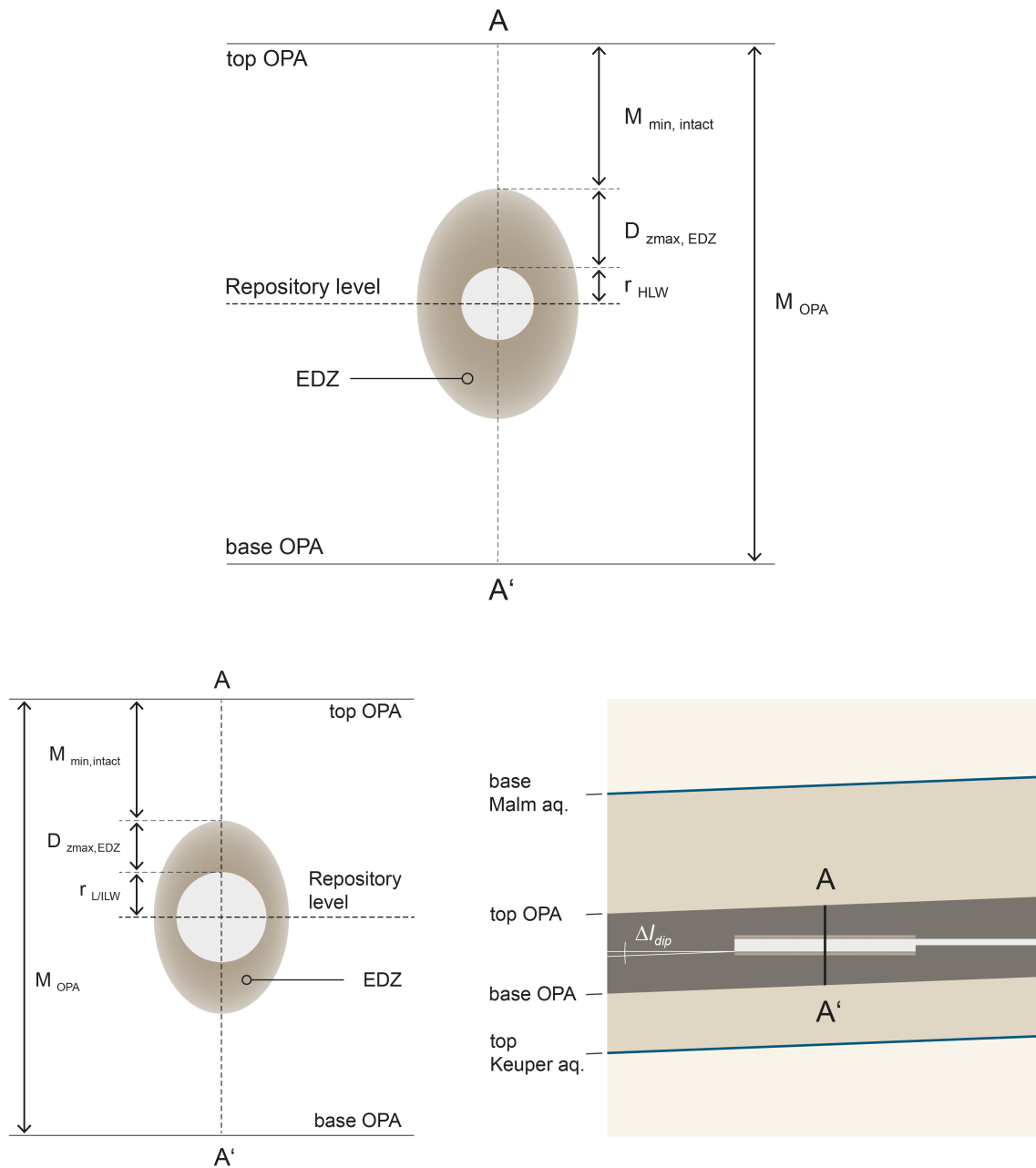


Fig. 5-1: Minimum thickness $M_{\min, \text{intact}}$ of the zone of intact host rock above/below the repository structures

(top) sketch of the minimum thickness $M_{\min, \text{intact}}$, representative for an emplacement room which is placed in the centre of the Opalinus Clay (from Leupin et al. 2016a and Leupin et al. 2016b; (bottom) modified formulation of the minimum thickness $M_{\min, \text{intact}}$, representative for a horizontally placed L/ILW cavern in a gently dipping Opalinus Clay formation.

The minimum required thickness of the zone of intact host rock above / below the HLW drifts was estimated to be 35 m, as reported in Section 4.1.1. It is based on simplified 1-D transport calculations, assuming that the HLW disposal drifts are placed in the centre of the host rock. For the L/ILW caverns, the minimum required thickness is 20 m as derived in Section 4.1.2. $M_{min,intact}$ represents the performance target, which is required to derive a normalised performance index “*Reduced path length in the intact host rock - RPL*”.

Assuming that the HLW disposal drifts are placed in the centre of the host rock, the RPL performance index is defined as:

$$RPL_{HLW} = \frac{M_{min,intact}}{0.5 \cdot M_{OPA} - r_{HLW} - D_{zmax,EDZ}}$$

where, M_{OPA} is the thickness of the host rock, r_{HLW} is the radius of the HLW drift and $D_{zmax,EDZ}$ is the maximum vertical extension of the EDZ around the HLW drift.

The specification of the RPL indicator for the L/ILW repository is complicated by the fact, that the L/ILW caverns will be placed horizontally in a slightly dipping host rock formation (see Fig. 5-1b). Therefore, a further term Δl_{dip} must be considered in the specification of the RPI indicator, which represents the distance of the mid-point of the L/ILW cavern to the centre of the Opalinus Clay:

$$RPL_{L/ILW} = \frac{M_{min,intact}}{0.5 \cdot M_{OPA} - r_{L/ILW} - D_{zmax,EDZ} - \Delta l_{dip}}$$

where, M_{OPA} is the thickness of the host rock, $r_{L/ILW}$ is the radius of the L/ILW cavern, $D_{zmax,EDZ}$ is the maximum vertical extension of the EDZ around the L/ILW cavern and Δl_{dip} is the maximum distance of the mid-point of the L/ILW cavern to the centre of the Opalinus Clay.

Determination of the vertical extent of EDZ for the site-specific HLW projects

The assessment aspect *Effects of the EDZ* is evaluated by numerical calculation of the vertical extent of the EDZ above / below the HLW emplacement tunnels. For this, the vertical extent $D_{zmax,EDZ}$ of the EDZ around a circular cavity in an anisotropic elastic medium is calculated, feeding in the aforementioned quantitative performance index “*Reduced path length in the intact host rock – RPL*”. The general modelling approach is based on a semi-analytical solution of stress distribution around a circular cavity in a transversely isotropic linear elastic rock mass (7App. D). Calculations of the vertical extent $D_{zmax,EDZ}$ of the EDZ were performed on a regular grid displaying the footprint of the HLW-disposal field of the provisional repository projects HLW-JO, HLW-NL and HLW-ZNO (Fig. 5-2). The local components of vertical and horizontal stress were determined at each grid point using stress ratios S_V/S_H according to the geomechanical reference data given in Nagra (2024c). Furthermore, two complementary sets of stiffness and strength parameters of the Opalinus Clay were extracted from the geomechanical reference data base. The two data sets represent a wide spectrum of geomechanical conditions in the provisional repository nearfield, ranging from *expected* to *unfavourable* conditions (Tab. 5-1). Following the general guidelines of the regulator (ENSI 2018), the site selection process must be based on the comparison of the repository projects assuming realistic, but unfavourable geomechanical conditions.

Tab. 5-1: Geomechanical data sets used for the estimation of vertical thickness of the EDZ

The two data sets are based on the geomechanical reference data (Nagra 2024c) and represent a wide spectrum of geomechanical conditions in the repository nearfield, ranging from *expected to unfavourable conditions* (abbreviations: d – drained, BE/LE – best estimate / lower estimate, pp – post peak strength, S_{ref} / S_{hmin} – stress ratios representing the reference/ minimum stress regime).

Parameter	Minimum	Reference	Maximum
Young's modulus (I) (GPa)	3.0	4.0	7.0
Young's modulus (II) (GPa)	8.0	13.0	16.0
Poisson's ratio (I)	0.1	0.2	0.43
Poisson's ratio (II)	0.13	0.26	0.38
Cohesion (MPa)	0.5	1.3	2.0
Friction angle (degree)	20.0	24.0	28.0

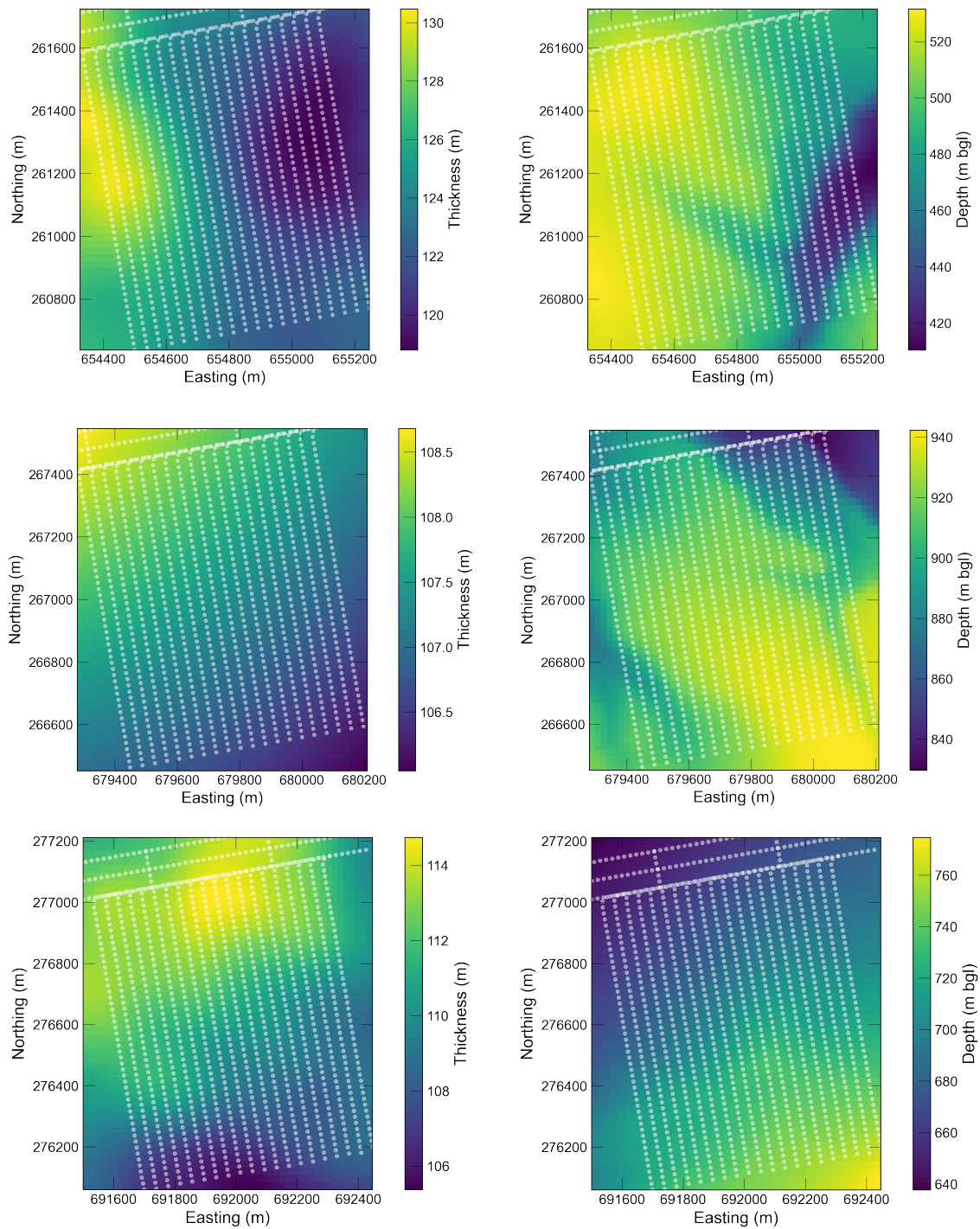


Fig. 5-2: Calculations of the vertical extent $D_{\text{zmax,EDZ}}$ of the EDZ were performed on a regular grid displaying the footprint of the HLW-disposal field of the provisional repository projects HLW-JO, HLW-NL and HLW-ZNO

Top figure: JO, middle: NL, bottom: ZNO

Left row: thickness of the Opalinus Clay formation. Right row: HLW repository depth

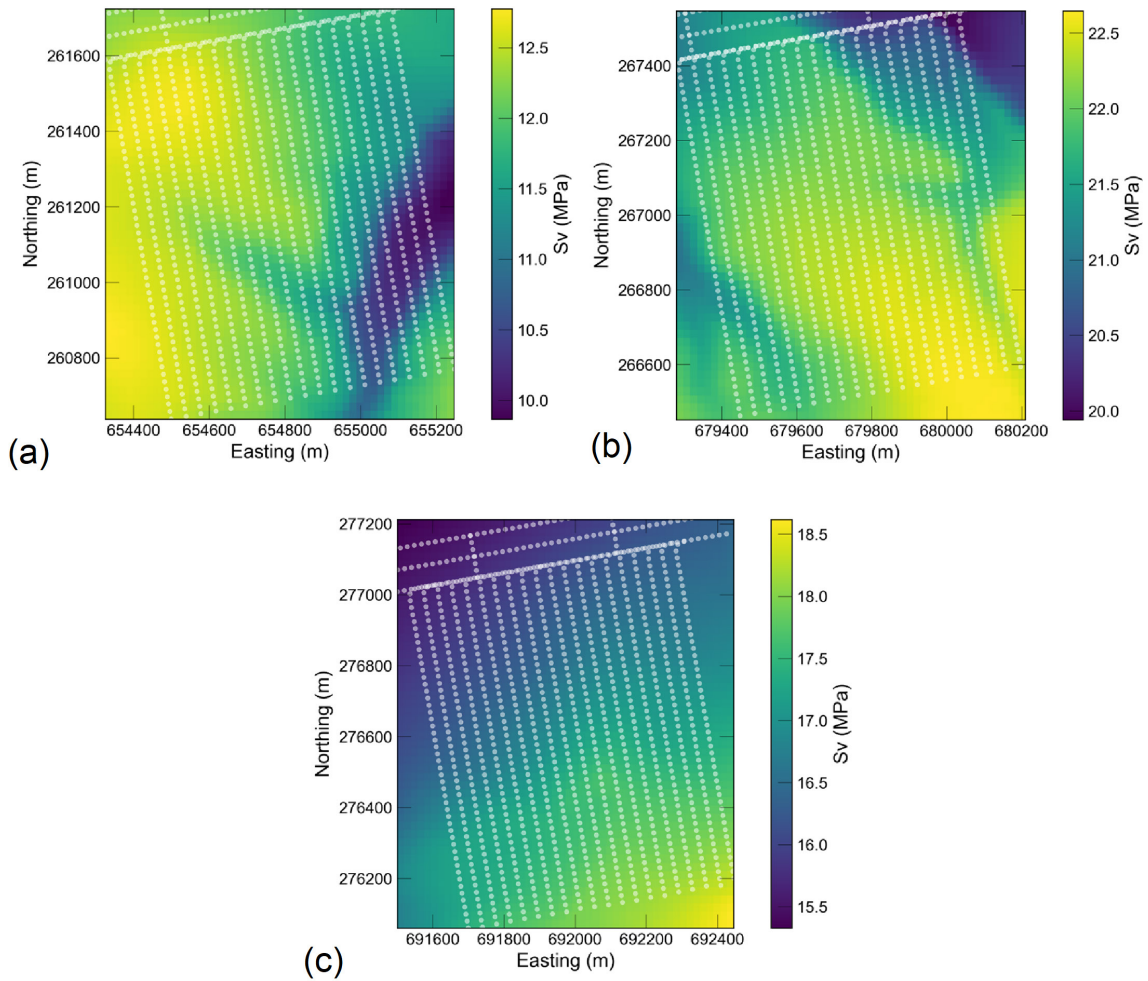


Fig. 5-3: Vertical stress distribution at repository level the HLW-disposal field of the repository projects HLW-JO (top left), HLW-NL (top right) and HLW-ZNO (bottom)

For each repository, the vertical extent $D_{zmax,EDZ}$ of the EDZ is calculated on a 50 cells by 50 cells structured grid enclosing the HLW disposal field at the centre of the Opalinus Clay (Fig. 5-2). Vertical and horizontal stresses are calculated on the same grid (Fig. 5-3). A Monte Carlo simulation is performed to evaluate the influence of key parameters on the vertical EDZ extent, in particular the anisotropic Young's moduli and Poisson's ratios (perpendicular and parallel to bedding), the coefficient of friction and the cohesion. The distributions of the parameters considered are based on the geomechanical reference parameters, given in Tab. 5-1, which are used to generate a set of 10,000 Latin Hypercube samples, as shown in Fig. 5-4 for the HLW-JO project (scatter plots from all repository projects are presented in App. D). For each sample, the vertical and horizontal stress values are randomly chosen (with repetition) among the 2,500 cells composing the structured grid. The diameter of the emplacement tunnel is assumed to be 3.9 m for all sites.

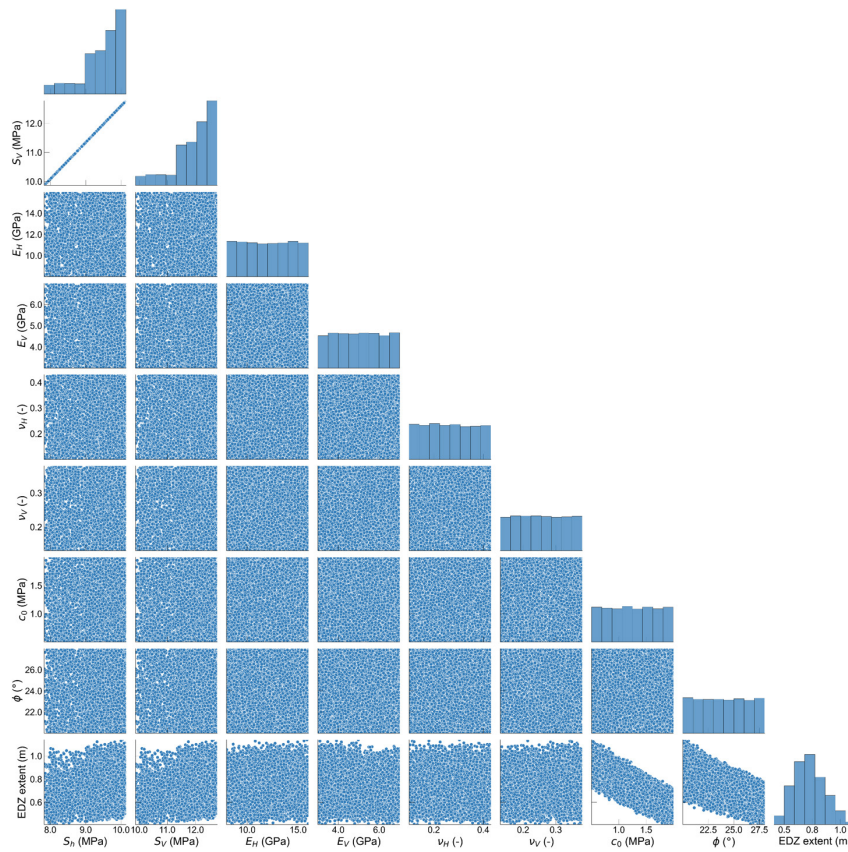


Fig. 5-4: Scatter plot matrix of the 10,000 Latin Hypercube samples for all model parameters considered for the HLW-JO project

The subplots along the diagonal show the marginal distributions (as a histogram) of the samples, while the off-diagonal subplots of the matrix represent a pairwise scatter plot between the different model parameters.

The multiple calculations of vertical extent of the EDZ on a regular grid of the HLW-disposal fields lead to histograms of $D_{z,EDZ}$ for the three provisional repository projects HLW-JO, HLW-NL and HLW-ZNO. The results are displayed in Fig. 5-5, representing bandwidth of $D_{z,EDZ}$ (graphs in the left column) and the dimensionless RPI performance index (right column). The vertical extent of the EDZ ranges between 0.4 and 1.1 m for HLW-JO with a mean value $\langle D_{z,EDZ} \rangle = 0.7$ m. For HLW-NL ($\langle D_{z,EDZ} \rangle = 0.9$ m) and HLW-ZNO ($\langle D_{z,EDZ} \rangle = 0.8$ m) the extent is slightly higher due to the greater repository depth. The results match well with the fracture network simulations, which were carried out in the context of the performance assessment for the prospect repository at the Haberstal site (Nagra 2024l, see also App. D.5).

Performance indices RPL are expressed in terms of the 95th percentile (P95) of the RPI frequency distribution (“histogram”). The RPI_{P95} -values are low for each of the repository projects HLW-JO ($RPI_{P95} = 0.625$), HLW-NL ($RPI_{P95} = 0.675$) and HLW-ZNO ($RPI_{P95} = 0.675$), indicating favourable barrier performance of the host rock at all sites. The RPI_{P95} -value is smallest for HLW-JO because the thickness of the Opalinus Clay is the largest. The RPI_{P95} -values are presented in Tab. 5-2 as input for the qualitative assessment of the CRZ based on the 13 SGT criteria (Nagra 2024h).

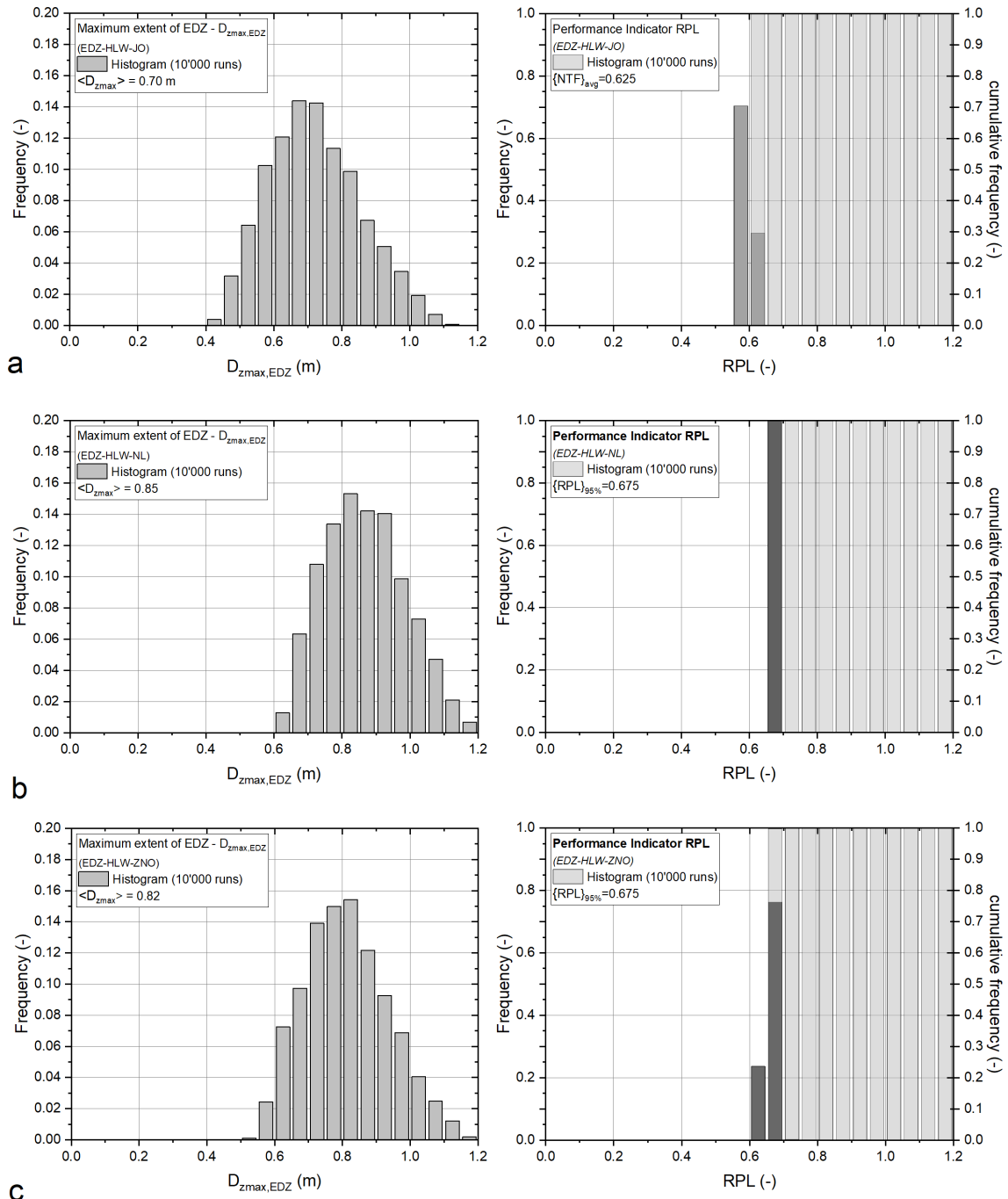


Fig. 5-5: Indicator of vertical extension of the EDZ above/below the HLW tunnels, based on 10,000 simulations for the repository projects HLW-JO, HLW-NL and HLW-ZNO

Determination of the vertical extent of EDZ for the site-specific L/ILW projects

The assessment aspect *Effects of the EDZ* is also evaluated for the provisional L/ILW repository projects by numerical calculation of the vertical extent of the EDZ above / below the L/ILW emplacement caverns. The general modelling approach corresponds to the modelling approach for the HLW drifts, assuming a circular L/ILW cavern with a diameter of 12.2 m. For each site, the vertical extent $D_{z,EDZ}$ of the EDZ and vertical and horizontal stresses were calculated on a 50 cells by 50 cells structured grid (2,500 cells in total) displaying the footprint of the L/ILW-disposal field of the repository projects L/ILW-JO, L/ILW-NL and L/ILW-ZNO as shown in Fig. 5-6 and Fig. 5-7. The same geomechanical data sets as for the HLW repository projects were used for the L/ILW configurations, covering the *expected* and the *unfavourable* conditions at the 3 sites (Tab. 5-1). A Monte Carlo simulation was performed to evaluate the influence of key parameters on the vertical EDZ extent, in particular the anisotropic Young's moduli and Poisson's ratios (perpendicular and parallel to bedding), the coefficient of friction and the cohesion. The distributions of the parameters considered are used to generate a set of 10,000 Latin Hypercube samples, as shown in Fig. 5-8 for the L/ILW-JO project (scatter plots from all repository projects are presented in App. D). For each sample, the vertical and horizontal stress values are randomly chosen (with repetition) among the 2,500 cells composing the structured grid.

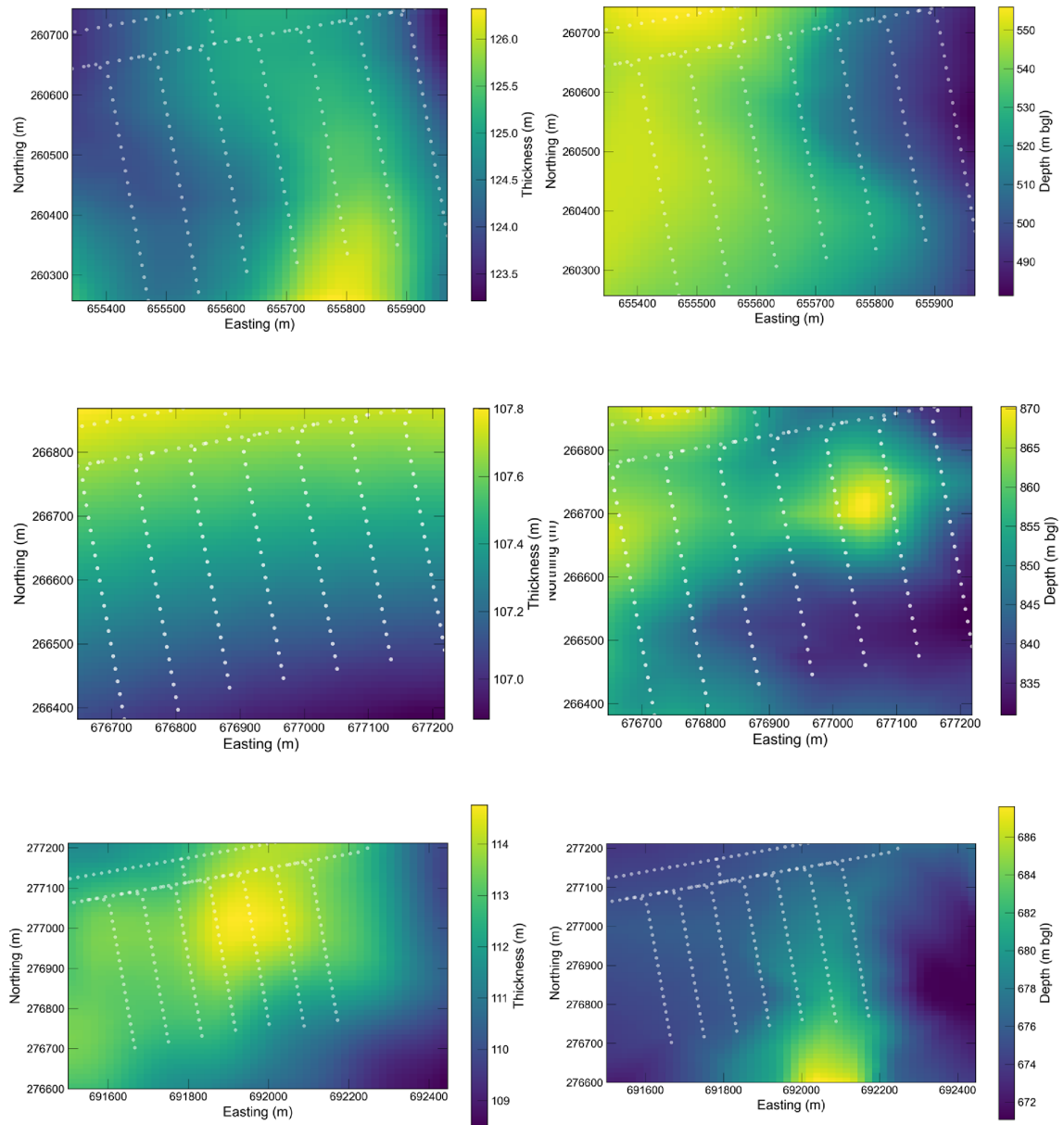


Fig. 5-6: Calculations of the vertical extent $D_{zmax,EDZ}$ of the EDZ were performed on a regular grid displaying the footprint of the L/ILW-disposal field of the provisional repository projects L/ILW-JO, L/ILW-NL and L/ILW-ZNO

Top figure: JO, middle: NL, bottom: ZNO.

Left row: thickness of the Opalinus Clay formation. Right row: L/ILW repository depth.

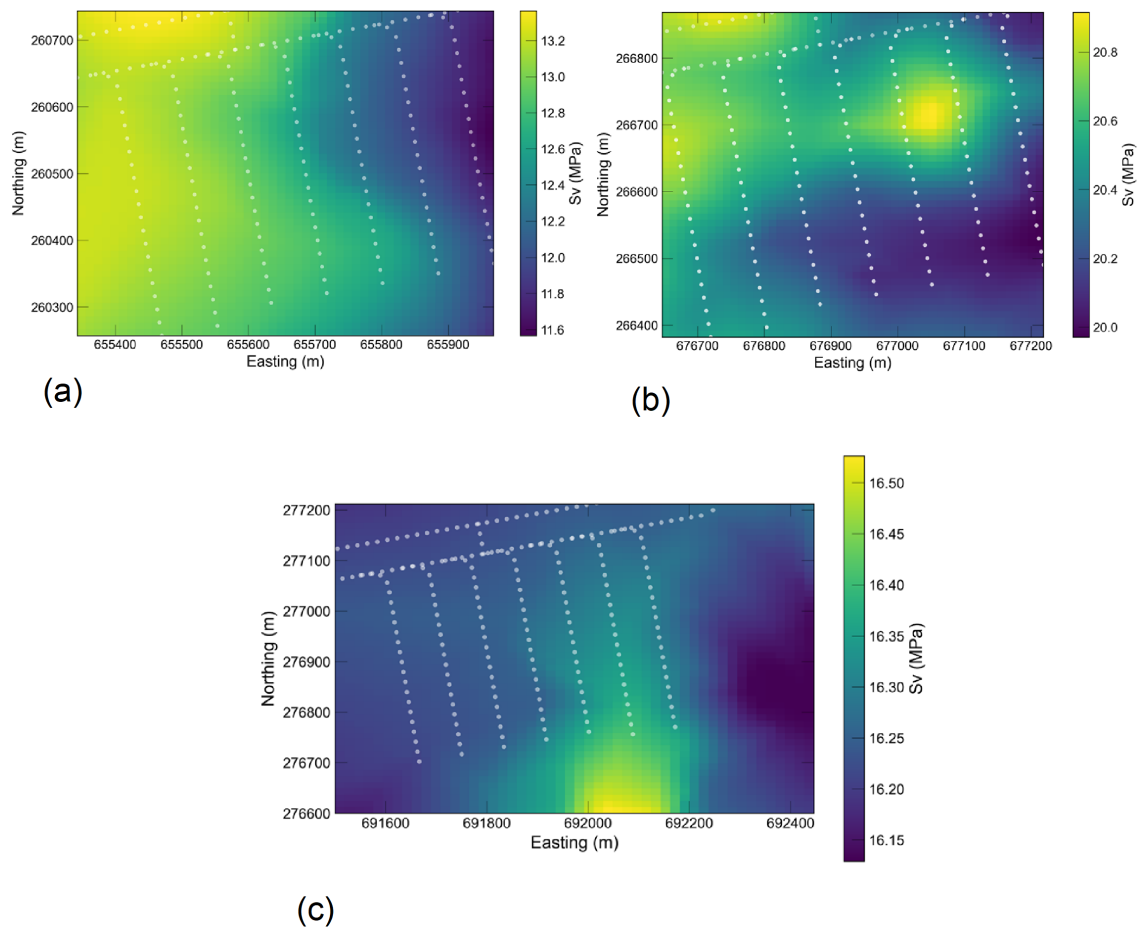


Fig. 5-7: Vertical stress distribution at repository level the ILW-disposal field of the repository projects ILW-JO (top left), ILW-NL (top right) and ILW-ZNO (bottom)

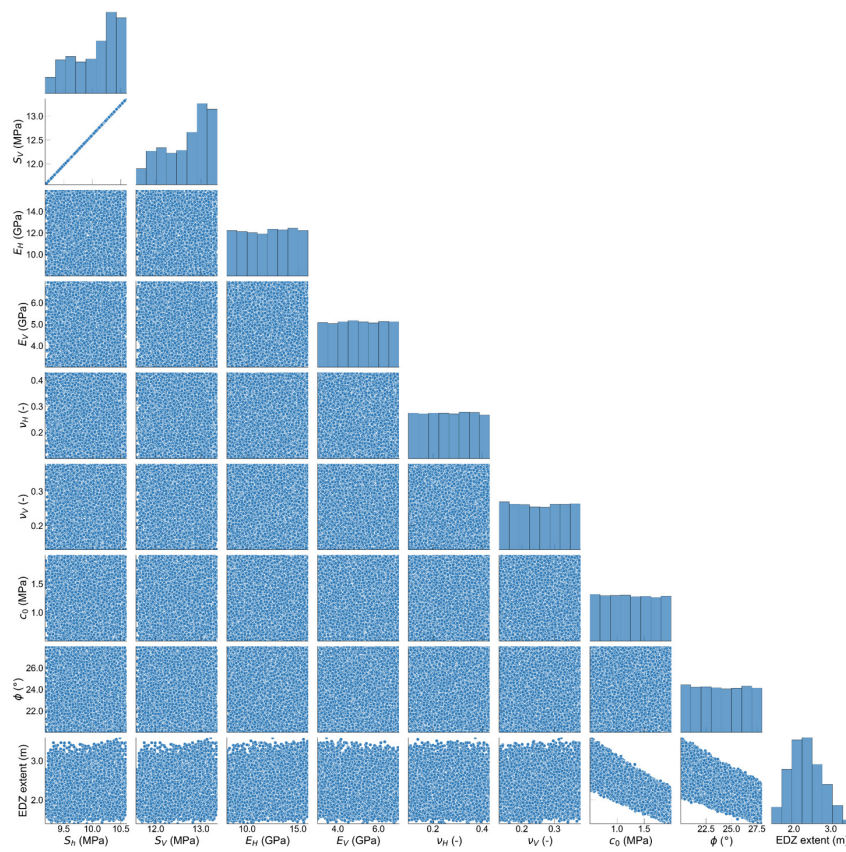


Fig. 5-8: Scatter plot matrix of the 10,000 Latin Hypercube samples for all model parameters considered for the L/ILW-JO project

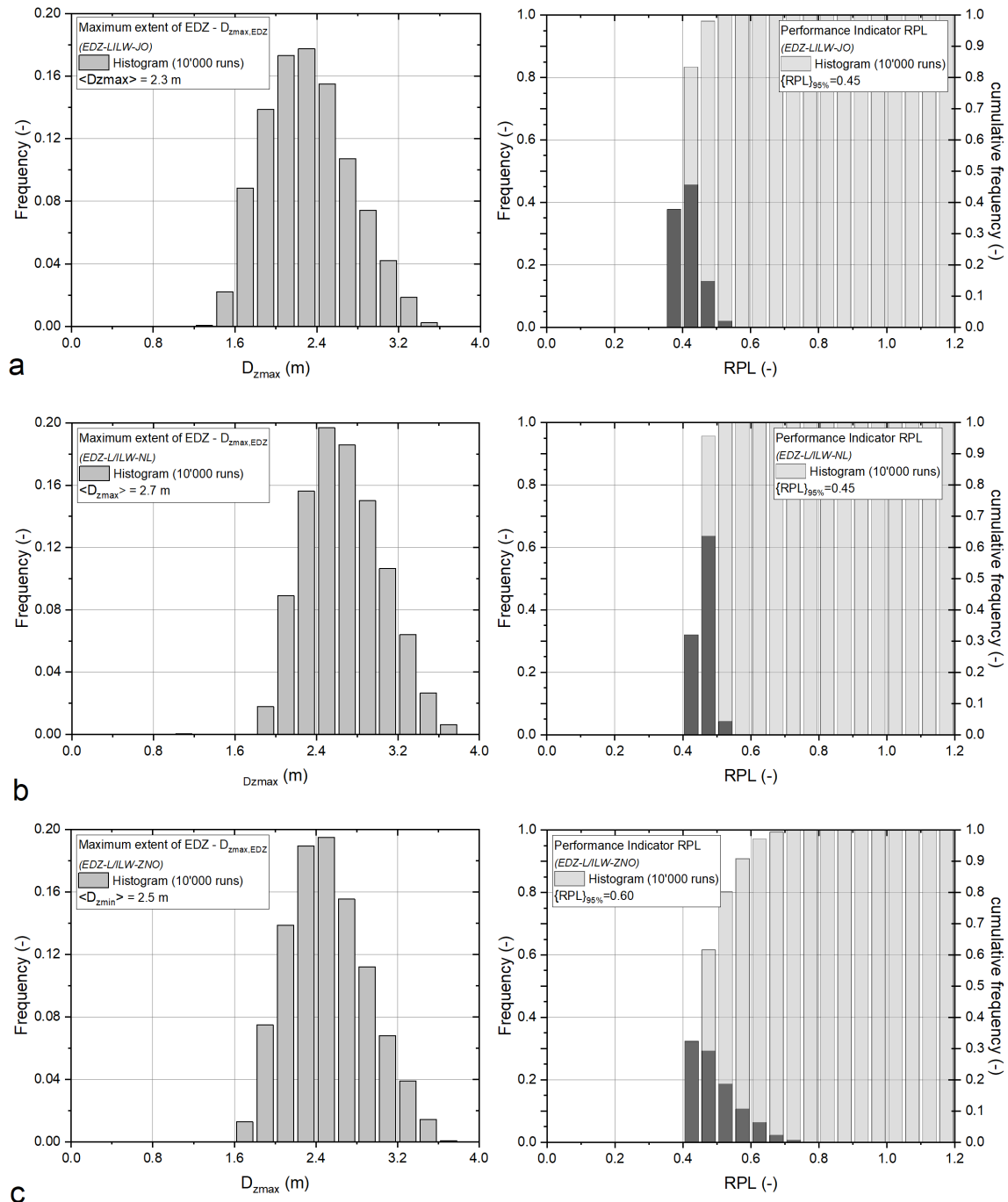


Fig. 5-9: Indicator of vertical extension of the EDZ above/below the L/ILW caverns, based on 10,000 simulations for the repository projects L/ILW-JO, L/ILW-NL and L/ILW-ZNO

The multiple calculations of vertical extent of the EDZ on a regular grid of the L/ILW-disposal fields lead to histograms of $D_{z,EDZ}$ for the three repository projects L/ILW-JO, L/ILW-NL and L/ILW-ZNO. The results are displayed in Fig. 5-9, representing bandwidth of $D_{z,EDZ}$ (graphs in the left column) and the dimensionless RPL performance index (right column). The vertical extent of the EDZ ranges between 1.6 and 3.3 m for L/ILW-JO with a mean value $\langle D_{z,EDZ} \rangle = 2.3$ m. For L/ILW-NL ($\langle D_{z,EDZ} \rangle = 2.7$ m) and L/ILW-ZNO ($\langle D_{z,EDZ} \rangle = 2.5$ m) the extent is slightly higher

due to the greater repository depth. The results match well with the fracture network simulations, which were carried out in the context of the performance assessment for the prospect repository at the Haberstal site (NTB 24-22, see also App. D.5).

Performance indices RPL are expressed in terms of the 95th percentile (P95) of the RPI frequency distribution (“histogram”). The RPI_{P95}-values are low for each of the repository projects L/ILW-JO (RPI_{P95} = 0.45), L/ILW-NL (RPI_{P95} = 0.45) and L/ILW-ZNO (RPI_{P95} = 0.60), indicating favourable barrier performance of the host rock at all sites. The RPI_{P95}-value is smallest for L/ILW-JO because the thickness of the Opalinus Clay is the largest. The RPI_{P95}-values are presented in Tab. 5-2 as input for the qualitative assessment of the CRZ based on the 13 SGT criteria (Nagra 2024h, see also App. D.5).

Length of release path in the intact host rock – input for the qualitative assessment of the CRZ based on the 13 SGT criteria

In the context of the qualitative assessment of the CRZ based on the 13 SGT criteria (Nagra (2024h), the assessment aspect *Effects of the EDZ* is evaluated by numerical calculation of the vertical extent of the EDZ above / below the emplacement rooms, both for the HLW and the L/ILW repository projects. The corresponding performance index RPL (“reduced path length in the intact host rock”) is provided in Tab. 5-2 as input for the qualitative assessment of the CRZ, documented in Nagra (2024h).

Tab. 5-2: Performance index RPL for the model-based assessment of the CRZ, corresponding to the three HLW and L/ILW repository projects, contributing to the criterion 2.3 “repository induced effects”

Note that the minimal values of the bars are reported here for HLW and L/ILW, whereas in the text and figures for HLW, midpoints of bars are used.

Performance indicator	JO HLW	NL HLW	ZNO HLW	JO L/ILW	NL L/ILW	ZNO L/ILW	Remarks
Assessment aspect: length of release path in the intact host rock							
RPL (normalised length of release path in the intact host rock)	0.60	0.65	0.65	0.45	0.45	0.60	
	criterion 2-3 (Repository induced effects)						

5.1.2 Thermal effects

Decay heat from SF and HLW will increase temperatures within and around the repository for long periods of time. From a long-term safety perspective, the key aspects to address are the thermal impacts on the host rock and on the bentonite buffer, respectively (Nagra 2024l). Adverse effects on the mechanical integrity of the host rock are expected, when (i) the peak temperature in the host rock exceeds significantly the maximum value attained during its burial history or (ii) when thermally induced pore pressures in the repository nearfield exceed the shear strength of the rock. The impacts of repository-generated heat on the safety functions of the multi-barrier system of an HLW repository are discussed in length in Leupin et al. (2016a) and in Nagra (2024l).

In the L/ILW repository heat is produced mainly by hydration processes, whereas the effects of radioactive decay of the waste are negligible. Further discussion concerning the thermal impacts on the multi-barrier system of an L/ILW repository are reported in Leupin et al. (2016b). In the context of the site comparison, thermal aspects are not relevant for distinguishing the L/ILW repository projects in the three sites.

Quantitative performance indicator “*thermally induced porewater overpressures in the host rock*”

At none of the candidate HLW sites it is expected that the peak temperature in the Opalinus Clay around the HLW drifts will exceed the so-called paleo-temperature, which is the maximum value attained during its burial history. On the other hand, thermally induced pore pressures will develop in the repository nearfield, which could give rise to unfavourable stress conditions in the host rock above the HLW drifts. Therefore, “*thermally induced porewater overpressures in the host rock*” are used as a quantitative performance indicator for the evaluation of the mechanical integrity of host rock, when subjected to thermal loads. The corresponding dimensionless performance index FPI_{heat} (failure potential of the intact host rock – thermal effects) is defined in the following paragraphs.

Assuming the applicability of the Mohr-Coulomb criterion for shear failure, the FPI indicator can be expressed as:

$$FPI = \frac{\tau}{\tau_{\max}} = \frac{q}{q_{\max}}$$

where τ is shear stress and $\tau_{\max}$ is the maximum shear stress that can be accommodated by the rock without failure; q and $q_{\max}$ are the corresponding deviator stresses. According to the Mohr-Coulomb relationship, the deviator stress at failure $q_{\max}$ depends on mean total stress p and porewater pressure p_w :

$$q_{\max} = a + M \cdot p' = a + M \cdot (p - p_w))$$

where a and M are the intercept and slope of the Mohr-Coulomb failure line. An in-depth discussion of FPI indicator is found in 7E.1. The FPI indicator is used for both, heat and gas induced porewater overpressures (FPI_{heat} , FPI_{gas}).

Probabilistic assessments – model set up, source terms and parameters

The model-based assessment of the thermal impact on repository performance was carried out for the three site provisional repository projects HLW-JO, HLW-NL and HLW-ZNO in a probabilistic framework. The two-phase modelling of the thermo-hydraulic (TH) evolution of the repository nearfield were performed using the EOS5 Equation-of-State module of the TOUGH3 code (Jung et al. 2018) for simulating the isothermal or non-isothermal, fully coupled flow and transport of hydrogen and water in porous media. A 2-D model set-up was elaborated for the probabilistic assessment, representing a vertical cross-section through the centre of the HLW repository. The meshes of the HLW repository projects at the three sites are presented in Fig. 5-10. Further technical details about the numerical code and the model set-ups are found in Nagra (2024e).

The parameter assignment for the deterministic / probabilistic assessments was based on the reference values for the two-phase properties provided in Nagra (2024g) and Nagra (2024e). Tab. 5-3 presents an overview of relevant TH parameters of the EBS materials and the host rock,

respectively. These reference values are forming input for the so-called *base case* simulation, which is the deterministic case used in criterion 2.3 for the calculation of the site-specific performance indicators “*thermally induced porewater overpressures in the host rock*” and the corresponding performance indices FPI_{heat} . The full data set of reference parameters used in the probabilistic assessments is given in Nagra (2024e).

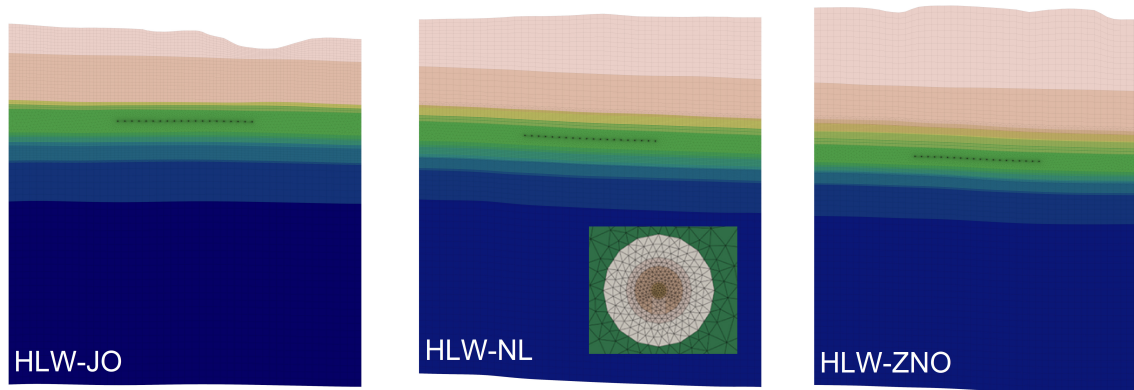


Fig. 5-10: Meshes of the models used for the simulation of 2-D simulation of thermally induced porewater overpressures in the HLW nearfield

2-D vertical cross-section through the centre of the HLW repository: repository projects HLW-JO (left), HLW-NL (middle) and HLW-ZNO (right). Mesh refinement in the HLW nearfield is shown in the close-up.

Monte Carlo simulations were performed to evaluate the influence of uncertainty of key parameters on the performance indicator FPI and estimate the confidence intervals around the best estimate. These simulations were carried out to substantiate criterion 3.3, referring to the predictability of long-term changes (see Tab. 2-1). For the heat simulations, parameters were selected based on their sensitivity to maximum pressures in the Opalinus Clay (Papafotiou et al. 2017). Based on previous probabilistic sensitivity analyses (Papafotiou et al. 2017), the following parameters were identified as the most sensitive ones: the permeability, porosity, pore compressibility, and saturated thermal conductivity of the Opalinus Clay, and the saturated thermal conductivity of the EDZ. The parameters considered were used to generate a set of 100 Latin Hypercube samples, as depicted in Fig. 5-11. Further details about parameter correlations and the assumed property distributions are given in Nagra (2024e).

Tab. 5-3: Reference hydraulic and thermal parameters of materials in the repository nearfield, which are relevant for the thermally induced overpressures around the HLW drifts
Extracted from Nagra (2024e).

ρ is the density, $T_{c,dry}$ and $T_{c,wet}$ are the thermal conductivity in unsaturated and saturated conditions, respectively, T_x is the thermal expansivity, K_h and K_v are the horizontal and vertical permeabilities, respectively, ϕ is the porosity, and C_p is the pore compressibility.

Material	ρ [kg/m ³]	$T_{c,dry}$ [W/m/ °C]	$T_{c,wet}$ [W/m/ °C]	T_x [1/ °C]	K_h [m ²]	K_v [m ²]	ϕ [-]	C_p [1/Pa]
CAN	7,850	52.5	52.5	1.5E-5	1E-20	1E-20	0.001	0
PELL	2,699	0.35	1.3	2.5E-5	3.5E-20	3.5E-20	0.33	3E-9
BLOCK					2.5E-21	2.5E-21	0.33	
LINER	2,650	1.4	2.3	1.5E-5	1E-18	1E-18	0.1	7E-10
EDZ	2,700	1.36	1.7	1.7E-5	4.54E-20	9.08E-21	0.12	1.7E-9
OPA	2,700	1.36	1.7	1.7E-5	4.54E-20	9.08E-21	0.12	1.7E-9

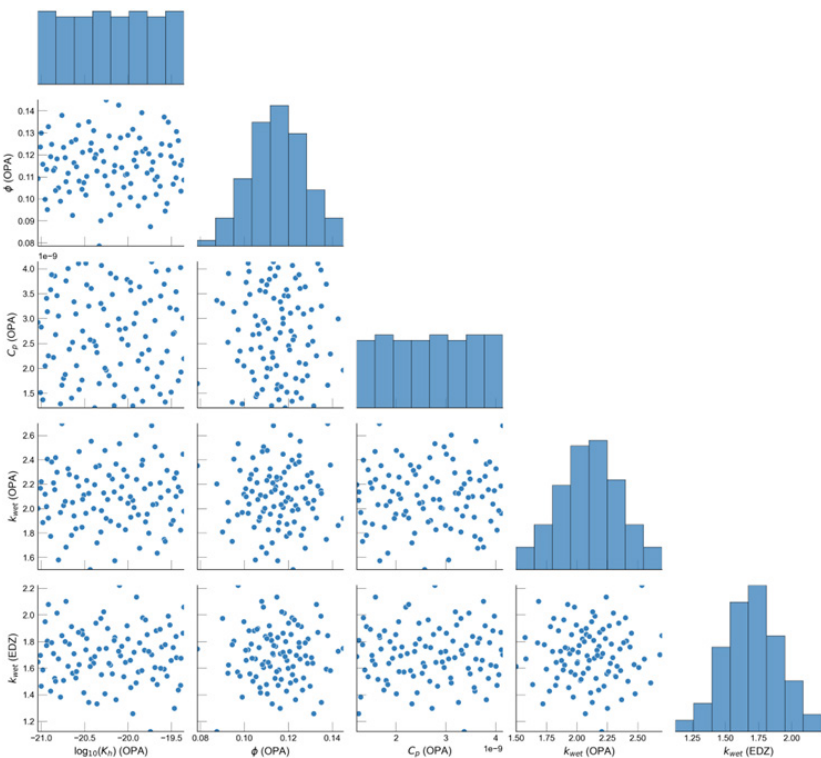


Fig. 5-11: Scatter-plot matrix of the 100 Latin Hypercube samples for all model parameters
From Nagra (2024e)

The subplots along the diagonal show the marginal distributions (as a histogram) of the samples, while the off-diagonal subplots of the matrix represent a pairwise scatter plot between the different model parameters.

Boundary and initial conditions typically correspond to near hydrostatic pressure conditions with constant pressure at the top of the model equal to atmospheric pressure. Temperature was fixed to 10 °C at the top while a 120 mW/m² basal heat flux was imposed at the bottom of the Permo-Carbonate layer. Thus, the top boundary was opened to flow, and the bottom boundary was closed to flow where the constant heat flux was imposed. All lateral boundaries were also assumed to be closed to flow.

The model domain was assumed to be initially fully water saturated. The initial pressure assigned to the model elements (including boundary elements) were calculated on the elevation respectively depth below ground level of each element assuming a 9.81 kPa/m vertical gradient, and initial temperature was calculated assuming a 0.043 °C/m geothermal gradient. For all simulations, a steady-state run was first carried out until pressure and temperature reach equilibrium (corresponding to undisturbed rock prior to repository construction).

In simulations of gas and heat transport, a 2-year long ventilation run was also performed where atmospheric pressure and a temperature of 28 °C were prescribed in the open tunnels (i.e., materials CAN, PELL, BLOCK, and LINER). For this ventilation phase, the initial water saturation of the emplacement tunnel elements was assumed to be 50%, except for the liner for which a 70% initial water saturation is prescribed.

The transition from ventilation to emplaced tunnels was assumed instantaneous. At emplacement the canister elements were assumed to be fully saturated with gas, while the bentonite buffer (PELL) and pedestal (BLOCK) elements were prescribed an initial water saturation of 20% and 50%, respectively (Nagra 2024e).

In the context of the site selection process, the model-based assessments of the repository induced effects were carried out with reference source terms for heat and gas generation according to Nagra (2024g) and Nagra (2024e) (Fig. 5-12). Gas generation rates were calculated using the gas generation tool (Nagra 2024g) for HLW components and multiplied by the density of hydrogen (0.082 kg/m³). Heat and gas generated by wastes were volumetrically distributed to canister elements (CAN), and gas generated by tunnels to liner elements (LINER).

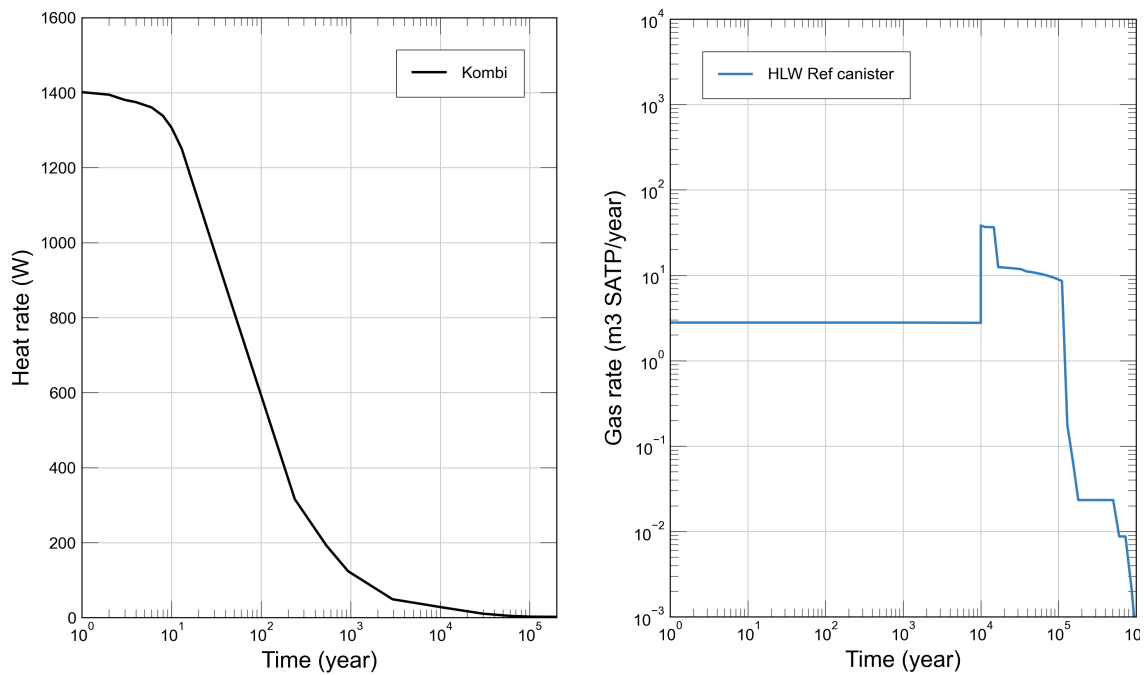


Fig. 5-12: Thermal source terms (left) and gas source terms (right) used for the indicator-based assessment of repository induced effects

See also Nagra (2024g) and Nagra (2024e).

Assessment of the thermal effects for the site-specific HLW projects

The model-based assessment of the thermal impact on repository performance was carried out for the three provisional repository projects HLW-JO, HLW-NL and HLW-ZNO, feeding in two different criteria:

- Criterion 2.3 (repository induced effects): the deterministic base case simulations for the 3 sites are compared with each other by use of the calculated performance index FPI.
- Criterion 3.3 (predictability of long-term changes): probabilistic simulations are carried out and the histograms of the FPI indicator are calculated for each site. The 95th percentile value ($FPI_{heat,P95}$) of the FPI_{heat} histogram is used.

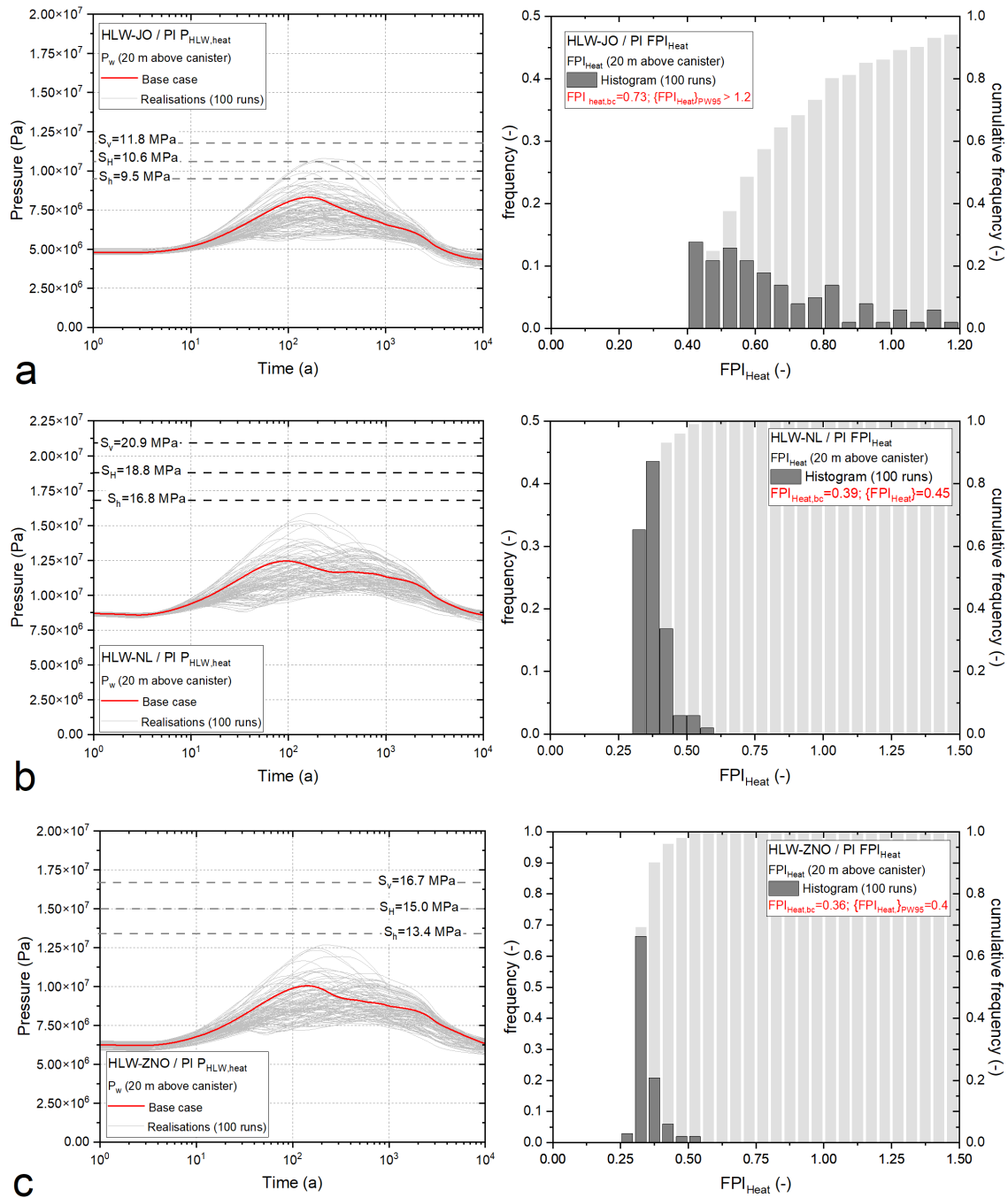


Fig. 5-13: Probabilistic simulations of thermally induced porewater overpressure in the host rock (left column) and histogram of the dimensionless FPI indicator (right column)

Results for the provisional HLW repository projects in JO (a), NL (b) and (c) ZNO. The FPI values calculated for the deterministic base case simulation correspond to criterion 2.3, whereas the P95-values are used in the evaluation of criterion 3.3.

The deterministic base case simulation and the probabilistic calculations of the evolution of pore pressure in the repository nearfield were carried out for the three repository projects HLW-JO, HLW-NL and HLW-ZNO. The results are shown in Fig. 5-13. The three graphs in the left column present transients of pore pressure at a control point 20 m above the HLW drift in the centre of the repository. The red line indicates the pore pressure evolution of the deterministic base case simulation, which is relevant for the evaluation of criterion 2.3. The family of gray lines represents the Monte Carlo simulations, contributing to the assessment of prediction uncertainties in criterion 3.3. In each diagram, the magnitudes of the three principal stress component S_h , S_H and S_v are indicated, referring to the initial stress at the control point in the host rock 20 m above the HLW drift. The derivation of failure stress is based on the Mohr-Coulomb relationship, assuming the residual strength parameters for the Opalinus Clay, which are provided in Nagra (2024c) (see also App. E). The thermally induced overpressures of the base case (red line) reach a maximum of about 3.5 – 4 MPa above hydrostatic, which is similar for all repository projects. However, for HLW-JO the thermal peak pressure is significantly closer to the minimum stress S_h than for the other configurations HLW-NL and HLW-ZNO. The minimum stress is often seen as a pessimistic estimator for the pore pressure at failure and gives a qualitative indication for lower safety margins of the HLW-JO project. The failure potential FPI is a better estimator, because it takes into account not only the local stress conditions but also the rock strength. The calculation of the FPI value for the base cases of the 3 configurations confirms this, revealing a significantly higher failure potential for HLW-JO ($FPI_{heat} = 0.73$), whereas the failure potential for HLW-NL ($FPI_{heat} = 0.39$) and HLW-ZNO ($FPI_{heat} = 0.36$) remains moderate.

The three graphs in the right column of Fig. 5-13 present histograms of the FPI index, representative for the failure potential at a control point 20 m above the HLW drift in the centre of the repository. The 95th percentile of the FPI frequency distribution is one of the performance indices for the evaluation of criterion 3.3. The comparison of the histograms of the 3 repository configurations indicates clearly, that the HLW-JO repository configuration is much more prone to failure, when geomechanical rock properties or stress conditions at the site are uncertain. A significant number of simulation cases indicate failure ($FPI \geq 1$), whereas significant safety margins are derived for the configurations HLW-NL ($FPI_{heat,P95} = 0.45$) and HLW-ZNO ($FPI_{heat,P95} = 0.4$). The reason for this is obviously the larger repository depth.

Thermally induced porewater overpressures in the host rock – input for the qualitative assessment of the CRZ based on the 13 SGT criteria

In the context of the qualitative assessment of the CRZ based on the 13 SGT criteria (Nagra (2024h)), the assessment aspect *thermal effects* is evaluated by TH simulations of the pore pressure evolution in the HLW repository nearfield. The corresponding performance index FPI_{Heat} (“*failure potential of the intact host rock – thermal effects*”) is provided in Tab. 5-4 as input for the qualitative assessment of the CRZ, documented in Nagra (2024h).

Tab. 5-4: Performance indices FPI for the model-based assessment of the CRZ, corresponding to the provisional HLW repository projects for the criteria 2.3 “Repository induced effects” and 3.3 “Predictability of long-term changes”

Performance index	JO HLW	NL HLW	ZNO HLW	JO L/ILW	NL L/ILW	ZNO L/ILW	Remarks
Performance indicator: “Thermally induced porewater overpressure in the host rock”							
FPI _{Heat} (Failure potential for intact host rock)	0.73	0.39	0.36	-	-	-	Deterministic base case simulation
	criterion 2.3 (Repository induced effects)						
FPI _{Heat,P95} (Failure potential for intact host rock)	>1.2	0.45	0.40	-	-	-	100 Monte Carlo simulations
	criterion 3.3 (Predictability of long-term changes)						

5.1.3 Gas effects

Gas will be generated in the HLW and L/ILW repository by anaerobic corrosion of metals and degradation of organic matter. From a performance assessment perspective, the accumulation of gases and gas pressure build-up in the backfilled repository structures could impair the mechanical integrity of the engineered barriers and the host rock, if gas pressures exceed the failure stresses of the barrier components. Furthermore, porewater overpressures in the emplacement rooms could enhance the release of dissolved radionuclides. Both safety issues are addressed in criterion 2.3 (repository induced effects) as part of the assessment aspect “*gas impacts*”.

Quantitative performance indicator “gas induced porewater overpressures in the host rock”

The enhanced release of dissolved radionuclides by the build-up of overpressures in the backfilled emplacement rooms of a repository has been proven to be of very limited safety relevance (e.g., Nagra 2024l). On the other hand, gas induced pore pressures will develop in the repository nearfield, which could give rise to unfavourable stress conditions in the host rock above the emplacement rooms (HLW drifts, L/ILW caverns). Therefore, “*gas induced porewater overpressures in the host rock*” are used as a quantitative performance indicator for the evaluation of the mechanical integrity of host rock, when subjected to gas overpressures. The corresponding dimensionless performance index FPI_{Gas} (failure potential of the intact host rock – gas effects) is defined as presented in Section 5.1.2. However, the highest gas overpressures are expected to occur in the HLW- and L/ILW emplacement rooms, whereas the thermal effects create the overpressures in the host rock around 20 m above the HLW drifts. The control point for the calculation of the FPI is a grid cell above the central HLW drift at the interface between EDZ and intact host rock. An in-depth discussion of the FPI index and the corresponding control points for FPI_{heat} and FPI_{Gas} is found in App. E.

Probabilistic assessments – model set up, source terms and parameters for the HLW projects

The model-based assessment of the gas impact on repository performance was carried out for the three provisional repository projects HLW-JO, HLW-NL and HLW-ZNO using the same models (Fig. 5-10), the same parameters (Tab. 5-3) and the same source terms (Fig. 5-12) that were presented in Section 5.1.2. Likewise, the reference values are forming input for the so-called *base case* simulation, which is the deterministic case used in criterion 2.3 for the calculation of the site-specific performance indicators “*gas induced porewater overpressures in the host rock*” and the corresponding performance indices FPI_{gas} .

Assessment of the gas effects for the site-specific HLW projects

Analogous to the procedure for assessing the thermal impacts, the model-based assessment of the gas impact on repository performance was carried out for the three provisional repository projects HLW-JO, HLW-NL and HLW-ZNO, feeding in two different criteria:

- Criterion 2.3 (repository induced effects): the deterministic base case simulations for the 3 sites are compared with each other by use of the calculated performance index FPI_{gas} .
- Criterion 3.3 (predictability of long-term changes): probabilistic simulations are carried out and the histograms of the FPI indicator are calculated for each site. The 95th percentile value ($FPI_{\text{gas},P95}$) of the FPI_{gas} histogram is used.

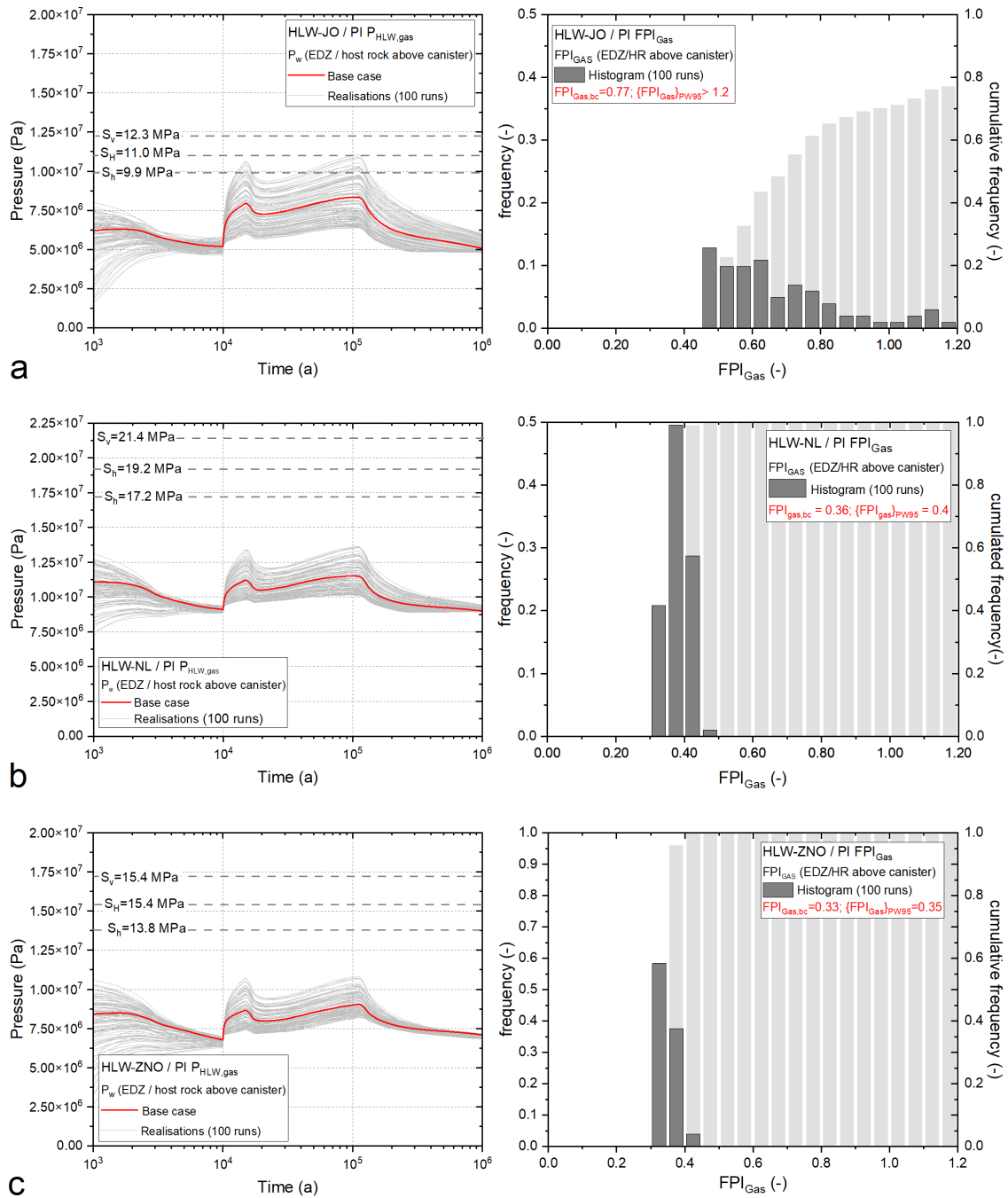


Fig. 5-14: Probabilistic simulations of thermally induced porewater overpressure in the host rock (left column) and histogram of the dimensionless FPI indicator (right column)

Results for the three provisional HLW repository projects in JO (a), NL (b) and (c) ZNO. The FPI values calculated for the deterministic base case simulation corresponds to criterion 2-3, whereas the P95-values are used for the evaluation of criterion 3-3.

The deterministic base case simulation and the probabilistic calculations of the evolution of pore pressure in the repository nearfield were carried out for the three repository projects HLW-JO, HLW-NL and HLW-ZNO. The results are shown in Fig. 5-14. The three graphs in the left column present transients of pore pressure at a control point at the interface between EDZ and intact host rock above the HLW drift in the centre of the repository. The red line indicates the pore pressure evolution at the control point for the deterministic base case simulation, which is the relevant case for the evaluation of criterion 2.3. The pressure transient exhibits two peaks after $\approx 20,000$ and $100,000$ years, which are caused by the characteristic changes of the gas generation rates (see Fig. 5-12). The second peak is slightly higher, and therefore used to calculate the FPI index. The family of gray lines represents the Monte Carlo simulations, contributing to the assessment of prediction uncertainties in criterion 3.3. In each diagram, the magnitudes of the three principal stress component S_h , S_H and S_v are indicated, referring to the initial stress at the control point, located at the interface between EDZ and host rock above the HLW canister. The derivation of failure stress is based on the Mohr-Coulomb relationship, assuming the residual strength parameters for the Opalinus Clay, which are provided in Nagra (2024c) (see also App. E). The gas induced overpressures of the base case (red line) reach a maximum of about $3 - 3.5$ MPa above hydrostatic, which is similar for all repository projects. Similar to the thermally induced overpressures, the gas-related simulations show for HLW-JO that the gas peak pressure is significantly closer to the minimum stress S_h than for the other configurations HLW-NL and HLW-ZNO, indicating a higher risk of gas induced failure. The calculation of the FPI value for the base cases of the 3 configurations confirms this, revealing a significantly higher failure potential for HLW-JO ($FPI_{Gas} = 0.77$), whereas the failure potential for HLW-NL ($FPI_{Gas} = 0.36$) and HLW-ZNO ($FPI_{Gas} = 0.33$) remains moderate.

The three graphs in the right column of Fig. 5-14 present histograms of the FPI index, representative for the failure potential at a control point 20 m above the HLW drift in the centre of the repository. The 95th percentile of the FPI frequency distribution is one of the performance indices for the evaluation of criterion 3.3. The comparison of the histograms of the 3 repository configurations indicates clearly that the HLW-JO repository configuration is much more prone to failure, when geomechanical rock properties or stress conditions at the site are uncertain. A significant number of simulation cases indicate failure ($FPI \geq 1$), whereas significant safety margins are derived for the configurations HLW-NL ($FPI_{gas,P95} = 0.40$) and HLW-ZNO ($FPI_{Gas,P95} = 0.35$). The reason for the better geomechanical performance of HLW-NL and HLW-ZNO is obviously the larger repository depth.

Probabilistic assessments – model set up, source terms and parameters for the L/ILW projects

The model-based assessment of the gas impact on performance of the L/ILW repositories was carried out for the three provisional repository projects L/ILW-JO, L/ILW-NL and L/ILW-ZNO in a probabilistic framework. Modelling of the thermo-hydraulic (TH) evolution of the L/ILW repository nearfield were also performed using the EOS5 Equation-of-State module of the TOUGH3 code. A 2-D model set-up was elaborated for the probabilistic assessment, representing a vertical cross-section through the centre of the L/ILW repository. To account for the gas dissipating through the tunnels, the 2-D mesh is extruded along the Y axis to a 2.5-D mesh consisting of three sections. The first section corresponds to the initial 2-D mesh with the waste packages where the gas is generated, the second section corresponds to the V1 plug (PLUG), and the third section corresponds to the branch tunnel and operation tunnels up to V2-HLW. The 2.5-D model with seven L/ILW caverns was generated, referred to as $2.5D-L/ILW \times 7$. To reduce the total number of elements in the 2.5-D mesh, all the geological layers except for the OPA are removed from the Chapters 2 and 3, as pressure changes are expected to be negligible in these layers. In addition, single L/ILW half-cavern models representing half (width-wise) of the middle L/ILW emplacement cavern are generated in the same manner and referred to as $2.5D-L/ILW \times 1$,

which are used in the probabilistic assessments. The volumes of the L/ILW half-cavern and adjacent tunnels are scaled down accordingly. The meshes of the L/ILW 2.5D-L/ILW $\times$ 7 models at the three sites are presented in Fig. 5-15. Further technical details about the numerical code and the model set-ups are found in Nagra (2024e).

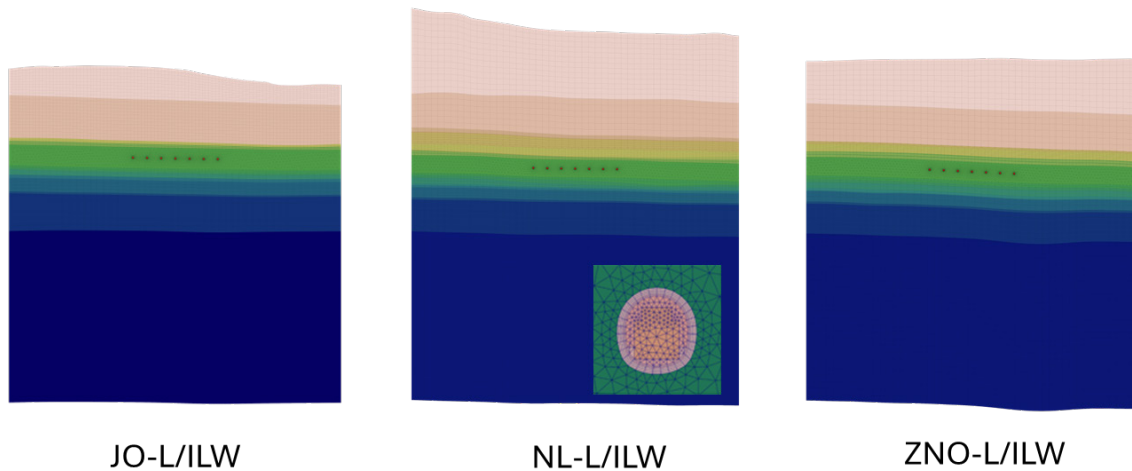


Fig. 5-15: Meshes of the models used for the simulation of 2.5-D simulation of gas induced porewater overpressures in the L/ILW nearfield

2-D vertical cross-section through the centre of the L/ILW repository: repository projects L/ILW-JO (left), L/ILW-NL (middle) and L/ILW-ZNO (right). Mesh refinement in the L/ILW nearfield is shown in the close-up. Note that single L/ILW half-cavern models representing half (width-wise) of the middle L/ILW emplacement cavern are employed in the probabilistic assessment.

The parameter assignment for the deterministic / probabilistic assessments was based on the reference values for the two-phase properties provided in Nagra (2024g) and Nagra (2024e). Tab. 5-3 presents an overview of relevant TH parameters of the EBS materials and the host rock, respectively. These reference values are forming input for the so-called *base case* simulation, which is the deterministic case used in criterion 2-3 for the calculation of the site-specific performance indicators “*thermally induced porewater overpressures in the host rock*” and the corresponding performance indices FPI_{Gas} . The full data set of reference parameters used in the probabilistic assessments is given in Nagra (2024e).

In the context of the site selection process, the model-based assessments of the repository induced effects were carried out with reference source term for gas generation according to Nagra (2024g) and Nagra (2024e) (Fig. 5-16).

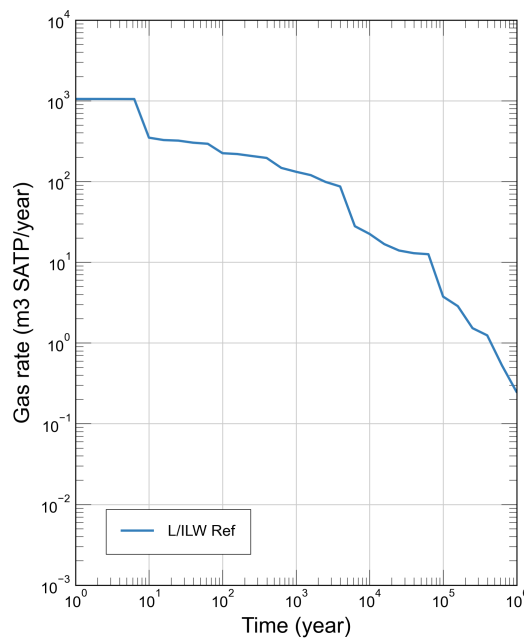


Fig. 5-16: Gas source term, representing reference gas generation rates in the L/ILW repository used for the indicator-based assessment of repository induced effects

See also Nagra (2024g) and Nagra (2024e).

Assessment of the gas effects for the site-specific L/ILW projects

Analogous to the procedure for HLW projects, the model-based assessment of the gas impact on repository performance was carried out for the three provisional repository projects L/ILW-JO, L/ILW-NL and L/ILW-ZNO, feeding in two different criteria:

- Criterion 2.3 (repository induced effects): The deterministic base case simulations for the 3 sites are compared with each other by use of the calculated performance index FPI_{gas} .
- Criterion 3.3 (predictability of long-term changes): Probabilistic simulations are carried out and the histograms of the FPI indicator are calculated for each site. The 95th percentile value ($FPI_{gas,P95}$) of the FPI_{gas} histogram is used.

The deterministic base case simulation and the probabilistic calculations of the evolution of pore pressure in the repository nearfield were carried out for the three repository projects L/ILW-JO, L/ILW-NL and L/ILW-ZNO. The results are shown in Fig. 5-17. The three graphs in the left column present transients of pore pressure at a control point at the interface between EDZ and intact host rock above the L/ILW cavern in the centre of the L/ILW repository. The red line indicates the pore pressure evolution at the control point for the deterministic base case simulation, which is the relevant case for the evaluation of criterion 2.3. For all simulations the peak pressure is reached after $\approx 80,000$ years, caused by a marked decrease of the gas generation rate (see Fig. 5-16). The family of gray lines represents the Monte Carlo simulations, contributing to the assessment of prediction uncertainties in criterion 3.3. In each diagram, the magnitudes of the three principal stress component S_h , S_H and S_v are indicated, referring to the initial stress at the control point, located at the interface between EDZ and host rock above the L/ILW cavern. The derivation of failure stress is based on the Mohr-Coulomb relationship, assuming the residual strength parameters for the Opalinus Clay, which are provided in Nagra (2024c) (see also App. E). The gas induced overpressures of the base case (red line) reach a maximum of about

2.8 – 3.8 MPa above hydrostatic, with L/ILW-JO indicating the highest overpressures (3.8 MPa). Similar to the HLW results, the gas-related simulations show for L/ILW-JO, that the gas peak pressure is significantly closer to the minimum stress S_h than for the other configurations L/ILW-NL and L/ILW-ZNO, indicating a higher risk of gas induced failure. The calculation of the FPI value for the base cases of the 3 configurations confirms this, revealing a significantly higher failure potential for L/ILW-JO ($FPI_{Gas} = 0.66$), whereas the failure potential for L/ILW-NL ($FPI_{Gas} = 0.33$) and L/ILW-ZNO ($FPI_{Gas} = 0.48$) remains moderate.

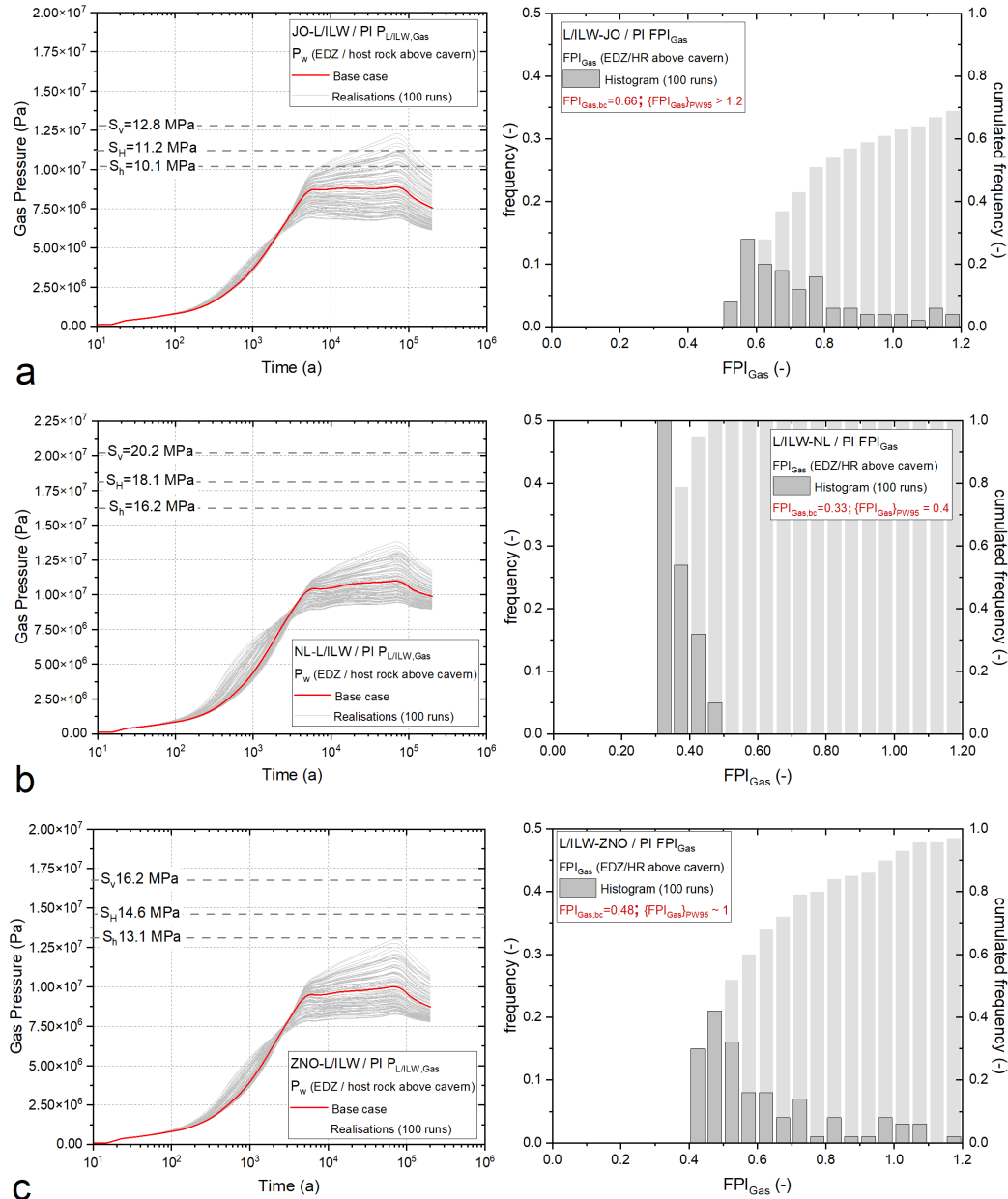


Fig. 5-17: Probabilistic simulations of gas induced porewater overpressure in the host rock (left column) and histogram of the dimensionless FPI indicator (right column)

Results for the three provisional L/ILW repository projects in JO (a), NL (b) and (c) ZNO. The FPI values calculated for the deterministic base case simulation corresponds to criterion 2.3, whereas the P95-values are used for the evaluation of criterion 3-3.

The three graphs in the right column of Fig. 5-17 present histograms of the FPI index, representative for the failure potential in the ceiling of the L/ILW cavern (control point located at the interface between EDZ and host rock above the L/ILW cavern). The 95th percentile of the FPI frequency distribution is one of the performance indices for the evaluation of criterion 3.3. The comparison of the histograms of the 3 repository configurations indicates, that the HLW-JO repository configuration ($FPI_{Gas,p95} > 1.2$). and, to lesser extent L/ILW-ZNO ($FPI_{Gas,p95} \approx 1$) are prone to failure, whereas large safety margins are derived for the configuration HLW-NL ($FPI_{Gas,p95} = 0.4$). The reason for the better geomechanical performance of HLW-NL is obviously the larger repository depth.

Gas induced porewater overpressures in the host rock (HLW and L/ILW)– input for the qualitative assessment of the CRZ based on the 13 SGT criteria

In the context of the qualitative assessment of the CRZ based on the 13 SGT criteria (Nagra (2024h)), the assessment aspect *gas effects* is evaluated with TH simulations of the pore pressure evolution, both in the HLW and the L/ILW repository nearfield. The corresponding performance index FPI_{Gas} (“*failure potential of the intact host rock – gas*”) is provided in Tab. 5-5 as input for the qualitative assessment of the CRZ, documented in Nagra (2024h).

Tab. 5-5: Performance index FPI_{Gas} for the model-based assessment of the CRZ, corresponding to the three provisional HLW and L/ILW repository projects, contributing to the criteria 2.3 “repository induced effects” and 3.3 “predictability of long-term changes”.

Performance index	JO HLW	NL HLW	ZNO HLW	JO L/ILW	NL L/ILW	ZNO L/ILW	Remarks
Performance indicator “Gas induced porewater overpressures in the host rock”							
FPI _{Gas} (Failure potential for intact host rock)	0.77	0.36	0.33	0.66	0.33	0.48	Deterministic base case simulation
	criterion 2.3 (Repository induced effects)						
FPI _{Gas,P95} (Failure potential for intact host rock)	>1.2	0.40	0.35	>1.2	0.40	~1	100 Monte Carlo simulations
	criterion 3.3 (Predictability of long-term changes)						

5.2 Criteria Group 3

Criteria Group 3 is dedicated to the remaining uncertainties concerning the barrier performance of the host rock and the CRZ, that cannot be reduced with geoscientific investigations from the surface. Three criteria were specified in the sectoral plan (Tab. 2-1):

- Criterion 3.1: ease of characterisation of the rock;
- Criterion 3.2: explorability of spatial conditions;
- Criterion 3.3: predictability of long-term changes.

Model-based assessments were performed to evaluate the impact of parametric, conceptual and scenario uncertainties on the barrier efficiency of the host rock and the CRZ in the three siting regions. Modelling workflows and results are presented in the following sections.

5.2.1 Criterion 3.1 (“Ease of characterisation of the rock”)

From a long-term safety perspective, it is advantageous if the safety properties of the host rock and the confining units above and below the host rock exhibit only little variability and can be determined without overly destructive investigations. Three assessment aspects are to be considered:

- effects of the spatial variability of transport properties of the host rock;
- the role of the hard beds in the upper confining units
- effects of the spatial variability of transport properties of the upper / lower confining units.

Model-based quantitative assessments were carried out for the three HLW repository configurations (HLW-JO, HLW-NL, HLW-ZNO) to evaluate the performance of the host rock and the CRZ as a transport barrier for dissolved radionuclides. The simulations were conducted with the TOUGH3 code using the EOS1 Equation-of-State module (Jung et al. 2018) for the simulation of non-isothermal transport of a non-sorbing tracer, which is dissolved in the porewater. Quantitative assessments of three L/ILW repository configurations (L/ILW-JO, L/ILW-NL, L/ILW-ZNO) were omitted; it has been demonstrated in Nagra (2024I) for the prospect repository project at the Haberstal site, that the dose relevant radionuclides of the L/ILW repository will be retained safely in the L/ILW caverns over the entire period of assessment. The released doses always remained many orders of magnitude below the regulatory dose limit. The results from L/ILW-NL can be transferred to the conditions at the two other sites.

Quantitative performance indicator “tracer flux of a conservative tracer”

The performance indicator *tracer flux (TF) of a conservative tracer* is used in the context of criteria group 3 for the evaluation of the barrier performance of the host rock and the CRZ for the three HLW repository configurations. The concept is briefly discussed in the following paragraphs, a more detailed discussion is found in App. E.

The TF of a conservative tracer, representing a dose-relevant, non-sorbing radionuclide from the nuclide inventory of the HLW repository, is used as a performance indicator for the evaluation of the radionuclide retention capacity of the multi-barrier system. It is assumed that the radionuclide is dissolved in the porewater and released as an instantaneous pulse from the buffer near-field into the host rock, from where it spreads out towards regional aquifer systems at the top/bottom of the CRZ. The dose-relevant radionuclide for the HLW repository is ^{129}I and the corresponding performance indicator is called $\text{TF}_{\text{I-129}}$. Realistic source terms are used in the numerical simulations to ensure representative estimates of the expected maximum tracer fluxes (for ^{129}I , it is assumed that 10% of the total inventory of radionuclide are released instantaneously after canister breaching). The total tracer flux, $\text{TF}_{\text{I-129}}$ in [Bq/a], is calculated as the sum of tracer fluxes passing the base of the Malm and top of the Keuper aquifers. The conversion of the units from [Bq/a] in [mSv/a] is performed with biosphere dose conversion factor, which represents the present-day climate. The performance index *normalized tracer flux* (NTF) is derived from the transients of the tracer flux by picking the maximum flux from the time series of tracer breakthrough:

$$\text{TF}_{\text{max}} = \max \{ \text{TF}_{\text{I-129}}(t) \}$$

and normalizing the maximum tracer flux $TF_{\max}$ with the regulatory dose limit:

$$NTF = \frac{TF_{\max} [mSv/a]}{0.1 [mSv/a]}$$

Probabilistic assessments – model set up, source terms and parameters

The model-based assessment of the barrier performance of the host rock and the CRZ was carried out for the three provisional repository projects HLW-JO, HLW-NL and HLW-ZNO in a probabilistic framework. 2-D model set-ups were used for the probabilistic assessment of the HLW repository projects at the three sites, which are based on the meshes presented in Fig. 5-10. Further technical details about the model set-ups are found in Nagra (2024e).

For the assessment of criteria group 3, it was assumed that diffusion of the dissolved and non-sorbing radionuclides is the dominating transport process at all sites. The parameter assignment for the deterministic / probabilistic assessments was based on the lithostratigraphic layer model and the reference values for the flow and transport properties are provided in Nagra (2024c). Minor modifications of the lithostratigraphic layer model were implemented (documented in Nagra 2024m) to reduce the numerical efforts in the probabilistic simulations. Tab. 5-6 presents an overview of the effective diffusion coefficients for iodine used in the base case simulations (best estimates). The full data set of reference parameters used in the probabilistic assessments is given in Nagra (2024e).

Monte Carlo simulations were performed to evaluate the influence of uncertainty of key parameters on the performance index NTF and estimate the confidence intervals around the best estimate. These simulations were carried out to substantiate the three criteria of criteria group 3 (see Tab. 2-1). The uncertain flow and transport parameters considered were used to generate a set of 100 Latin Hypercube samples, as depicted in Fig. 5-18. Further details about parameter correlations and the assumed property distributions are given in Nagra (2024e).

Tab. 5-6: Effective diffusion coefficient for Iodine for various stratigraphic units respectively formations and their representation in the PA

Effective diffusion coefficient D_{eff} (Iodine)							
Unit	NL (East and West)			PA modelling			PA material code
	Min. [m ² /s]	Best [m ² /s]	Max. [m ² /s]	Min. [m ² /s]	Best [m ² /s]	Max. [m ² /s]	
CM (Malm aquifer)	-	-	-	-	-	-	MALM
MM2	1.81E-12	6.05E-12	1.59E-11	1.81E-12	6.05E-12	1.59E-11	MM2
NL-CM	1.24E-12	4.72E-12	1.33E-11	1.24E-12	4.72E-12	1.33E-11	CM
MM1	1.96E-12	6.15E-12	1.58E-11	1.96E-12	6.15E-12	1.58E-11	MM1
AD	1.58E-12	3.66E-12	8.27E-12	1.58E-12	3.66E-12	8.27E-12	AD
E/W-CD (Herrenwis Unit)	9.00E-13/ 1.53E-12	3.40E-12/ 5.57E-12	9.76E-12/ 1.52E-11	9.00E-13/ 1.53E-12	3.40E-12/ 5.57E-12	9.76E-12/ 1.52E-11	HERRE/ HERRW
NL-ARD	1.43E-12	3.14E-12	6.93E-12	1.43E-12	3.35E-12	7.25E-12	DOGG
SCD	1.86E-12	6.47E-12	1.72E-11				
SAD	1.43E-12	3.35E-12	7.25E-12				
OPA	1.22E-12	2.65E-12	5.48E-12	1.22E-12	2.65E-12	5.48E-12	OPA
ML	1.96E-12	5.76E-12	1.45E-11	1.96E-12	5.76E-12	1.45E-11	ML
AL	1.80E-12	4.28E-12	1.05E-11	1.80E-12	4.28E-12	1.05E-11	AL
CL	1.66E-12	5.02E-12	1.24E-11	1.54E-12	3.87E-12	8.59E-12	KEUK
AK3 and JO-AK2/3	1.53E-12	3.72E-12	8.16E-12				
NL-DK2	1.46E-12	5.20E-12	1.42E-11	1.56E-12	5.32E-12	1.42E-11	KAU
AK2	1.81E-12	5.61E-12	1.44E-11				
NL-DK1	1.05E-12	3.85E-12	1.08E-11	1.23E-12	2.97E-12	6.51E-12	KAL
AK1	1.12E-12	2.45E-12	5.10E-12				
SK	1.97E-12	5.36E-12	1.34E-11				
AAK	1.63E-12	5.17E-12	1.35E-11	1.63E-12	5.17E-12	1.35E-11	GIPSK
MAK	3.48E-13	1.33E-12	3.94E-12	3.48E-13	1.33E-12	3.94E-12	MAK
DAK	4.84E-13	1.83E-12	5.37E-12				
DM	-	-	-	-	-	-	MUSCH

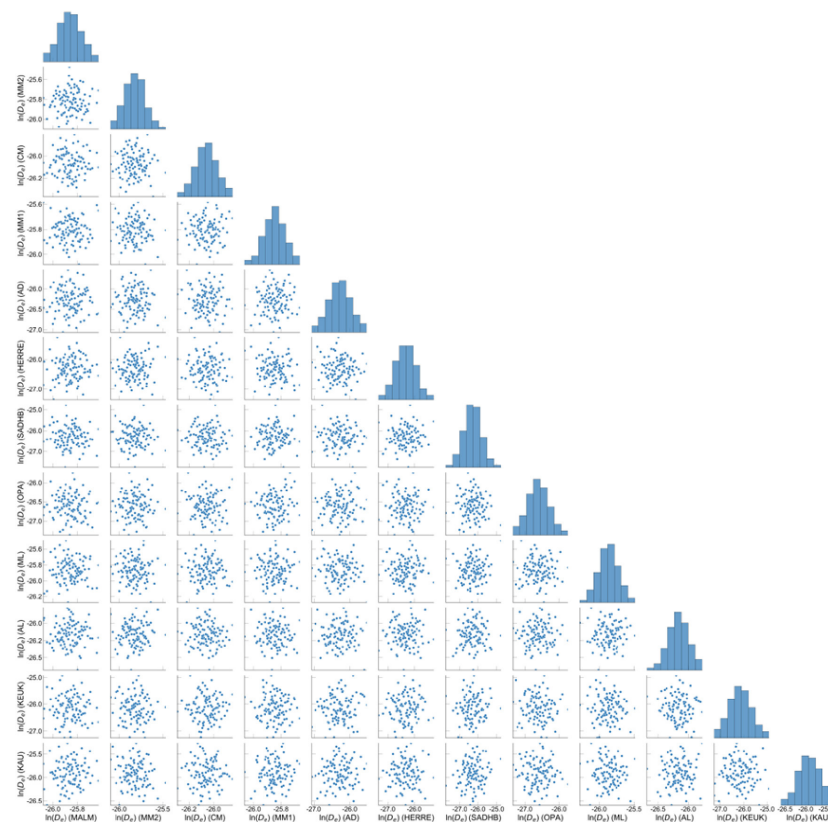


Fig. 5-18: Scatter-plot matrix of the 100 Latin Hypercube samples for all model parameters
From Nagra (2024e)

The subplots along the diagonal show the marginal distributions (as a histogram) of the samples, while the off-diagonal subplots of the matrix represent a pairwise scatter plot between the different model parameters.

Assessment of the effects of the spatial variability of transport properties of the host rock

As stated in Nagra (2024d), the Opalinus Clay is the most clay-mineral-rich unit in all three siting regions considered in SGT Stage 3, with no systematic differences in the mineralogical composition between the siting regions. The lateral and vertical lithological variability is generally small compared with other Mesozoic formations. A recent subfacies classification of the Opalinus Clay has been reported in Nagra (2024d), which was also applied to represent the host rock in the siting area NL. It comprises six subunits, with two dominant facies. The subfacies classification scheme served as a basis for a generic stochastic model, aimed at investigating the role of facies variability on the performance of the host rock as a transport barrier for dissolved radionuclides (Nagra 2024l). A stochastic realisation is shown in Fig. 5-19a, which presents a vertical cross-section through the centre of the HLW repository. The stochastic facies distribution was used to derive stochastic distributions of the effective diffusion coefficient $D_{\text{eff}}(x,z)$ in the Opalinus Clay formation by the use of known property correlations for clay content, porosity and diffusion coefficient (see details in Nagra 2024l). Fig. 5-19b shows a single realisation of the $D_{\text{eff}}(x,z)$ distribution in the Opalinus Clay formation as used for the probabilistic PA calculations. It is worth noting that the spread of the D_{eff} -values in the Opalinus Clay is modest, typically in the

range $2 - 3 \times 10^{-12} \text{ m}^2/\text{s}$ (arithmetic mean: $2.6 \times 10^{-12} \text{ m}^2/\text{s}$; geometric mean: $2.4 \times 10^{-12} \text{ m}^2/\text{s}$; harmonic mean: $2.3 \times 10^{-12} \text{ m}^2/\text{s}$). The homogeneous D_{eff} -values of the other rock units represent the reference values according to Tab. 5-6.

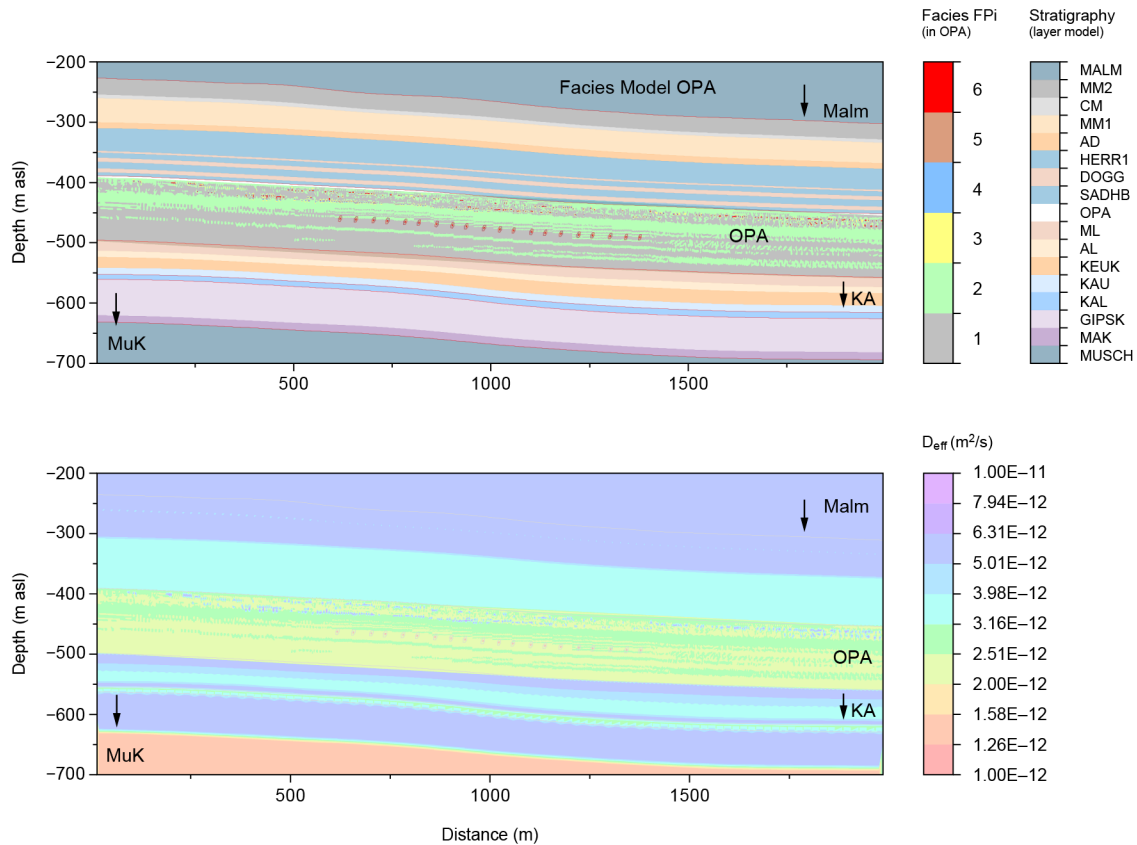


Fig. 5-19: Generic stochastic facies model of the Opalinus Clay in the NL siting region embedded in the layer stack between Muschelkalk and Malm

Vertical cross-sections through the centre of the HLW repository section (the 20 HLW tunnels are marked in red): (a) single realisation of the spatial distribution of the six facies in the Opalinus Clay formation; (b) single realisation of the random distribution of $D_{\text{eff}}(x,z)$ in the Opalinus Clay formation. Note that the homogeneous D_{eff} -values of the other rock units represent the best estimates according to Tab. 5-6.

Probabilistic transport simulations were carried out with the 2D model setup shown Fig. 5-19b. For this, a total of 100 realisations of the $D_{\text{eff}}(x,z)$ distribution in the Opalinus Clay were generated. A non-sorbing tracer, representing the dose-relevant radionuclide ^{129}I , was released from the HLW repository drifts into the CRZ, finally reaching the regional aquifer systems. The tracer flux $\text{TF}_{\text{I-129}}$ defined above was used as the performance indicator that evaluates the efficiency of the Opalinus Clay to retain the ^{129}I .

100 Monte Carlo simulations were conducted with the stochastic $D_{\text{eff}}(x,z)$ distributions and the sum of the tracer fluxes at the top and base of the Opalinus Clay⁷ was calculated. The results were compared with the corresponding tracer fluxes derived for a homogeneous representation of the Opalinus Clay with a constant effective diffusion coefficient, representing the geometric mean of

⁷ Note: tracer flux is extracted at top / base Opalinus Clay to address the barrier efficiency of the Opalinus Clay only.

the stochastic D_{eff} distributions. Fig. 5-20 presents the results of the probabilistic simulations, indicating that the 100 simulations with stochastic property distributions are practically indistinguishable from the simulations with the homogeneous Opalinus Clay. This is because the spread of diffusion coefficients in the 6 facies of the Opalinus Clay is quite modest, in the range $2 - 3 \times 10^{-12} \text{ m}^2/\text{s}$. The simulation with homogeneous host rock properties (geometric mean of $D_{\text{eff}} = 2.4 \times 10^{-12} \text{ m}^2/\text{s}$) represents the barrier efficiency of the host rock without significant loss of accuracy.

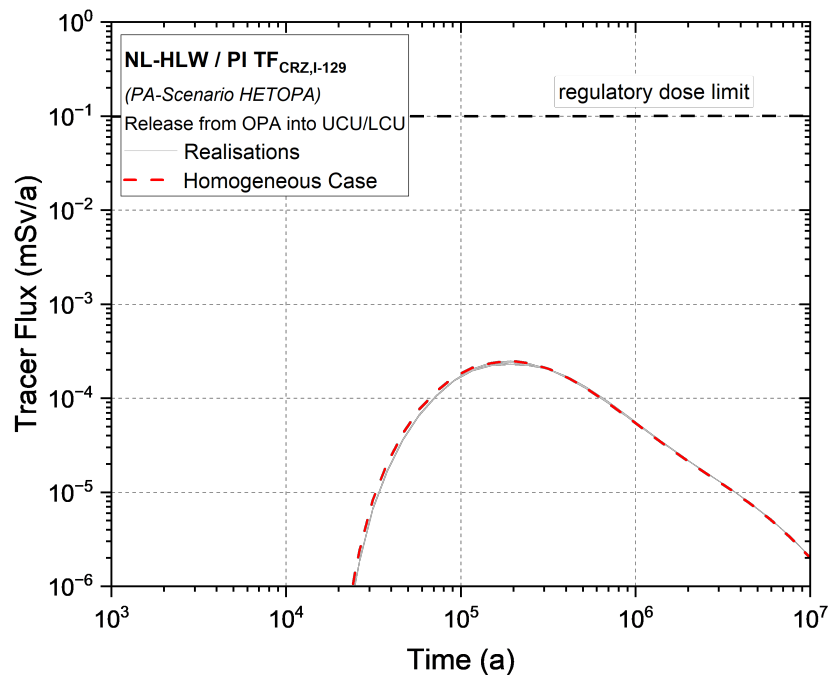


Fig. 5-20: Generic Tracer flux released from the Opalinus Clay into the upper and lower confining units (diffusion-dominated transport is assumed)

Probabilistic simulations with 100 stochastic property distributions of $D_{\text{eff}}(x,z)$ are practically indistinguishable from the simulation with the homogeneous Opalinus Clay (red dotted line)

The role of the hard beds in the upper confining units

The role of the hard beds in the upper confining units as a potential lateral release pathway was discussed intensively in Stage 2 of the Sectoral Plan. In the context of the deep borehole campaign carried out during Stage 3 of the Sectoral Plan, considerable efforts were dedicated to the hydraulic characterisation of the hard beds in the three siting regions. The existing hydro-geological database was confirmed, indicating very limited porewater circulation in the hard beds of the upper confining units. Furthermore, the parametric uncertainties of the relevant flow and transport properties were reduced for all siting regions. The site selection process required that the main repositories for HLW and L/ILW must be placed with a minimum lateral distance of 200 m from any major fault systems, as these could act as potential release pathways towards the regional aquifer systems (see Section 4.2).

A special PA scenario *HRDBED* was specified in NTB 24-22 for the prospected repository project at the Haberstal site NL, aimed at investigating the role of the hard beds in the upper confining units as a possible release pathway for dissolved radionuclides. The results from the NL site region can be extrapolated to the effects of similar lithostratigraphic features on the barrier performance of the CRZ in the other two siting regions. The *HRDBED* scenario considers three

hard beds in the so-called Sandy-Argillaceous Dogger unit above the host rock, each of them characterised by an elevated hydraulic conductivity, but still in the parameter range specified in Nagra (2024c) (Fig. 5-21a). Furthermore, it is assumed that a high lateral hydraulic gradient $i = 0.1 \text{ m/m}$ applies. A hypothetical vertical fault at a distance of 200 m from the HLW repository section mimics a potential release pathway towards the regional aquifer systems. Fig. 5-21b shows a snapshot of tracer concentration after 1 million years, assuming that the tracer is released instantaneously from the HLW drifts into the CRZ. The simulation represents the base case of the HRDBED scenario, which means that the hydraulic conductivities and effective diffusions coefficients of the layer stack correspond to the reference values as specified in Nagra (2024e). The tracer plume exhibits a peculiar shape with a uniform diffusive tracer front, propagating from the HLW drifts downwards to the Keuper aquifer and with a somewhat deformed front towards the Malm aquifer. The shape of the tracer front towards the Malm aquifer can be explained by the effect of lateral porewater through the hard beds which exhibit a higher horizontal permeability than the Opalinus Clay. The high lateral hydraulic gradient of 0.1 m/m in the hard beds creates a significant lateral porewater flow, which carries the tracer towards the virtual fault and reduces diffusive flux towards the Malm aquifer.

The probabilistic assessment of the *HRDBED* scenario is based on a set of 100 Monte Carlo simulations. The performance indicator $\text{TF}_{\text{CRZ},\text{I-129}}$ (Fig. 5-21c) is used to infer the total tracer flux into the regional aquifer systems, including the release into the steeply dipping fault. The corresponding histogram of the performance index $\text{NTF}_{\text{CRZ},\text{I-129}}$ is presented in Fig. 5-21d. The simulations reveal that tracer flux increases by around 0.5 orders of magnitude with respect to the EXPERF PA scenario of expected performance. The barrier performance of the CRZ is still favourable, meaning that the expected dose remains around 3 orders of magnitude below the regulatory dose limit. Keeping in mind that the assumed high lateral porewater flow in the hard beds is not supported by the observed hydrogeological evidence, such as natural tracer profiles in the deep boreholes drilled in NL, the *HRDBED* scenario can be classified as having a low probability of occurrence.

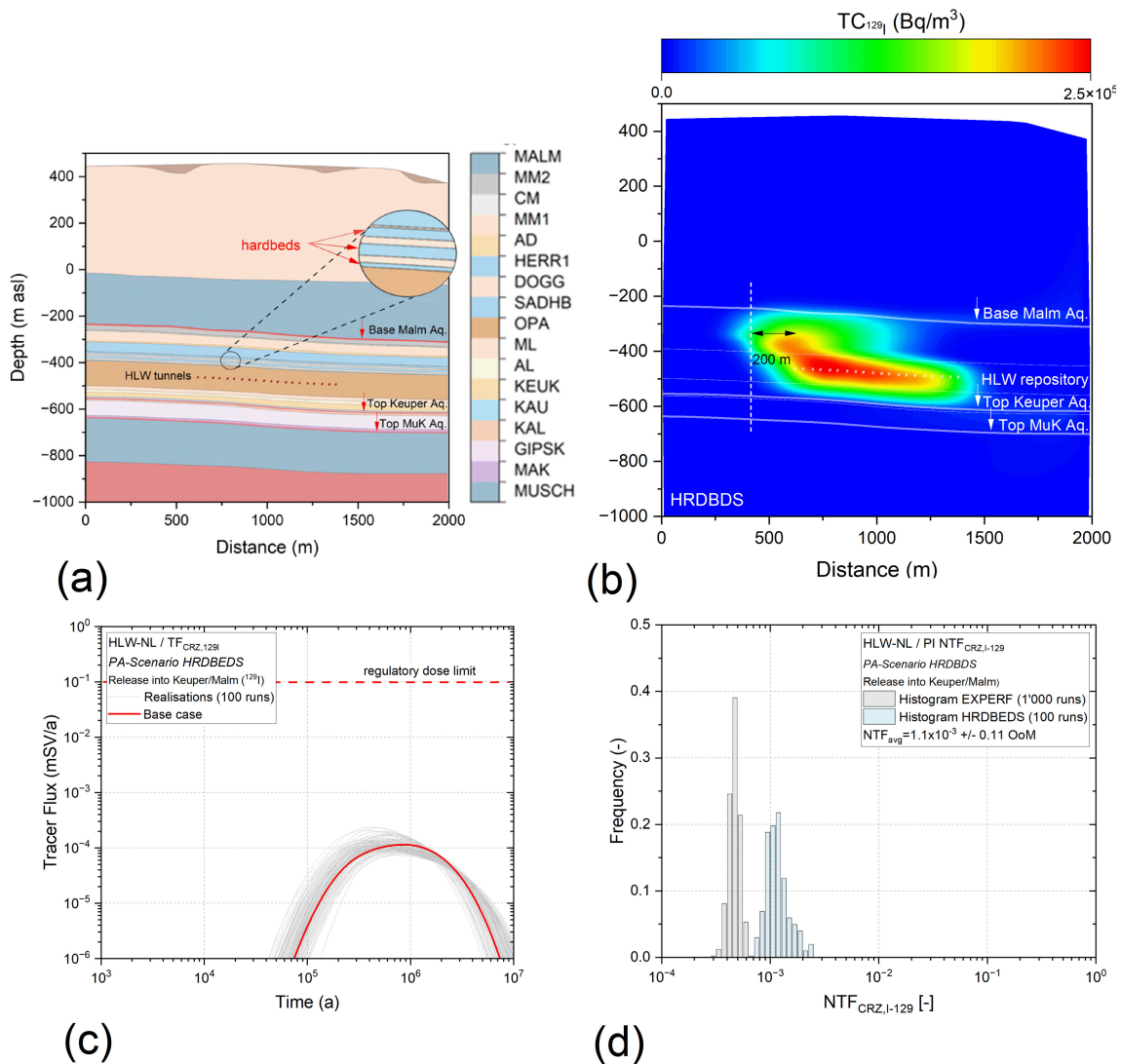


Fig. 5-21: Generic Tracer flux released from the CRZ into the regional aquifer systems (diffusion-dominated transport is assumed)

(a) Representation of the hard beds in the upper confining units, implemented in the HRDBED scenario; (b) snapshot of tracer concentration in the CRZ after 1 million years; (c) transients of tracer flux $TF_{CRZ,I-129}$ and (d) histogram of normalised performance index $NTF_{CRZ,I-129}$.

Assessment of the effects of the spatial variability of transport properties of the upper / lower confining units

At each of the three candidate repository sites the upper and lower confining units, as part of the CRZ, serve as additional effective transport barriers. Lithostratigraphy, mineralogical composition and thickness of the Mesozoic layer stack differs from one site to the other. This lateral and vertical lithological variability could affect the barrier performance of the CRZ and differentiate between the repository projects. Model based assessments were carried out to evaluate the performance of the CRZ at the three HLW sites (HLW-JO, HLW-NL, HLW-ZNO). The *tracer flux (TF) of a conservative tracer* was used as the performance indicator. Probabilistic transport simulations were carried out with the 2D model set-ups shown in Fig. 5-10. For this, a total of 100 realisations of the $D_{\text{eff}}(z)$ distribution in the Mesozoic layer stack were generated, assuming that the diffusion coefficient is constant within each lithostratigraphic unit. The corresponding scatter plots of the uncertain model input parameters are shown in Fig. 5-18.

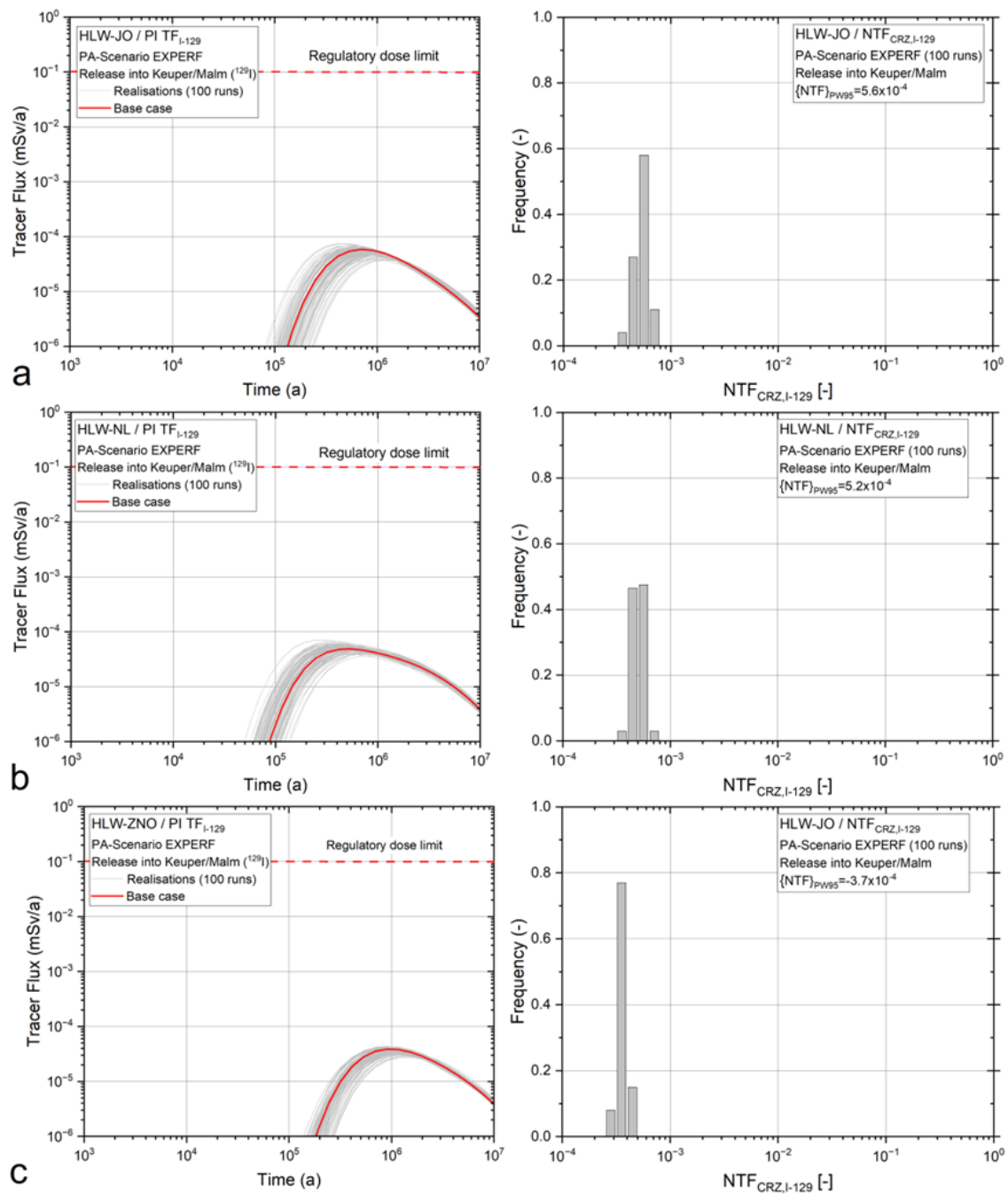


Fig. 5-22: Generic Tracer flux released from the CRZ into the upper and lower confining units (diffusion-dominated transport is assumed)

Probabilistic simulations with 100 stochastic property distributions of $D_{eff}(z)$ distribution in the Mesozoic layer stack were generated, assuming that the diffusion coefficient is constant within each lithostratigraphic unit (red dotted line: base case parameter set).

The results of the Monte Carlo simulations for the three repository configurations are presented in Fig. 5-22. A very favourable performance of the CRZ can be stated for all repository projects with peaks of tracer flux remaining more than 3 orders of magnitude below the regulatory dose limit. The differences between the three sites are small as indicated in the small differences of the NTF_{p95} index (HLW-JO: $\text{NTF}_{p95} = 5.6 \times 10^{-4}$; HLW-NL: $\text{NTF}_{p95} = 5.2 \times 10^{-4}$; HLW-ZNO: $\text{NTF}_{p95} = 3.7 \times 10^{-4}$).

Ease of characterization of the rock – input for the qualitative assessment of the CRZ based on the 13 SGT criteria

In the context of the qualitative assessment of the CRZ based on the 13 SGT criteria (Nagra 2024h), the criterion 3.1 (“ease of characterization of the rock and the CRZ”) is evaluated by numerical transport simulations, indicative for the performance of the CRZ as a transport barrier for dissolved radionuclides. For the comparison of the HLW repository configurations, the corresponding performance index NTF_{L-129} (“normalized tracer flux”) is provided in Tab. 5-7 as input for the qualitative assessment of the CRZ, documented in Nagra (2024h). Transport simulations for the L/ILW repository were omitted, because the released doses of relevant radionuclides from the L/ILW repository remained many orders of magnitude below the regulatory dose limit at all times.

Tab. 5-7: Performance indices NTF for the model-based assessment of the CRZ, corresponding to the three HLW repository projects for the criterion 3.1 “Ease of characterization of the rock”

Performance index	JO HLW	NL HLW	ZNO HLW	JO L/ILW	NL L/ILW	ZNO L/ILW	Remarks
Assessment aspect “Effects of the spatial variability of transport properties of the host rock”							
Normalised tracer flux released from CRZ (NTF _{p95})	Simulation performed for NL only. Heterogeneous cases undistinguishable from homogeneous simulations			<0.001	<0.001	<0.001	See Nagra (2024h) for in-depth analyses (Haberstal site)
				No simulations performed			
Assessment aspect “Effects of the spatial variability of transport properties of the upper / lower confining units”							
Normalised tracer flux released from CRZ (NTF _{p95})	0.00056	0.00052	0.00037	<0.001	<0.001	<0.001	
				No simulations performed			

5.2.2 Criterion 3.2 (“Explorability of spatial conditions”)

The impact of conceptual uncertainties regarding the spatial conditions and the vertical delimitation of the CRZ are addressed in the assessment aspect “*Impact of uncertainties regarding the delimitation of the CRZ*”. In all three siting areas, the CRZ is limited by the Keuper aquifer. The structure of the Keuper aquifer occurring in the Klettgau formation is complex and varies between the siting areas. In ZNO and JO, all deep boreholes provide evidence of flow paths in the Klettgau formation. In NL, however, this is not the case; there, such paths occur locally in connection with local sandy deposits. Where there are no sandy channel deposits in NL, the thickness of the EG is therefore significantly greater, namely around 400 m to the Muschelkalk aquifer. In this situation, the transport path for radionuclides to the lower boundary of the EG is also considerably longer. Probabilistic assessments of tracer release show that the retention effect

is thereby significantly increased for the HLW repository at NL (Nagra 2024l). Fig. 5-23a presents a comparison of the barrier performance of the CRZ for the two scenarios. The corresponding performance index $\text{NTF}_{\text{I-129}}$ indicates, that the barrier performance improves by nearly factor of two, when the Muschelkalk aquifer represents the lower boundary of the CRZ. For the Muschelkalk scenario, the HLW-NL repository project performs better than HLW-JO and HLW-ZNO, respectively (Fig. 5-23b).

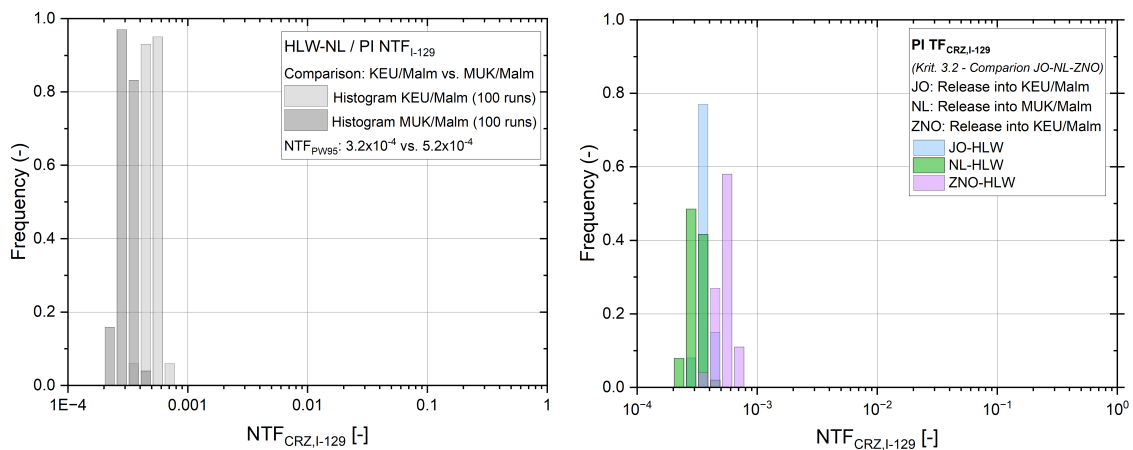


Fig. 5-23: Comparison of the barrier performance of the CRZ for the two scenarios “release to Keuper/Malm aquifers” and “release to Keuper/Muschelkalk aquifers”

(a) HLW-NL – comparisons Keuper/Malm versus Muschelkalk/Malm; (b) comparison HLW-JO and HLW-ZNO (both Keuper/Malm) with HLW-NL Muschelkalk/Malm. The performance index $\text{NTF}_{\text{I-129}}$ indicates, that the barrier performance improves by nearly factor of two, when the Muschelkalk aquifer represents the lower boundary of the CRZ.

5.2.3 Criterion 3.3 (“Predictability of long-term changes”)

In criterion 3.3, the assessments formulated in criteria 2.2 and 2.3 for the expected long-term geological evolution and repository induced effects are reviewed, taking into account the remaining uncertainties that cannot be further reduced by geological investigations. The two assessment aspects “thermal effects” and “gas effects” were evaluated with the probabilistic modelling workflows described in Sections 5.1.2 and 5.1.3. The results of the assessments are given in Tab. 5-4 and Tab. 5-5.

6 Summary and conclusions

The primary aim of the present report has been to provide a traceable documentation of the model-based assessments, supporting the safety-related site comparison in the context of SGT-Stage 3. Emphasis was on the following evaluations:

- Vertical and lateral delimitation of the containment-providing rock zone (CRZ) for a HLW and L/ILW repository project in the 3 siting regions.
- Indicator-based assessment of the barrier performance of the CRZ for a HLW and L/ILW repository project in the 3 siting regions.

Vertical and lateral delimitation of the CRZ

The CRZ is the part of the geological barriers which, with the expected evolution of the repository for the period under consideration, ensures the effective containment and retention of the radioactive substances contained in the waste. The sectoral plan requires that the CRZ is to be delimited laterally and vertically at a suitable depth. The indicator-based approach presented in this report ensures a traceable demarcation of the favourable areas and, within these areas, the vertical and lateral delimitation of the CRZ. The approach is founded on dedicated delimitation indicators, reliable performance targets and evaluation scales.

The thickness of the Opalinus Clay is a delimitation indicator for the vertical extent of the CRZ, which is required to assess the efficiency of the CRZ as a transport barrier for radionuclides. The minimum thickness of the host rock $L_{\min, \text{HLW}}$ represents the corresponding performance target for the HLW repository. Based on a dimensionless representation of advective-diffusive transport processes in the host rock, a minimum thickness above and below the emplacement tunnels of 20 - 35 m was estimated for the HLW repository to provide acceptable performance as a transport barrier for dissolved radionuclides (the lower value of 20 m refers to the best estimate D_{eff} values of the Opalinus Clay and modest advective flow component; the upper value represents an even stricter performance target, referring to the upper bound D_{eff} values and a strong vertical pore-water flow component in the Opalinus Clay). For the L/ILW repository with a diameter of approximately 10 m, a minimum thickness of the intact host rock package above and below the caverns of 20 m is estimated to ensure the confinement of the waste and the mechanical and chemical integrity of the repository system as a whole.

The delimitation indicator for lateral delimitation of the CRZ is called “distance to steeply dipping faults”. The corresponding performance target $L_{\min, \text{fault}} = 200$ m has been specified as a minimum distance of the HLW and L/ILW disposal areas from any fault systems. Model-based assessments confirm that the lateral release to a steeply dipping fault is not relevant, when the respect distance of 200 m is maintained. Complementary simulations indicate that even for 100 m distance, the radionuclide release rates are expected to be negligible.

Another delimitation indicator used for lateral delimitation of the prospected protection zone is called “minimum lateral distance between the prospected protection zone and the next injection / pumping well”. The corresponding performance target $L_{\min, \text{well}} = 50$ m has been specified as a minimum distance of the prospected repository zone from any deep boreholes. Model-based assessments confirm that the lateral release into a deep borehole is not relevant, when the respect distance of 50 m is maintained. The tested scenarios encompass scenarios of unsealed abandoned wells and future geothermal applications.

A complementary workflow was pursued for setting out favourable repository areas and for delineation of the corresponding repository footprints in the three siting regions. The screening process was aimed at mapping lateral variations of barrier performance of the host rock. Significant lateral variations in barrier performance of the host rock could not be identified; it can be concluded that the entire prospected protection zone is equally well suited to host the repository.

Indicator-based assessment of the barrier performance of the CRZ

Model-supported assessments have been performed to identify safety-relevant differences between the site-specific repository projects. The indicator-based evaluations concentrated on the SGT criteria 2.3 (“repository induced influences”) and the three criteria in criteria group 3 (“reliability of findings”).

The effects of the excavation damaged zone (EDZ) were evaluated by numerical calculations of the vertical extent of the EDZ above / below the emplacement rooms, both for the HLW and the L/ILW repository projects. The analyses revealed that none of the repository projects is detrimentally affected by a safety-relevant loss of barrier function of the CRZ, caused by the vertical extent of the EDZ.

Thermally induced overpressures in the host rock around the HLW drifts have a significant power to distinguish between the three HLW repositories. The HLW-NL and HLW-ZNO repository configurations are characterized by significantly higher safety margins with regard to thermally induced shear failure than the HLW-JO project. A similar picture emerges when taking into account the parametric and conceptual uncertainties addressed in criteria group 3. The reason for the less favorable performance of the HLW-JO configuration is the lower repository depth at the JO site.

Gas induced overpressures develop both, in the HLW and the L/ILW repository structures. The gas impacts have a significant power to distinguish between the three repository sites. The repository projects at the NL site perform best due to the greatest repository depth, the configurations in ZNO performs also well, whereas low safety margins are seen for the JO projects due to the lowest repository depth.

Finally, model-based assessments were performed to evaluate the impact of parametric, conceptual and scenario uncertainties on the efficiency of the host rock and the CRZ in the three siting regions as a transport barrier for dissolved radionuclides. Tracer flux of a conservative tracer was used as a performance indicator which can be calculated with numerical modelling tools. Probabilistic simulations confirmed an excellent barrier performance of the CRZ for all repository configurations at all sites, indicating that the power to distinguish between the three repository sites is low.

7 References

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App. A An approach for the derivation of the performance target “minimum thickness of the intact host rock above/below the repository structures” from normalized tracer fluxes

A.1 Concept for the assessment of barrier performance of the host rock

In order to evaluate the potential of the geological barrier to perform as a transport barrier, the migration of a hypothetical, dissolved, non-sorbing, stable element through the host rock is considered. A step function / unit release rate is assumed as tracer source term from the repository, which results in a breakthrough $R(t)$ to the upper and lower confining units (UCU/LCU). Correspondingly, the breakthrough curve for a delta-function release of the stable solute is simply the derivative of $R(t)$, i.e. $R'(t)$ [kg/a²]. When decay of the radionuclide is included, the breakthrough curve $r(t)$ [Bq/a] for a pulse near-field release of a radionuclide is:

$$r(t) = M \cdot \frac{R'(t)}{R(\infty)} \cdot \exp^{-\lambda \cdot t} \quad (\text{A-1})$$

Where $R(\infty)$ [kg/a] is the modelled long-term, steady-state tracer release rate from the near field to the host rock and M [Bq] is the magnitude of the pulse release (Instant Release Fraction IRF). It also follows that the “unit” peak release rate of the radionuclide from the CRZ is:

$$r_{\max} = \max \left[\frac{R'(t)}{R(\infty)} \cdot \exp^{-\lambda \cdot t} \right] \quad (\text{A-2})$$

A.1.1 Specification of a dimensionless performance indicator

The performance indicator $I1$ (“maximum of the time-derivative of the release to the UCU/LCU”) represents a measure of spreading / dispersion of IRF. It is defined as follows:

$$I1_{Rn} = \frac{M \cdot BDCF_{Rn}}{10^{-4} \text{ Sv/a}} \cdot r_{\max} \quad (\text{A-3})$$

where $BDCF_{Rn}$ is the biosphere dose conversion factor of the radionuclide and the factor 10^{-4} Sv/a is the dose rate limit specified in Swiss regulations. The dose relevant non-sorbing radionuclides for HLW and L/ILW and the corresponding BDCF’s are:

- HLW: ^{129}I is the most penalising radionuclide in the case of the HLW repository.
 $BDCF_{w\&d} = 6.32 \cdot 10^{-13}$ Sv/Bq (present day climate)
 $M = 4.4 \cdot 10^{12}$ Bq (total inventory of ^{129}I)
 $\lambda_{I-129} = 4.41 \cdot 10^{-8}$ 1/a (decay rate of ^{129}I)
- L/ILW: ^{36}Cl was chosen to represent the in the case of the L/ILW repository.
 $BDCF_{w\&d} = 1.65 \cdot 10^{-14}$ Sv/Bq (present day climate)
 $M = 9.76 \cdot 10^{11}$ Bq (total inventory ^{36}Cl)
 $\lambda_{Ca-41} = 2.31 \cdot 10^{-6}$ 1/a (decay rate of ^{36}Cl)

A.1.2 Dimensionless representation of tracer flux

The 1-D diffusion equation in a homogeneous, isotropic medium can be written as follows:

$$\frac{\partial c}{\partial t} = D_{eff} \frac{\partial^2 c}{\partial x^2} \quad (A-4)$$

where c [kg/m³] is the concentration and D_{eff} [m²/s] is the effective diffusion coefficient. Dimensional analysis leads to a simpler representation of the diffusion equation by introducing the corresponding characteristic length and time scales L and T and reference concentration c_0 :

$$t \rightarrow t' \cdot T, \quad x \rightarrow x' \cdot L, \quad c \rightarrow c' \cdot c_0$$

The dimensionless diffusion equation is derived by substitution in Eq. (A-4):

$$\frac{\partial c'}{\partial t'} = \frac{T \cdot D_{eff}}{L^2} \cdot \frac{\partial^2 c'}{\partial x'^2} \quad (A-5a)$$

Fig. A-1 presents the numerical simulations of the 1-D diffusion equation for a tracer injection with step-function release rate in dimensional and dimensionless form, using $T = 10$ mio years and $L = 20, 35$ and 50 m as the characteristic time and length scales. It can be seen that all breakthrough curves in the dimensional representation (left side) collapse onto a single curve in the dimensionless representation (right side) of the time axis, where:

$$t' = \frac{t \cdot D_{eff}}{L^2} \quad (A-5b)$$

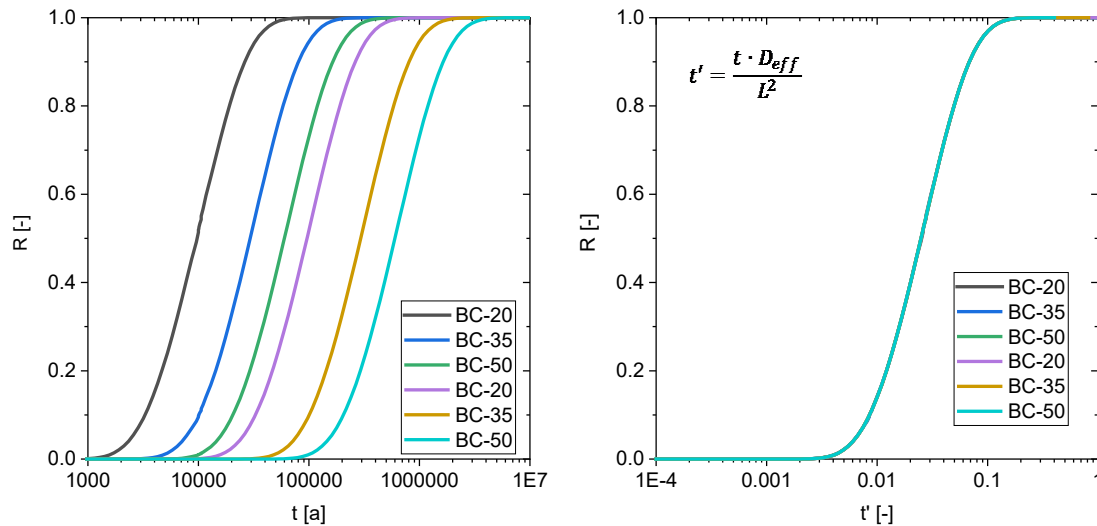


Fig. A-1: Step responses derived from 1-D numerical simulations representing a tracer injection with constant release rate

(a) normalised release rate in [-] and time in [y]; (b) dimensionless representation with characteristic time $T = 10$ mio years, characteristic length scales $L = 20, 35$ and 50 m and diffusion coefficient of 3.2×10^{-12} and 3×10^{-11} m²/s.

The dimensionless advection-diffusion equation can be derived in a similar manner:

$$\frac{\partial c'}{\partial t'} + \frac{\partial c'}{\partial x'} = \frac{1}{Pe} \cdot \frac{\partial^2 c'}{\partial x'^2} \quad (\text{A-6})$$

where Pe represents the Peclet number defined as:

$$Pe = \frac{L \cdot u}{D_L} = \frac{L \cdot v_f}{n \cdot D_L} \quad (\text{A-7})$$

D_L is the longitudinal dispersion coefficient, u is the particle velocity, n is porosity and v_f is the Darcy velocity.

$$D_L = \alpha_L \cdot |u| + D_{m,eff} \quad (\text{A-8})$$

where α_L is the longitudinal dispersivity and $D_{m,eff}$ is the effective diffusion coefficient in the porous medium. Due to the ultra-low Darcy velocity of porewater flow in Opalinus Clay, it is assumed here that $D_L \approx D_{m,eff}$, which holds for the examples in Fig. A-2a, when $\alpha_L < 5$ m. Empirical relationships for α_L have been developed for heterogeneous porous groundwater flow systems, whereas the available evidence for ultra-low permeability structures is limited to theoretical considerations concerning the microstructural characteristics of the medium.

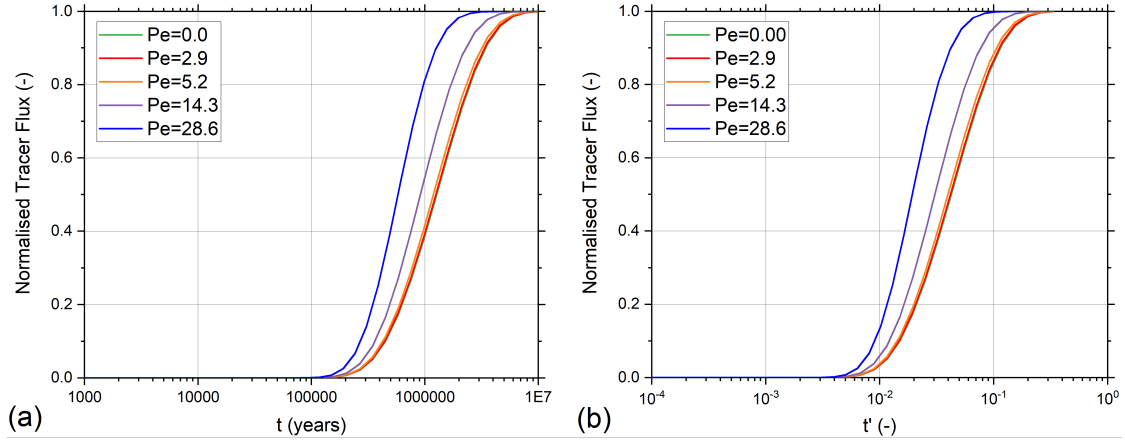


Fig. A-2: Typical breakthrough curves in response to a step injection (normalised to the injection rate)

- (a) numerical 1-D simulations of advective-diffusive transport with Darcy velocities up to 2×10^{-13} m/s. The effective diffusion coefficient is $D_{eff} = 3.2 \times 10^{-12}$ m²/s, the hydraulic conductivity is $K = 2 \times 10^{-14}$ m/s and the transport length is 55 m; (b) dimensionless representation of normalised breakthrough curves.

A.2 Derivation of the performance indicator for HLW from dimensionless step response

Fig. A-3 displays the normalised derivatives $r(t')/M$ according to equation (A-2) of the dimensionless step response functions of a non-decaying tracer ($\lambda = 0$) for the advective-diffusive flux with Peclet numbers ranging between 0 and 28.65 (corresponding to the graphs in Fig. A-2b). The values of the maximum derivative $r_{\max}$, corresponding (dimensionless) times of maximum derivative $t'_{\max}$ and the Peclet numbers are given in the appended table.

The maximum derivative $r_{\max}$ increases markedly with increasing Peclet number. Fig. A-4 presents the graph together with a polynomial fit of the function $r_{\max}(Pe)$ in the advection-diffusion regime with Peclet numbers up to $Pe = 28.65$. The performance indicator I_{HLW} (equation A-3) representing the radionuclide ^{129}I can be expressed as:

$$I_{HLW} = \frac{M \cdot BDCF_{I-129}}{10^{-4}} \cdot \max \left[\frac{R'(t)}{R(\infty)} \cdot e^{-\lambda_{I-129} \cdot t} \right] \rightarrow \text{decay neglected for } ^{129}\text{I} \quad (\text{A-9})$$

$$\rightarrow I_{HLW}(Pe) \approx \frac{M \cdot BDCF_{I-129}}{10^{-4}} \cdot \max \left[\frac{R'(t)}{R(\infty)} \right] = 2.78 \cdot 10^4 \cdot r_{\max}(Pe) \quad (\text{A-10})$$

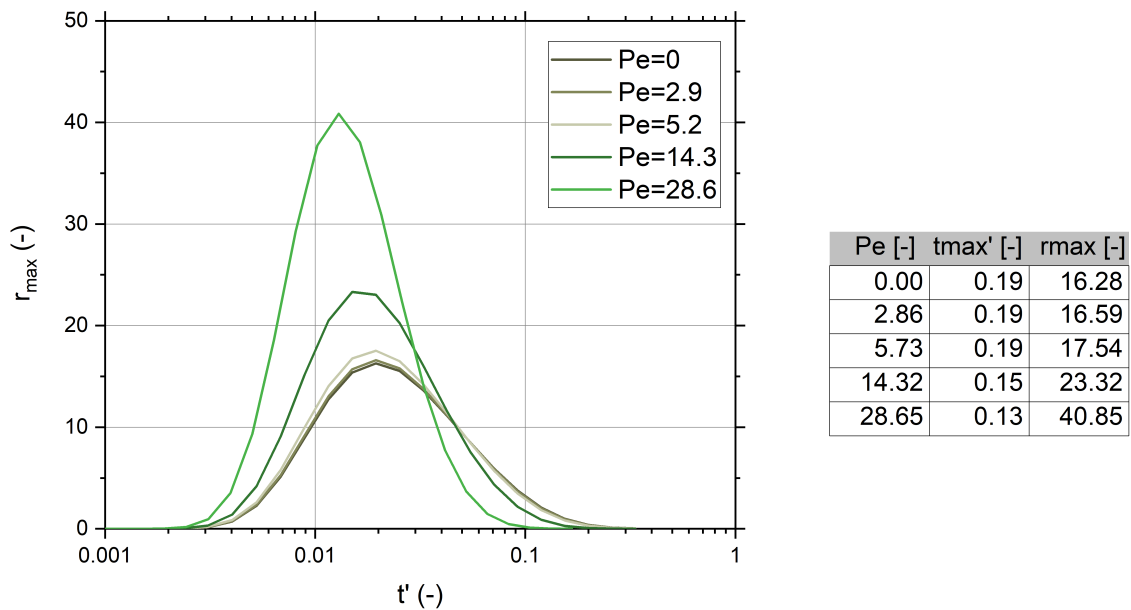


Fig. A-3: Normalised derivative $r(t')/M$ of the step response function $R(t')$ plotted versus dimensionless time t' for Peclet numbers ranging between 0 and 28.65

The values of the maximum derivative $r_{\max}$ and the corresponding (dimensionless) times of maximum derivative $t'_{\max}$ are given in the table.

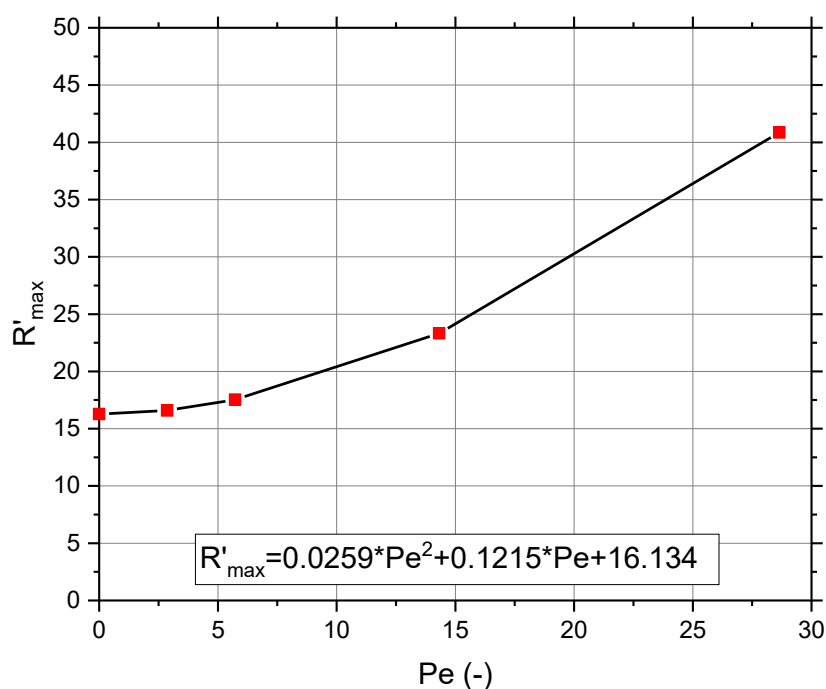


Fig. A-4: The max. derivative $r_{\max}$ of a non-decaying tracer is plotted versus Peclet number up to $Pe = 28.65$

The data are fitted with a polynomial of the order 2.

A.3 Minimum thickness of the host rock for the SF/HLW repository

The performance target «*minimum thickness of the Opalinus Clay* - $L_{\min,HLW}$ » ensures that the geological barrier is sufficiently thick to represent a reliable transport barrier for diffusive transport of dissolved radionuclides. It is derived from the dimensionless performance indicator for tracer transport I_{Rn} which has been specified in equation (A-3). The following evaluation scale is normalised to a limit state $I_1 = 1$ (regulatory dose limit reached) with the following quality levels:

Favourable:	$I_1 < 0.01$,
Less favourable:	$0.01 \leq I_1 < 0.1$,
Unfavourable:	$0.1 \leq I_1 < 1$,
Unacceptable:	$I_1 \geq 1$.

For the HLW repository, the performance indicator I_{I-129} is defined according to equation (A-9), based on a present-day climate. It can be expressed in terms of the Peclet number (equation A-10), using the polynom approximation given in Fig. A-4. The performance target “minimum thickness of the host rock” $L_{min,HLW}$ is specified such that the host rock provides barrier performance at the quality level “unfavourable” but still below the performance limit ($I_I = 1$):

$$\begin{aligned}
 L_{min,HLW} &\equiv I_{I-129,unfavourable} = 0.1 \approx 2.78 \cdot 10^4 \cdot R'_{w_max}(Pe) \cdot \frac{D_{eff}}{L^2} \\
 &= 2.78 \cdot 10^4 \cdot (0.0287 \cdot Pe^2 + 1.438 \cdot Pe + 16.3) \cdot \frac{D_{eff}}{L^2} \\
 \Rightarrow L_{min,HLW}(Pe) &= \sqrt{2.78 \cdot 10^4 \cdot (0.0259 \cdot Pe^2 + 0.1215 \cdot Pe + 16.134) \cdot D_{eff} \left[\frac{m^2}{y} \right]} \quad (A-11)
 \end{aligned}$$

In the case of the HLW repository the minimum thickness of the Opalinus Clay, $L_{min,HLW}$, depends not only on the transport properties of the Opalinus Clay (i.e. D_{eff} and K_f), but also on the vertical component of the hydraulic gradient across the Opalinus Clay. A graphical representation of the dependence of $L_{min,HLW}$ on the effective diffusion coefficient D_{eff} for Peclet numbers up to 50 is given in Fig. A-5. The diagram allows to determine $L_{min,HLW}$ for the HLW repository configuration for a given Peclet number and effective diffusion coefficient of the Opalinus Clay (dose relevant radionuclide: ^{129}I). A minimum thickness of 35 m above and below the emplacement tunnels within the Opalinus Clay is deemed a sensible value, covering a wide range of effective diffusion coefficients and Peclet numbers.

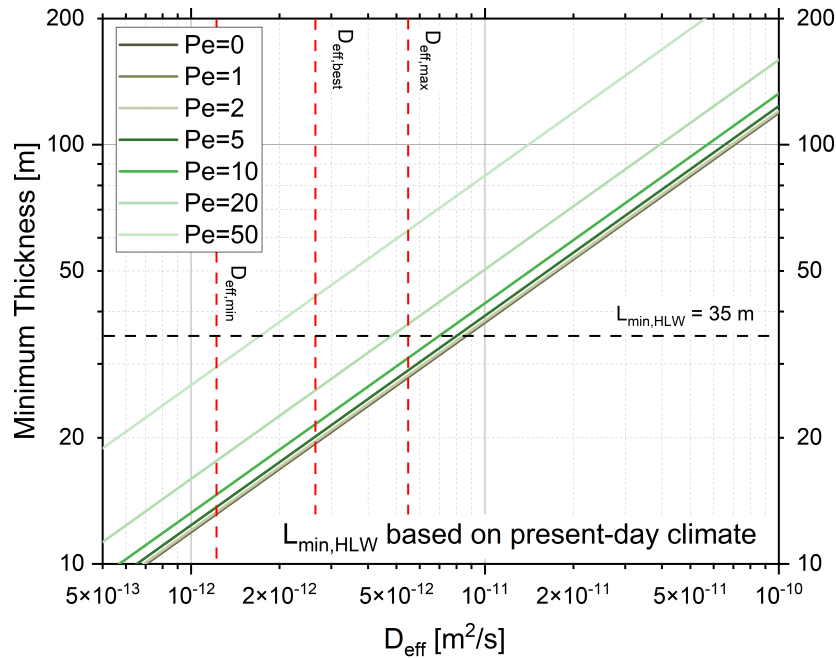


Fig. A-5: Minimum thickness of the Opalinus Clay above and below the HLW emplacement tunnel, derived from performance indicator I_{I-129} for the HLW repository at performance level “unfavourable”

Assessment based on a present-day climate scenario.

A.4 Concluding remarks

A similar approach was tested to determine the minimum thickness of the Opalinus Clay for the L/ILW repository. The dose relevant radionuclide was ^{36}Cl . The calculations indicated a required minimum thicknesses of less than 10 m above and below the caverns within the Opalinus Clay. Even if such a thickness of the host rock were sufficient to act as a transport barrier for dissolved radionuclides, the safety function of the mechanical protection of the EBS would not be guaranteed. From a PA perspective, the determination of the minimum thickness of the host rock must take into account other aspects in addition to the function as a transport barrier. Based on the diameter of the SMA caverns of approximately 10 m, a minimum thickness of the intact host rock package above and below the caverns of 20 m appears to be justified to ensure the confinement of the waste and the mechanical and chemical integrity of the repository system as a whole.

App. B Minimum distance to faults and wells

B.1 Problem statement

“Distance to wells” is a delimitation indicator in the site comparison process and the “minimum required distance to wells” is the corresponding performance target. The minimum required distance is derived by numerical modelling of tracer release from the HLW repository section of the prospect repository project at the Haberstal site. The model simulates advection and diffusion in a fully saturated porous medium. It accounts also for the for non-isothermal conditions in the repository near-field, including the natural heat flux from the basement to ground surface and the heat emitting wastes in the emplacement drifts. It is assumed that HLW canisters will breach 10,000 years after repository closure. At that time a conservative tracer, which represents the dose-relevant radionuclide ^{129}I , is released instantaneously from the HLW canisters. The prevailing transport mechanisms are diffusion and advection. Advective transport represents a superposition of a vertical flow component associated with the porewater overpressures in the Keuper aquifer and a radial flow component depending on the pressure conditions in the borehole.

Normalised tracer flux at top/base of the CRZ (i.e., base Malm and top Keuper aquifer) is deduced from the transport simulations, assuming that diffusion is the governing transport process (see also E.2). The simulations of tracer transport through the stack of geological formations are performed using the EOS1 module of TOUGH3.

B.2 Modelling concept

A hypothetical borehole (e.g., production or injection well) is assumed at a distance of 50 m from the HLW disposal area. Depending on the purpose of the borehole, different scenarios can be assessed to test whether the borehole could affect repository safety in a detrimental manner. Two scenarios were investigated:

- *Abandoned well scenario:* It is assumed that a deep borehole is drilled down to the base of the Keuper aquifer, an aquifer system of regional extent, exhibiting artesian conditions at the borehole location (1 MPa above hydrostatic). The borehole is placed at a lateral distance of 50 m from the outermost drift of the HLW repository in the siting region NL (see Fig. B-1). At the end of its service life, the borehole is insufficiently sealed. A permanent vertical flow of groundwater is established from the artesian Keuper aquifer to the hydrostatic Malm aquifer. The effect of this vertical flow in the abandoned well on the radionuclide release from the HLW repository is investigated by calculating the additional tracer flux into the well.
- *Geothermal well scenario:* It is assumed that in the distant future a geothermal well will be drilled to the aquifer systems below the Opalinus Clay (i.e., Keuper and Muschelkalk aquifer). Hydrostatic conditions prevail in both aquifers prior to the operational phase. The operating time of the geothermal well is 100 years and a pumping rate of 10 l/s is applied. The impact of the geothermal well on the barrier performance of the repository is evaluated by calculating the additional tracer flux into the well.

B.3 Model set-up

B.3.1 Mesh

The numerical model comprises the entire sequence of geological formations from the Permo-Carboniferous to the surface. The 3-D representation of the Mesozoic layer stack from top Malm to base Muschelkalk was from the geological model called LokMOD 2023 derived for Nördlich Lägern (see Nagra 2024m). The lateral extension of the model is restricted to the primary investigation perimeter. The HLW part of the repository was implemented with a nested rectangular IFD mesh in 3D based on the combined repository model in Nagra (2024g). The mesh was refined to model an additional well with an area of 1 m^2 at a distance of 50 m from the HLW repository, which connected the Malm with the Keuper aquifer. The model set up is shown in Fig. B-1.

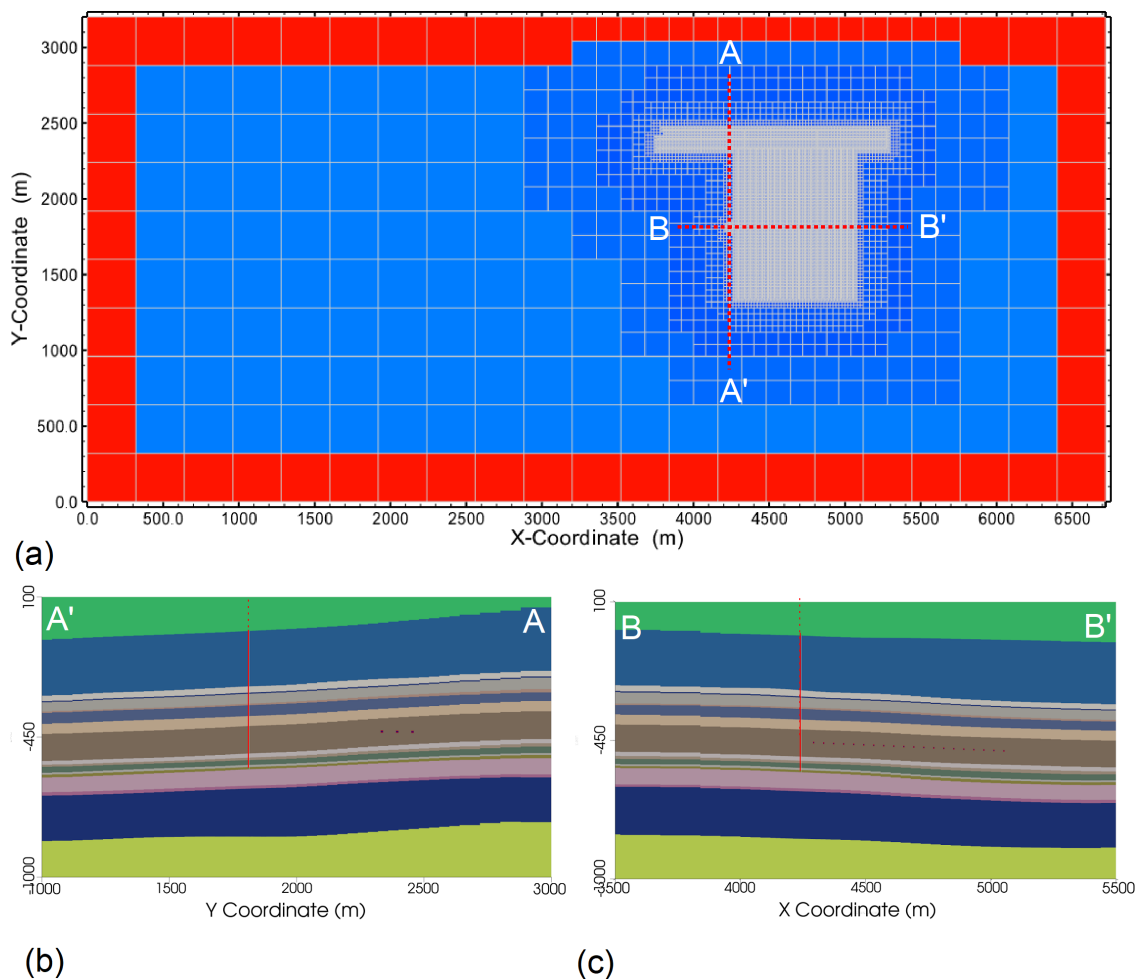


Fig. B-1: Model-based assessment of minimum distance to wells: model set-up

(a) Horizontal discretisation at repository level. The HLW repository and a well in 50 m distance of the HLW repository are implemented. Lateral boundary elements are indicated in the figure. Vertical cross-section through along the profiles A-A' and B-B' are presented in (b) and (c).

B.3.2 Parameters

Homogeneous hydraulic conductivities, diffusion coefficients and porosities are assigned to each lithostratigraphic unit, corresponding to the reference values (“best estimates”) given in Nagra (2024c). The properties of the site model and TH parameters for the geologic formations and the repository are based on the reference values provided in Nagra (2024m) and Nagra (2024e). A permeability of $1 \times 10^{-14} \text{ m}^2$ (transmissivity of $1 \times 10^{-7} \text{ m}^2/\text{s}$) was assigned to the well.

B.3.3 Boundary / initial conditions

Boundary and initial conditions typically correspond to near hydrostatic pressure conditions with constant pressure and temperature at the top of the model. The initial pressure assigned to the model elements (including boundary elements) were calculated on the elevation respectively depth bgl of each element assuming a 9.81 kPa/m vertical gradient, and initial temperature was calculated assuming a 0.043 °C/m geothermal gradient. A steady-state run was first carried out until pressure and temperature reach equilibrium (corresponding to undisturbed rock prior to a well construction). The model domain was assumed to be initially fully water saturated.

After the steady state run, Dirichlet boundary conditions were assigned to all lateral boundaries. A vertical flow through the abandoned well from the lower Keuper aquifer (KAL) to the Malm aquifer was activated by adding 1 MPa to the lateral boundary elements of the Keuper aquifer (KAL).

The abandoned well model was simulated for 2 million years to reach another equilibrium which was used to initialise the HLW repository model for the tracer simulation. To evaluate the tracer transport under consideration of an abandoned well, diffusive as well as advective transport was considered. The simulations of tracer transport through the stack of geological formations are performed using the EOS1 module of TOUGH3.

B.4 Source terms

For heat generation, average heat rates used for repository-scale modelling (Kombi) were used (see Nagra 2024e). The tracer source term used in the tracer simulations corresponds to an instantaneous release fraction (IRF₁₋₁₂₉) equal to 10% of initial activity of ¹²⁹I in the HLW inventory (Nagra 2024l), released at the HLW tunnel elements.

B.5 Results

Contour plots of tracer concentration for the abandoned well scenario are shown in Fig. B-2 for the time steps 100,000 years, 200,000 years and 1 mio years.

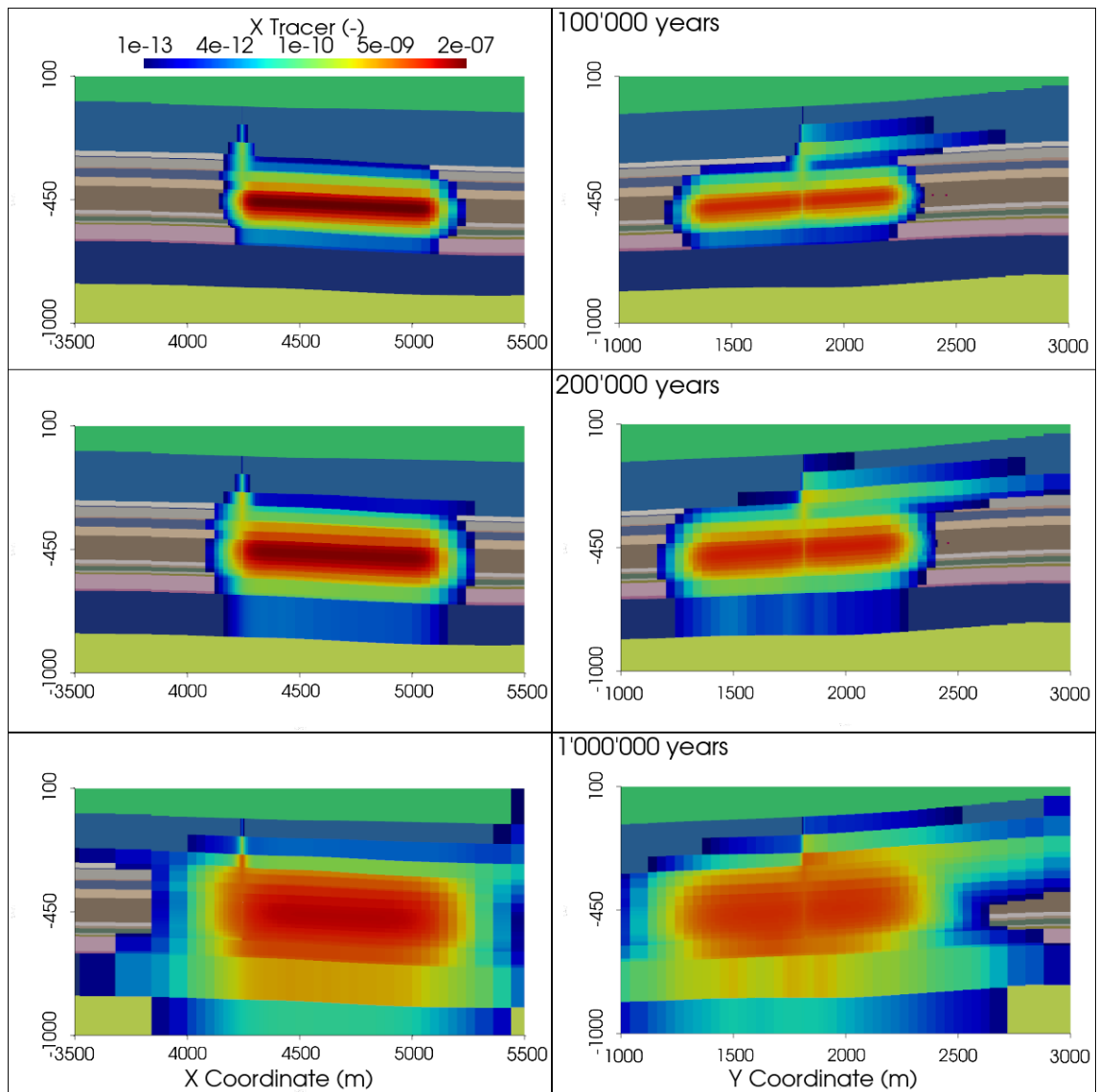


Fig. B-2: Abandoned well scenario: Contour plots of tracer concentration, released from the repository area at times steps 100,000, 200,000 and 1 million years

Left column: vertical cross section through the well perpendicular to the HLW drifts (profile A-A'); right column: vertical cross section through the well parallel to the HLW drifts (profile B-B').

App. C Confirmation of the repository footprint in the siting regions

C.1 Methodology

The screening process, aimed at mapping lateral variations of barrier performance of the host rock (Opalinus Clay) is carried out for generic footprint areas with a square base of $0.5 \times 0.5 \text{ km}^2$. Vertically, the repository is assumed to be located in the centre of the host rock formation. At repository level, a conservative, non-sorbing tracer is released with a constant source strength (i.e., as a step input function). Normalised tracer flux at top/base Opalinus Clay is deduced from the transport simulations, assuming that diffusion is the governing transport process. The simulations of tracer transport through the stack of geological formations are performed using the EOS1 module of TOUGH3.

C.1.1 Model geometry and transport parameters

A 3-D representation of the Mesozoic layer stack from top Malm to base Muschelkalk is derived for each site from the geological model called LOK-MOD 2023 (see Nagra 2024m). The lateral extension of the model is restricted to the primary investigation perimeter. Homogeneous hydraulic conductivities, diffusion coefficients and porosities are assigned to each lithostratigraphic unit, corresponding to the reference values (“best estimates”) given in Nagra (2024c). Note that the diffusion coefficients are corrected for the ambient temperature. For all sites, graphical representations of the geological models and tables with the flow and transport parameters are given in Tab. 5-6.

C.1.2 Boundary and initial conditions

Boundary and initial conditions typically correspond to near hydrostatic pressure conditions with constant pressure and temperature at the top and bottom of the model. No-flow conditions are assigned to all lateral boundaries.

The initial pressure assigned to the model elements (including boundary elements) are calculated on the elevation resp. depth bgl of each element assuming a 9.81 kPa/m vertical gradient.

The initial temperature distribution is obtained by interpolating borehole data available in the siting regions.

To allow for any redistribution and equilibration of pressure and temperature, a single-phase non-isothermal steady-state simulation is performed prior to any tracer release calculation (the steady-state simulation is repeated each time any of the materials or properties assigned to the model are changed). To evaluate diffusion effects separately, advection is turned off by setting absolute permeability to zero for all formations.

C.1.3 Tracer source terms

For the confirmation of repository placement, diffusion-dominated transport of a non-sorbing tracer is simulated with a single-phase transport simulation of tracer release. The considered locations of the repository are sampled throughout the model grid, either deterministically or stochastically. It is assumed that the footprint resp. release area has a size of $500 \times 500 \text{ m}^2$ with the tracer being released in the middle of the Opalinus Clay.

For simple model grids with a rectangular outer boundary (e.g., NL), a simpler deterministic approach is sufficient: each potential site is regularly spaced every 500 metres in both X and Y directions throughout the model.

However, for model grids with an arbitrarily shaped outer boundary (e.g., ZNO and JO), sampling regularly distributed point locations is not straightforward. In this case, the candidate site locations are sampled as follows:

- extract the outer boundary polygon (or convex hull) of the model grid;
- generate N samples evenly distributed on a 2D grid that covers the whole model grid (with N taken sufficiently large, e.g., $N = 10,000$);
- remove sampled points that fall outside of the outer boundary polygon;
- use the K-means clustering algorithm to cluster the remaining points into K regularly spaced groups;
- use the centroids of the K clusters as potential candidate site locations.

Once the site locations are sampled, the source elements where tracer is released are selected within a 500 by 500 m square centred around each sampled site location.

A hypothetical conservative tracer is released at a constant rate at the footprint of the emplacement field of the repository (total: 7.0×10^{-7} kg/s). Tracer is released in the transient transport simulation at a 1-m thick central layer representing the repository at the middle of the Opalinus Clay. Simulations of tracer breakthrough are carried out for all potential site locations, and tracer breakthrough curves are tracked at top Opalinus Clay.

C.1.4 Evaluation metrics

In the PA workflow the tracer flux TF of a conservative tracer, dissolved in the porewater and released from the repository field into the regional aquifer systems is the performance indicator for the model-supported assessment of safety function “immobilisation, retention and slow release of radionuclides”.

The evaluation metrics are based on the general assessment workflow developed for the performance indicator “tracer flux TF of a conservative tracer” (App. E.2). In brief, the following steps were executed:

- extraction of the breakthrough curves of tracer in terms of total tracer flux in [kg/s] from the Opalinus Clay to the upper confining units (“Brauner Dogger”);
- The total tracer flux is normalised by dividing by the total source term in [kg/s] released from the HLW near-field into the Opalinus Clay (Fig. C-1b, Fig. C-2b, Fig. C-3b).
- Calculation of the time derivative of the normalised tracer flux to get the normalised response of the system on an instantaneous release of the tracer. Derivation of the NTF index according to App. E.2.1.
- The calculated NTF indices are assigned to the 100 candidate site locations sampled (Fig. C-1a, Fig. C-2a, Fig. C-3a).
- The NTF values are interpolated on a regular grid which represents the siting regions (Fig. 4-8, Fig. 4-9, Fig. 4-10).

C.2 Results

C.2.1 Siting area JO

Tracer simulations were carried out at a total of 100 locations in the siting area JO (Fig. C-1a). Fig. C-1b shows the normalised tracer breakthrough curves for all the sampled release areas for JO. An average of 10% of the tracer has reached the upper confining unit after 1 million years.

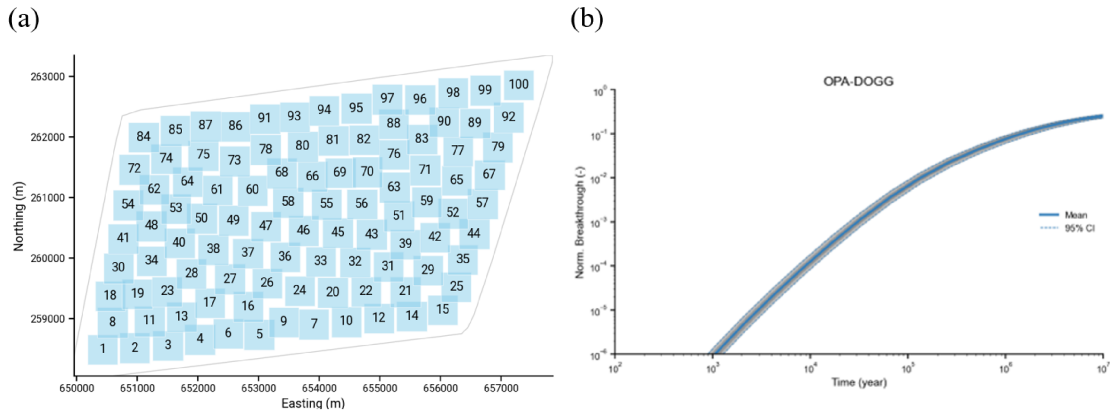


Fig. C-1: Confirmation of the repository footprint in the siting region JO

(a) Locations of sampled candidate sites for JO. (b) Normalised tracer breakthrough at the interface Opalinus-Dogger.

C.2.2 Siting area NL

Tracer simulations were carried out at a total of 100 locations in the siting area NL (Fig. C-2a). Fig. C-2b shows the normalised tracer breakthrough curves for all the sampled release areas for NL. An average of 10% of the tracer has reached the upper confining unit after 1 million years.

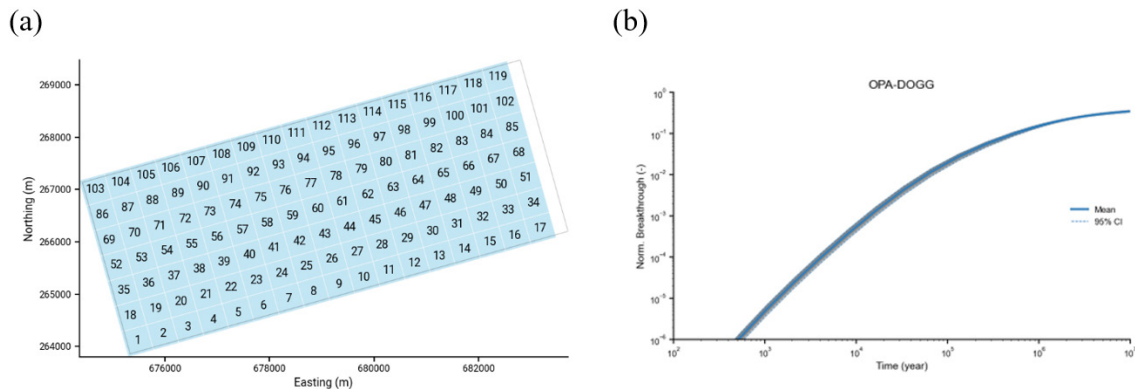


Fig. C-2: Confirmation of the repository footprint in the siting region NL

(a) Locations of sampled candidate sites for NL. (b) Normalised tracer breakthrough at the interface Opalinus-Dogger.

C.2.3 Siting area ZNO

Tracer simulations were carried out at a total of 100 locations in the siting area ZNO (Fig. C-3a). Fig. C-3b shows the normalised tracer breakthrough curves for all the sampled release areas for ZNO. An average of 10% of the tracer has reached the upper confining unit after 1 million years.

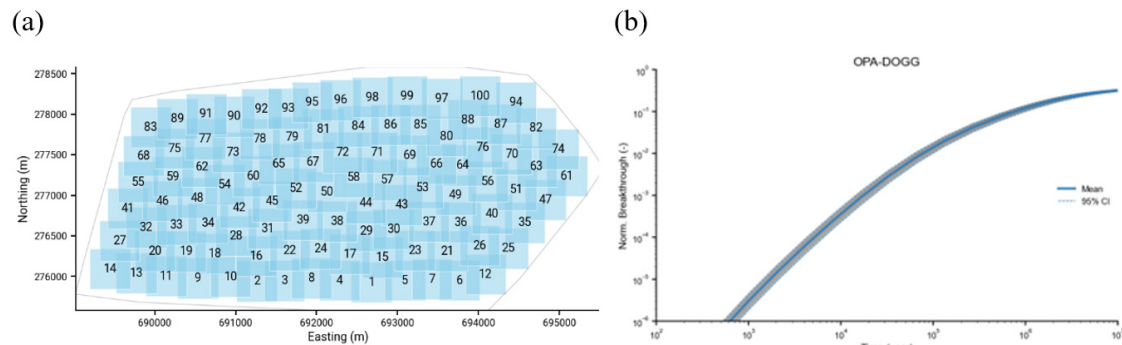


Fig. C-3: Confirmation of the repository footprint in the siting region ZNO

(a) Locations of sampled candidate sites for ZNO; (b) Normalised tracer breakthrough at the interface Opalinus-Dogger.

App. D Development of analytical solution for the extent of the EDZ

The Excavation Damaged Zone (EDZ) is one of the three assessment aspects (gas, heat, EDZ) to address as part of the qualitative assessment of the 13 SGT criteria (Criterion 2-3 “Repository-induced influences”). In all three siting regions, the Opalinus Clay formation is the host rock for the HLW and L/ILW repository projects, respectively. Known differences between the siting regions, which could have an impact on the extension of the EDZ are the thickness and the dip of the host-rock formation together with the depth of the repository level and the ambient stress regime.

D.1 Problem statement – performance indicator “Reduced Path Length in intact host Rock (RPL)”

The performance indicator “*Reduced Path Length in intact host Rock (RPL)*” was defined in Section 5.1.1 both for the HLW and the L/ILW repository. Assuming that the HLW disposal drifts are placed in the centre of the host rock, the RPI indicator was defined as:

$$RPL_{HLW} = \frac{M_{min,intact}}{0.5 \cdot M_{OPA} - r_{HLW} - D_{zmax,EDZ}}$$

where, M_{OPA} is the thickness of the host rock, r_{HLW} is the radius of the HLW drift and $D_{zmax,EDZ}$ is the maximum vertical extension of the EDZ around the HLW drift.

The specification of the RPL indicator for the L/ILW repository is complicated by the fact, that the L/ILW caverns will be placed horizontally in a slightly dipping host rock formation. Therefore, a further term Δl_{dip} must be considered in the specification of the RPI indicator, which represents is the distance of the mid-point of the L/ILW cavern to the centre of the Opalinus Clay:

$$RPL_{L/ILW} = \frac{M_{min,intact}}{0.5 \cdot M_{OPA} - r_{L/ILW} - D_{zmax,EDZ} - \Delta l_{dip}}$$

where, M_{OPA} is the thickness of the host rock, $r_{L/ILW}$ is the radius of the L/ILW cavern, $D_{zmax,EDZ}$ is the maximum vertical extension of the EDZ around the L/ILW cavern and Δl_{dip} is the distance of the mid-point of the L/ILW cavern to the centre of the Opalinus Clay.

D.2 Analytical solution development

Closed form solutions, although generally based on simplified geometric and constitutive assumptions, have the advantage that they allow large parametric studies to be carried out and can give a reliable estimation of the EDZ extent. Vu et al. (2013) proposed a semi-analytical solution which accounts for initial stress anisotropy as well as material anisotropy. The solution applies not only to the stresses and displacements along the tunnel wall, but also in the far field of the formation. In this section, only the principles of the solution are introduced but with a particular focus on validation of implementation. Details of the solution development can be found in the original publication of Vu et al. (2013).

D.2.1 Circular tunnel in a transversely isotropic linear elastic rock mass

During a rapid excavation in clay rock, the low permeability of the rock prevents significant water inflow, so the surrounding rock remains undrained. Because the rock is still saturated, the total stress concept can be applied. Vu et al. (2013) present an analytical solution for calculating the displacements and stresses around a circular tunnel in an infinite, transversely isotropic elastic medium under a uniform but cross-isotropic stress field. The model assumes a homogeneous and anisotropic initial stress state prior to excavation, with zero stress along the tunnel wall as a boundary condition, representing a fully excavated state. This analytical solution is implemented in Matlab and Python and validated through comparison with existing analytical solutions and numerical simulations.

D.2.2 Verification of implementation

The validation of the implementation consisted in comparing stresses and displacements at the tunnel wall, calculated using the implemented analytical solution of Vu et al. (2013), with those obtained from other numerical methods.

First, the results from Vu et al. (2013) were compared to an earlier analytical solution by Brady & Brown (1985) for an isotropic medium. Both solutions, applied to a tunnel of 1.5 meters in radius, showed excellent agreement in predicting stresses and displacements at the tunnel wall under anisotropic stress conditions. This demonstrates the accuracy of Vu et al.'s solution.

Additionally, another validation was carried out using finite element simulations (FEM) with Code_Aster software (Granet 2021) in a transversely isotropic medium to check the performance of Vu et al.'s solution across the entire domain surrounding the tunnel. The FEM model simulated a tunnel excavation under different elastic material properties and stress states. Three tests were conducted:

1. isotropic medium with isotropic stress
2. isotropic medium with anisotropic stress
3. transversely isotropic medium with anisotropic stress

For the first two tests (isotropic conditions), the analytical solution matched well with the FEM results. In the third test (transversely isotropic medium), slight deviations in horizontal stresses near the boundary were observed due to the finite model size used in FEM, compared to the infinite domain assumed in Vu et al.'s analytical solution.

In conclusion, the analytical solution of Vu et al. (2013) was successfully validated against both another analytical solution and finite element simulations, proving its robustness and accuracy for tunnel excavation problems.

D.3 Methodology for determination of EDZ extent

The methodology for determining the extent of the Excavation Damaged Zone (EDZ) consists in using plasticity models to identify areas where the material undergoes plastification due to stress changes after tunnel excavation. Two plasticity criteria are used:

1. Mohr-Coulomb model: This model uses cohesion (c) and the friction angle (ϕ) to assess failure based on the difference between the maximum (σ_1) and minimum (σ_3) principal stresses. Failure occurs when a specific function of these stresses equals zero.
2. McLamore & Gray (1967): This model adds complexity by considering the material's anisotropy, particularly for transversely isotropic rocks. It accounts for the dependence of the strength on the orientation of the maximum principle stress direction for transversely isotropic rocks. A modified cohesion parameter (c_0), dependent on the angle (θ) between the maximum principal stress and the bedding plane, is introduced.

The procedure to determine the plastic zone around the tunnel excavation consists of the following steps:

1. calculating the stress field after excavation using the implemented analytical solution;
2. determining the angle between the bedding plane and the maximum principal stress (if the McLamore and Gray model is adopted);
3. applying the selected plasticity model to compute the plastic potential;
4. estimating the maximum EDZ extents in the horizontal ($D_{EDZ,x}$) and vertical ($D_{EDZ,y}$) directions.

A hypothetical example is provided for a circular tunnel where the McLamore and Gray model is used to characterize the EDZ in a transversely isotropic material, with the vertical stress being higher than the horizontal (see Fig. D-1). The extents of the EDZ are determined in both the horizontal and vertical directions.

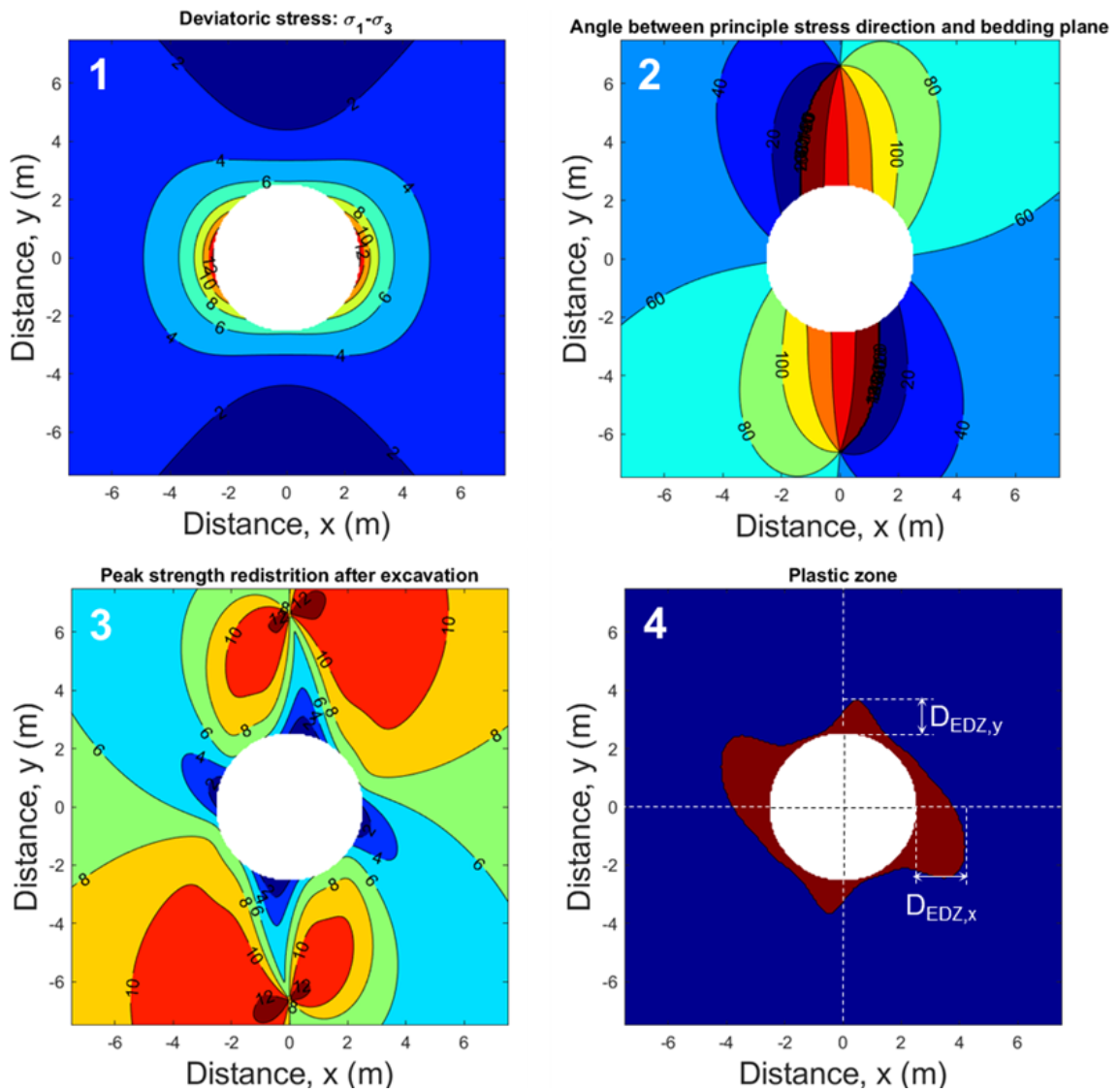


Fig. D-1: A hypothetical EDZ extent determination process for a circular tunnel (diameter 2.5 m)

The initial vertical stress is larger than the horizontal one, the material is transversely isotropic elastic and the McLamore and Gray plasticity model is adopted. The maximum EDZ extent is characterised in the horizontal and vertical directions by $D_{EDZ,x}$ and $D_{EDZ,y}$, respectively

D.4 Determination of the vertical extent of EDZ for the site-specific HLW projects

Stress conditions at the repository sites and geomechanical material properties of the Opalinus Clay were derived from NAB 24-10. The best guess parameters correspond to the base case calculations. Tab. D-1 provides the bandwidth of the principal stress components (S_h , S_H and S_v) in terms of “lowest”, “best guess” and “highest” values at depth levels between 400 and 1,000 m.

Tab. D-1: Principal stress components in the Opalinus Clay derived from NAB 24-10

The stresses are calculated for depths between 400 and 1,000 m b.g.).

	Shmin					SHmax					Sv
Depth [m.b.g.]	Shmin lowest [MPa]	Shmin lower bound [MPa]	Shmin best guess [MPa]	Shmin upper bound [MPa]	Shmin highest [MPa]	SHmax lowest [MPa]	SHmax lower bound [MPa]	SHmax best guess [MPa]	SHmax upper bound [MPa]	SHmax highest [MPa]	Approximate* [MPa]
400	6.8	7.4	7.6	7.9	8.5	7.0	7.8	8.5	9.1	10.4	9.6
450	7.7	8.3	8.6	8.8	9.5	7.9	8.8	9.5	10.3	11.7	10.8
500	8.5	9.2	9.5	9.8	10.6	8.7	9.7	10.6	11.4	13.0	12.0
550	9.4	10.1	10.5	10.8	11.7	9.6	10.7	11.7	12.6	14.2	13.2
600	10.2	11.1	11.4	11.8	12.7	10.5	11.7	12.7	13.7	15.5	14.4
650	11.1	12.0	12.4	12.8	13.8	11.3	12.7	13.8	14.8	16.8	15.6
700	11.9	12.9	13.3	13.8	14.9	12.2	13.6	14.8	16.0	18.1	16.8
750	12.8	13.8	14.3	14.7	15.9	13.1	14.6	15.9	17.1	19.4	18.0
800	13.6	14.8	15.3	15.7	17.0	14.0	15.6	17.0	18.3	20.7	19.2
850	14.5	15.7	16.2	16.7	18.0	14.8	16.5	18.0	19.4	22.0	20.4
900	15.3	16.6	17.2	17.7	19.1	15.7	17.5	19.1	20.5	23.3	21.6
950	16.2	17.5	18.1	18.7	20.2	16.6	18.5	20.2	21.7	24.6	22.8
1000	17.0	18.5	19.1	19.7	21.2	17.4	19.5	21.2	22.8	25.9	24.0

The geomechanical properties extracted from Nagra (2024c) comprise two complementary sets of stiffness and strength parameters of the Opalinus Clay. The two data sets represent a wide spectrum of geomechanical conditions in the repository nearfield, ranging from expected to unfavourable conditions (Tab. D-1). The parameters in Tab. D-1 were used to specify probability density functions of the input parameters for the probabilistic simulations of the extent of the EDZ.

Fig. D-2 to Fig. D-4 show the scatter plot matrices of 10,000 Latin Hypercube samples, comprising all uncertain model input parameters considered for the calculation of the vertical extent of the EDZ for all addressed repository configurations (JO-HLW & L/ILW; NL-HLW & L/ILW; ZNO-HLW & L/ILW).

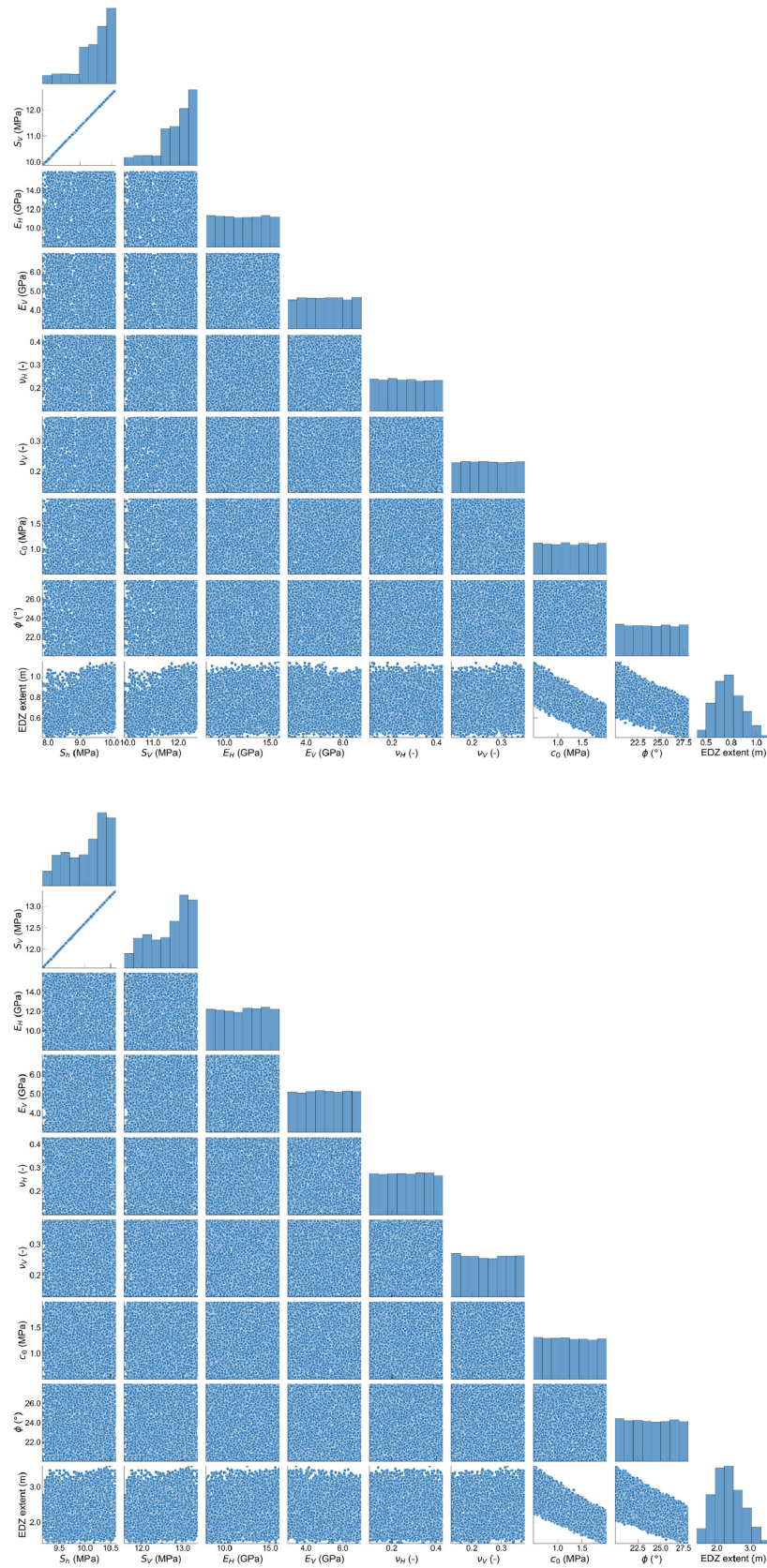


Fig. D-2: Scatter plot matrices of 10,000 Latin Hypercube samples for all model parameters considered for the repository projects HLW-JO (top) and L/ILW-JO (bottom)

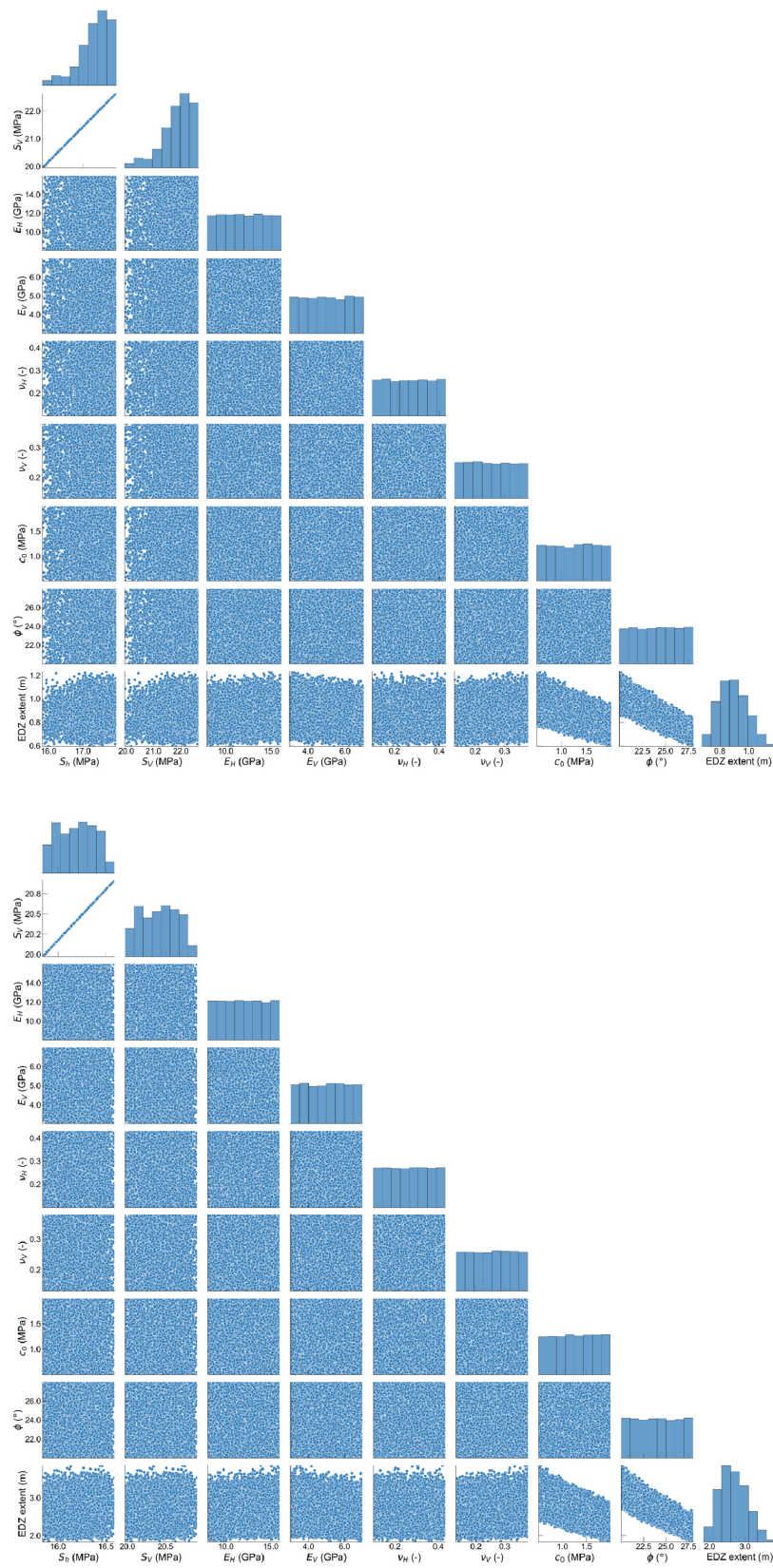


Fig. D-3: Scatter plot matrices of 10,000 Latin Hypercube samples for all model parameters considered for the repository projects HLW-NL (top) and L/ILW-NL (bottom)

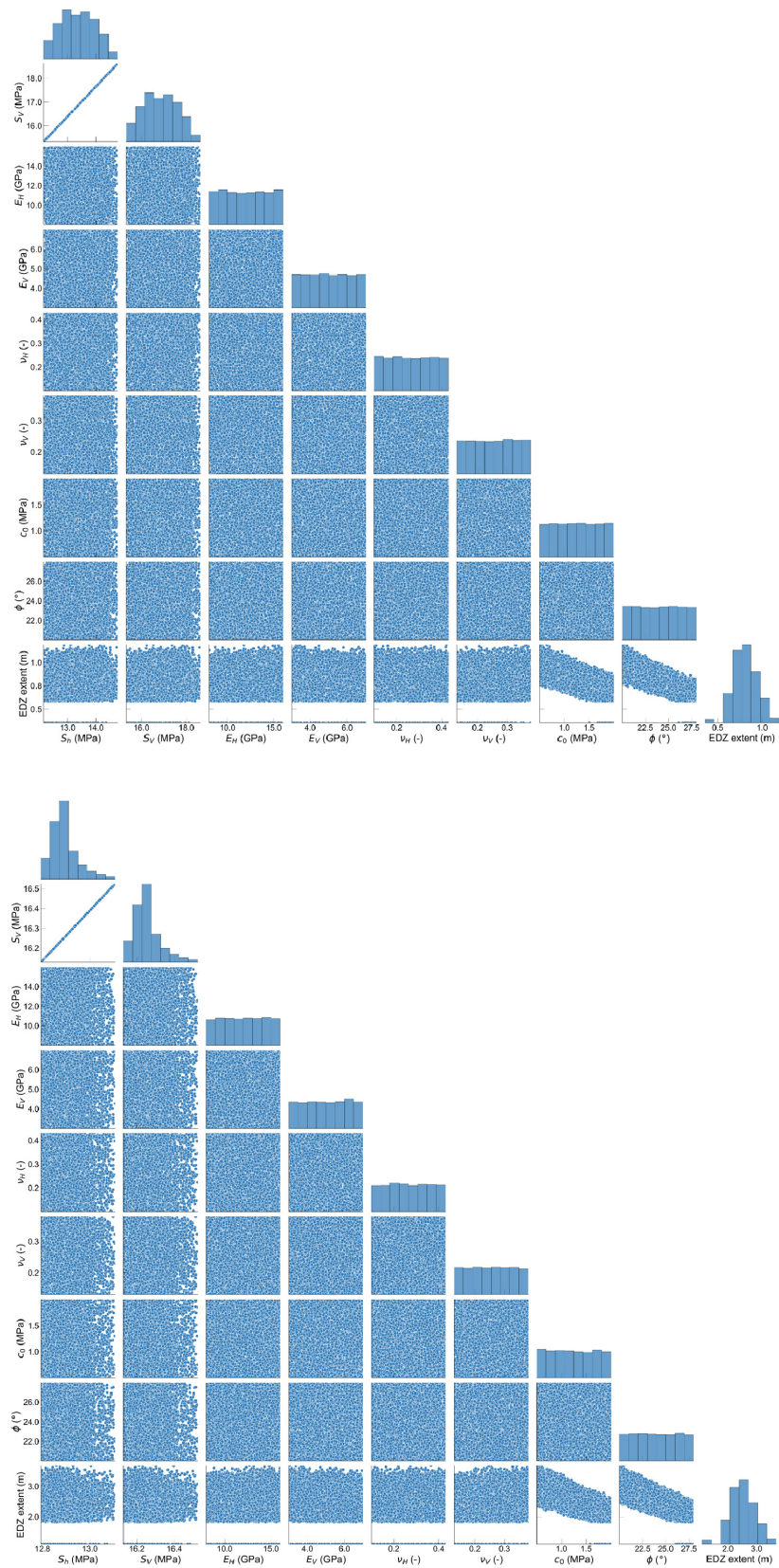


Fig. D-4: Scatter plot matrices of 10,000 Latin Hypercube samples for all model parameters considered for the repository projects HLW-ZNO (top) and L/ILW-ZNO (bottom)

D.5 Consistency with the results in support of license application

A numerical fracture network approach was developed in Nagra (2014) with emphasis on an adequate representation of the hydro-mechanical conditions in the EDZ, covering the full range of hydraulic regimes, from the fracture dominated, with localised pore-water flow during early times, to the matrix-dominated distributed flow in the late times. The workflow consists of three main steps carried out sequentially (Fig. D-5). First, a hybrid finite-discrete element method is used to simulate the geometry and geomechanical conditions of the discrete fracture networks forming the EDZ, which allows to solve the fluid motion equations in the excavation near-field. A salient feature of the suggested approach is that hydraulic parameters of both fracture and matrix evolve over time as a response to re-saturation of the tunnel surroundings. Finally, an abstraction of the complex model is made based on the late time behaviour (after full re-saturation) of the system.

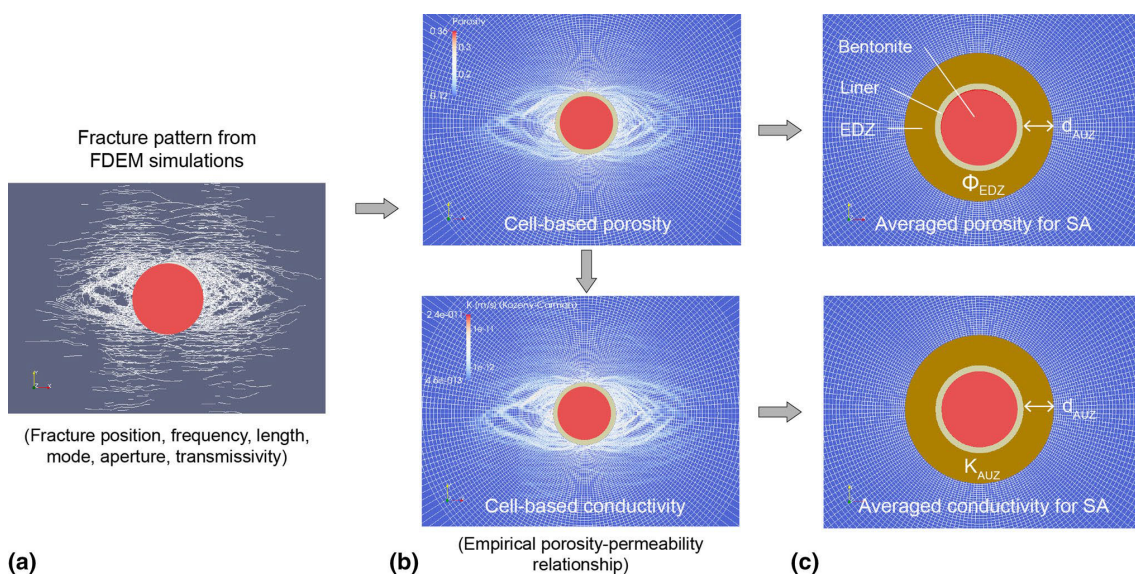


Fig. D-5: Concept of the EDZ abstraction procedure for safety assessment (SA) applicable for a circular tunnel

After NTB 14-02 / Dossier 4

(a) representative fracture patterns are simulated for relevant repository configurations with a discrete element model; (b) the discrete fracture patterns are converted in heterogeneous porosity and hydraulic conductivity distributions; (c) in a final abstraction process, the heterogeneous porosity and conductivity distributions are converted into a shell defined by a radius and homogeneous porosity and conductivity.

Fracture network simulations on the EDZ formation for L/ILW and SF/HLW emplacement tunnels and the operations shaft were carried out for repository for HLW and L/ILW at the Haberstal site (NTB 24-22 / Appendix B.2). Exemplarily, the simulated aperture and slip of the fractures for two cases with different rock strength is shown in Fig. D-6. As observed in the plot, the region near the excavation boundary has the greatest aperture and slip. Regions of significant shear displacement are bedding parallel fractures above/below the crown/floor and conjugate shear fractures in the sidewalls.

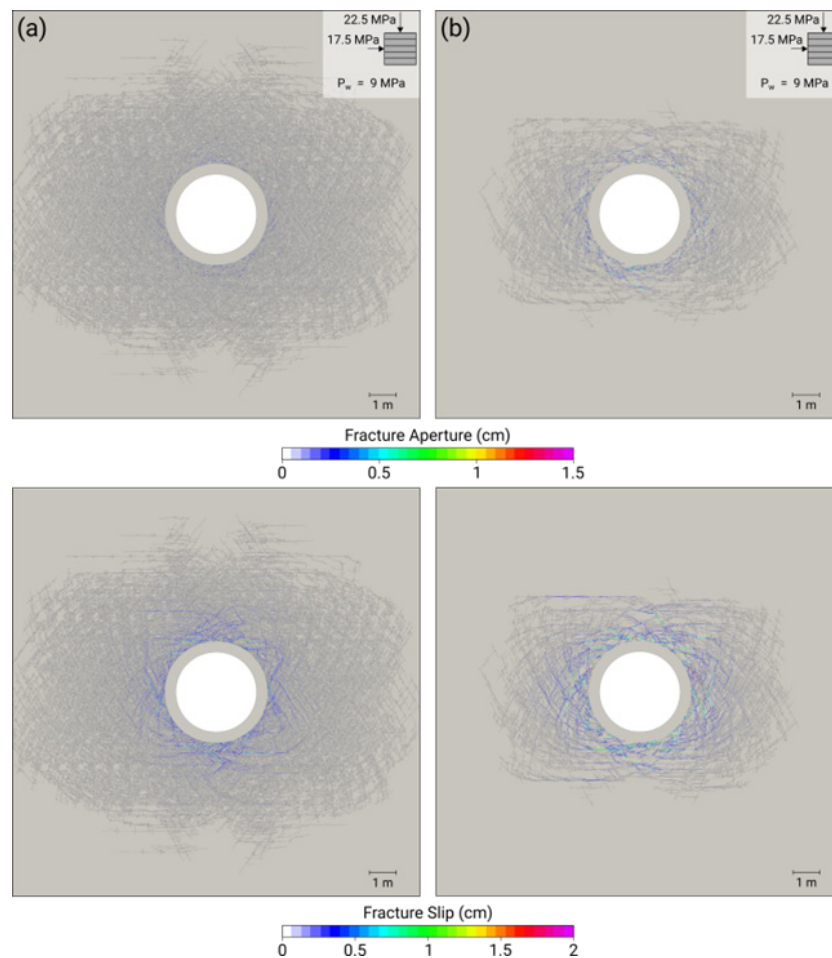


Fig. D-6: Fracture aperture (top) and slip (bottom) contours for HLW tunnel models with minimum horizontal in-situ stress ($\sigma_h = 17.5$ MPa) for (a) lower bound and (b) upper bound strength calibrations

From NTB 24-22 / Appendix B.2

The outputs of the fracture pattern simulations were analysed with the numerical approach in Nagra (2014). Following the abstraction procedure in Fig. D-5, radial porosity and radial conductivity profiles were calculated, which were finally converted into a shell defined by a radius and equivalent homogeneous porosity and conductivity (Fig. D-7).

Despite of the fundamental differences in the derivation of the extent of the EDZ, it can be concluded that both the analytical approach and the numerical fracture network approach lead to quite similar estimates of the extent of the EDZ. The fracture mechanics model indicates for the HLW drifts, that the zone of significant porosity and permeability changes is limited to around 1 m, whereas the zone of significant porosity changes around the L/ILW cavern ranges between 2.5 and 3 m. These results fit quite well with the semi-analytical solution, which has been used in the present report.

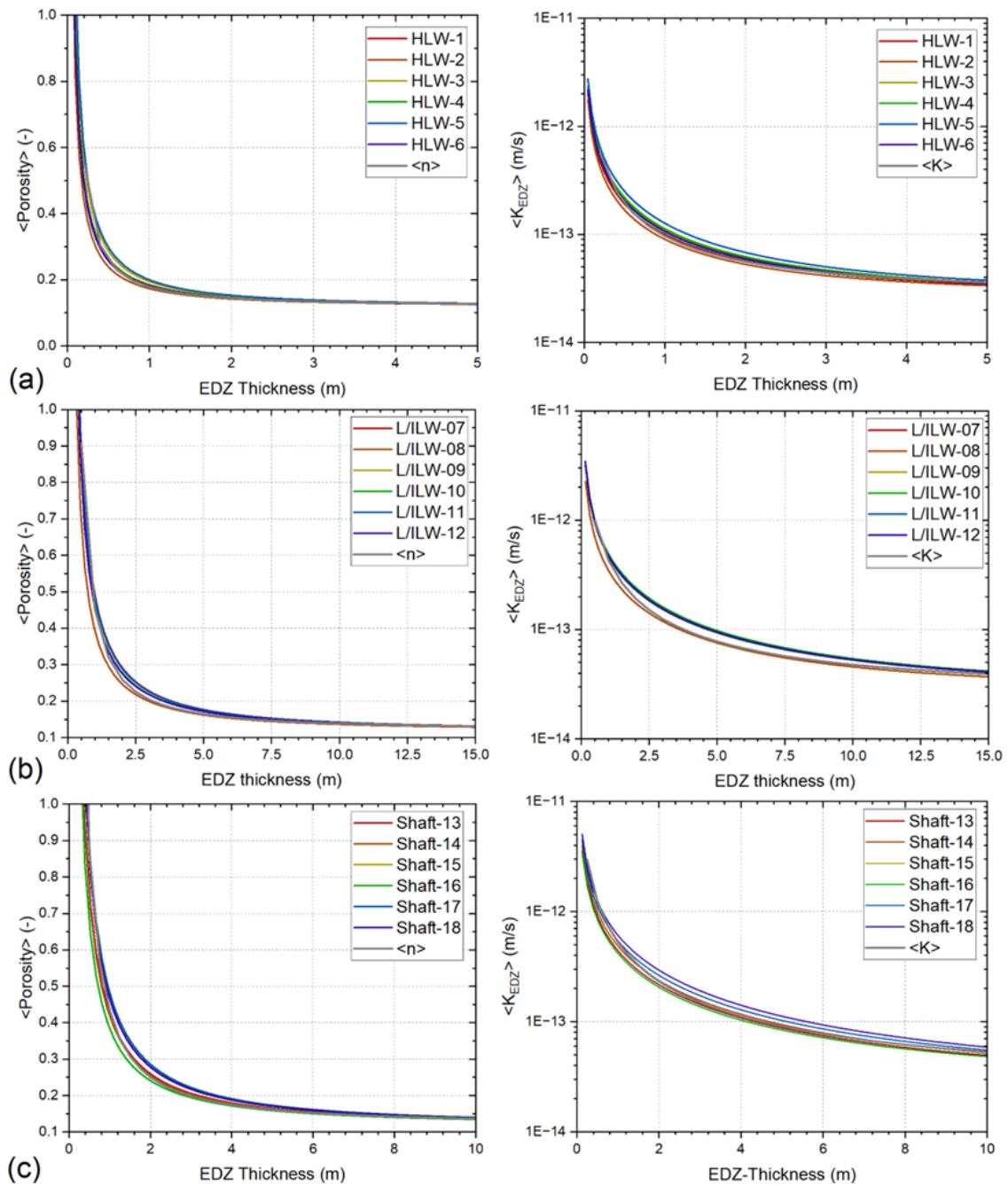


Fig. D-7: Radial profiles of equivalent porosity and equivalent hydraulic conductivity derived from the corresponding radial profiles

(a) HLW tunnels, (b) L/ILW caverns

From NTB 24-22 / Appendix B.2

App. E Performance indices

E.1 Dimensionless performance index FPI (failure potential of the intact rock)

E.1.1 Derivation of the performance index FPI

From a long-term safety perspective, it is desirable to avoid shear (or tensile) failure in the host rock due to gas-induced and thermally-induced overpressures. The possibility of shear/tensile failure can be assessed using the performance indicator FPI. In case of thermally induced porewater overpressures the indicator is called FPI_{Heat} , gas-induced overpressures are associated with the indicator FPI_{Gas} .

Assuming the applicability of the Mohr-Coulomb criterion for shear failure, the FPI can be expressed as:

$$FPI = \frac{\tau}{\tau_{max}} = \frac{q}{q_{max}} \quad E-1$$

where τ is the shear stress, τ_{max} is the maximum shear stress that can be accommodated by the rock without failure and q , q_{max} are the corresponding deviator stresses. For stress path analyses it is convenient to use the mean effective stress p' and the deviator stress q , which are formulated here as octahedral stresses:

$$q = \sqrt{\frac{(\sigma_H - \sigma_h)^2 + (\sigma_H - \sigma_v)^2 + (\sigma_h - \sigma_v)^2}{2}} \quad E-2$$

$$p' = \frac{\sigma_H + \sigma_h + \sigma_v}{3} - p_w \quad E-3$$

where σ_H , σ_h and σ_v are the principal stress components and p_w represents the pore pressure. The Mohr-Coulomb criterion is formulated in terms of a deviator stress q_{max} using:

$$q_{max} = a + M \cdot p' \quad E-4$$

where the slope M and the intercept a from the drained friction angle φ' and cohesion c' as:

$$M = \frac{6 \cdot \sin \varphi'}{3 - \sin \varphi'} \quad E-5$$

and

$$a = c' \cdot \frac{6 \cdot \cos \varphi'}{3 - \sin \varphi'} \quad E-6$$

In cases when non-isothermal conditions apply (e.g.; thermally induced porewater overpressures), temperature changes ΔT do not only affect the porewater pressure (thermal expansion of the fluid) but create also a change of total stress $\Delta\sigma_T$. In the TOUGH code, the impact of temperature changes on the fluid and the rock skeleton is addressed by the temperature dependence of fluid viscosity and fluid density and by the thermal expansion of the rock.

In the stress path analysis, temperature dependence of total stress can be considered in the effective stress formulation:

$$p'(T) = \left(\frac{\sigma_H + \sigma_h + \sigma_v}{3} \right)_{ini} - p_w(T) + \Delta\sigma_T \quad \text{E-7}$$

with:

$$\Delta\sigma_T = \frac{3 \cdot E \cdot \alpha_s \cdot \Delta T}{1 - 2 \cdot \nu} \quad \text{E-8}$$

and

$$\alpha_s = \frac{\alpha_T \cdot n}{3 \cdot (1 - n)} \quad \text{E-9}$$

where E is the Young's modulus, α_s is the thermal expansion coefficient of the solid, ν is Poisson's ratio, α_T is thermal pore expansivity and n is porosity. Note that the thermal stress component assumes constant volume conditions. In the case of gas induced porewater overpressures, temperatures does not significantly affect the stress path.

A graphical representation of the Mohr circle used to evaluate the failure potential is given in Fig. E-1. The increase of porewater pressure in the host rock due to gas production or thermal expansion of the porewater will shift the Mohr circle towards low effective stress. If a significant change of total stress $\Delta\sigma_T$ must be considered, this would cause a shift towards higher effective stresses. Shear failure occurs when the Mohr circle hits the Mohr-Coulomb failure line, corresponding to the performance target / performance limit $FPI = 1$. Shear failure is omitted when $FPI < 1$.

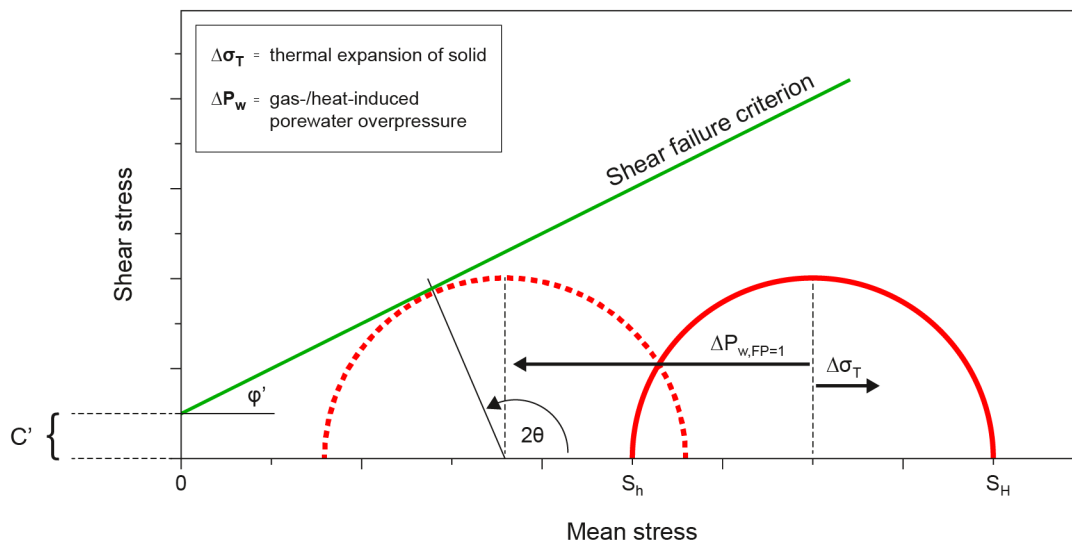


Fig. E-1: Shear failure of the intact host rock in response to gas- and heat induced porewater overpressures presented as a Mohr diagram

E.1.2 Indicator based assessments using of FPI_{Heat} and FPI_{Gas}

Model-based assessment using the performance index FPI were carried out for the assessment of:

- thermally induced overpressures in the host rock above the HLW drifts (FPI_{Heat});
- gas induced overpressures in the host rock above the HLW drifts (FPI_{Gas});
- gas induced overpressures in the host rock above the L/ILW caverns (FPI_{Gas}).

The calculation workflow for each version of the FPI index is described in greater detail in the following paragraphs.

Thermally induced overpressures in the host rock above the HLW drifts (FPI_{Heat})

TH-simulations of pore pressure evolution in the HLW repository nearfield are carried out with the 2-D models presented in Fig. 5-10. The control point for calculating the FPI index is located 20 m above the HLW drift in the centre of the repository as shown in Fig. E-2.

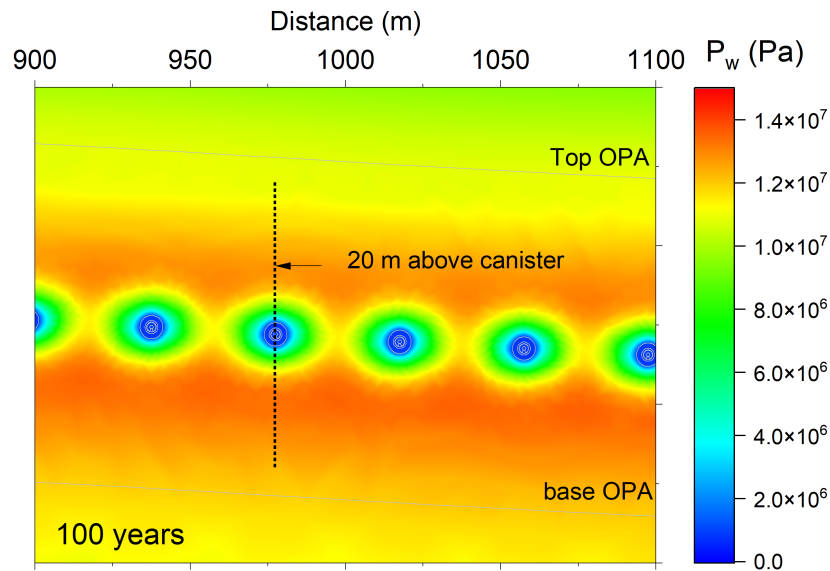


Fig. E-2: Control point for calculating the performance indicator FPI_{Heat}.

The strength parameters of the Opalinus Clay refer to post peak strength ($c' = 1.3$ MPa, $\phi' = 24^\circ$). The principal stress components at the location of the control point were derived by interpolation of depth from Tab. D-1. The estimation of the change of total stress $\Delta\sigma_T$ with temperature was carried out with the following parameters: $E = 7$ GPa, $\nu = 0.27$, $\alpha_T = 1.7 \times 10^{-5}$ 1/°C, $n = 0.115$.

Gas induced overpressures in the host rock above the HLW drifts (FPI_{Gas})

TH-simulations of heat- and gas-related pore pressure evolution in the HLW repository nearfield were carried out with the same 2-D models presented in Fig. 5-10. The control point for calculating the FPI_{Gas} index is at the interface between EDZ and host rock in the centre of the repository as shown in Fig. E-3.

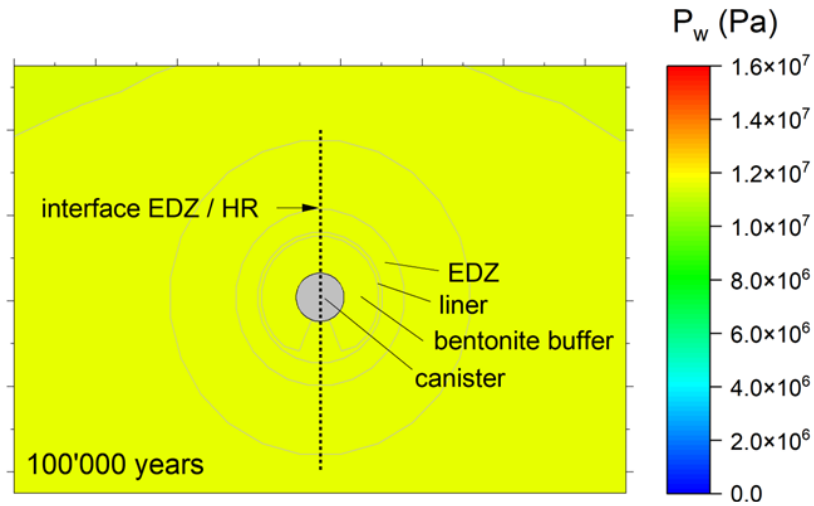


Fig. E-3: Control point for calculating the performance indicator FPI_{Gas}

The strength parameters of the Opalinus Clay refer to post peak strength ($c' = 1.3$ MPa, $\phi' = 24^\circ$). The principal stress components at the location of the control point were derived by interpolation of depth from Tab. D-1. The estimation of the change of total stress $\Delta\sigma_T$ with temperature was omitted, because temperature changes at late times are small.

Gas induced overpressures in the host rock above the L/ILW caverns (FPI_{Gas})

TH-simulations of gas-related pore pressure evolution in the L/ILW repository nearfield were carried out with the 2.5-D models presented in Fig. 5-15. The control point for calculating the FPI_{Gas} index is at the interface between EDZ and host rock in the centre of the repository as shown in Fig. E-4.

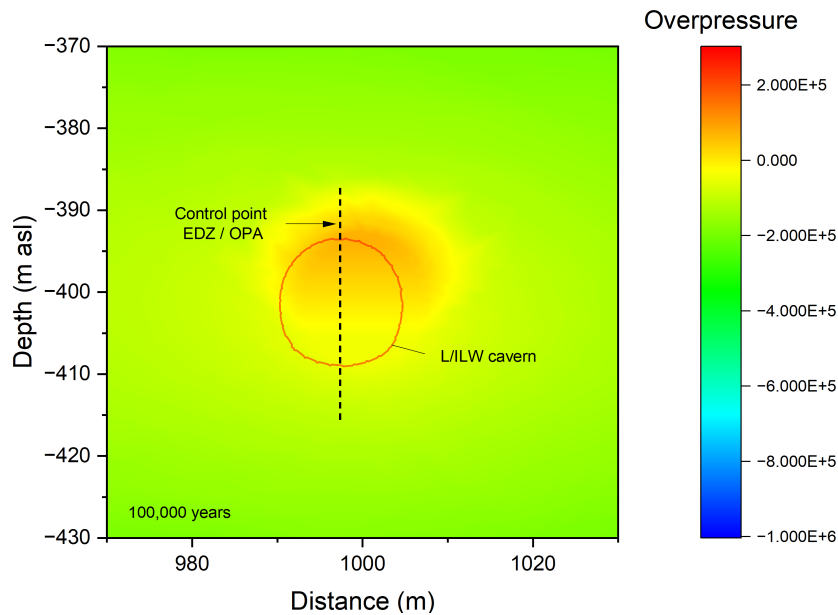


Fig. E-4: Control point for calculating the performance indicator FPI_{Gas}

The strength parameters of the Opalinus Clay refer to post peak strength ($c' = 1.3$ MPa, $\phi' = 24^\circ$). The principal stress components at the location of the control point were derived by interpolation of depth from Tab. D-1. The estimation of the change of total stress $\Delta\sigma_T$ with temperature was omitted, because temperature changes at late times are small.

E.2 Dimensionless Performance index NTF

In the PA workflow the tracer flux TF of a conservative tracer, dissolved in the porewater and released from the repository field into the regional aquifer systems is the performance indicator for the model-supported assessment of safety function “immobilisation, retention and slow release of radionuclides”. It is assumed that the dissolved radionuclide released as an instantaneous pulse from the buffer near-field into the host rock, from where it spreads out towards regional aquifer systems at the top/bottom of the CRZ. Tracer flux is calculated with a 2D transport model (TOUGH3/EOS1), representing a vertical cross-section through the centre of the HLW repository and comprising the entire Mesozoic layer stack. Fig. E-5a presents the example of the HLW repository at NL from surface to the base of the Permo-Carbonate. Base Malm, top Keuper and top Muschelkalk are also indicated, representing the upper and lower bounds of the CRZ (note: the Muschelkalk represents the regional aquifer below the Opalinus Clay in the alternative scenario used in criterion 3.2). The 20 HLW drifts in the centre of the Opalinus Clay formation are marked in red. Fig. E-5b presents the concentration of the non-sorbing tracer after 1 mio years released from the HLW drift and propagating towards the upper and lower regional aquifers.

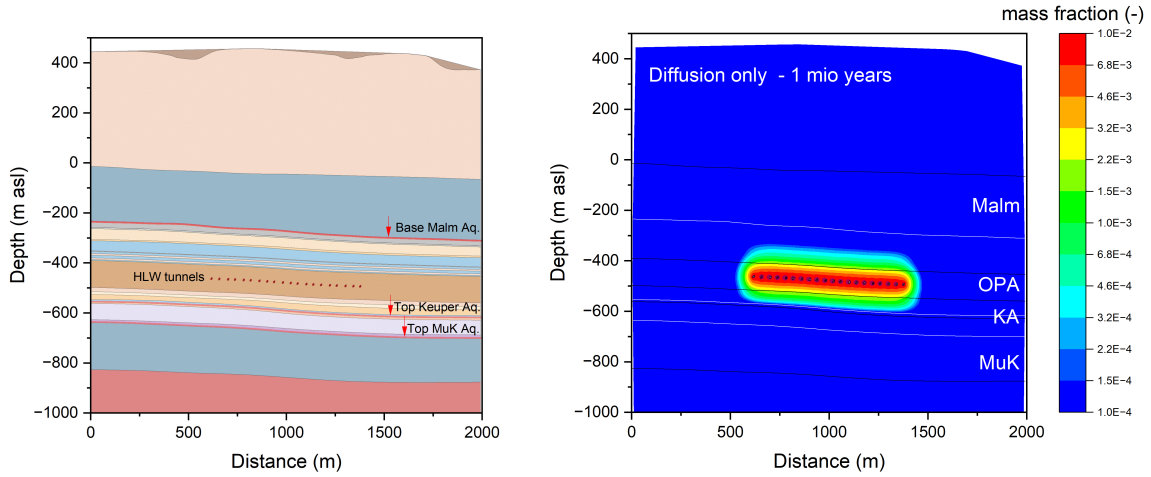


Fig. E-5: Model setup for the derivation of the HLW performance indicator TF_{I-129}

From Nagra (2024l)

(a) vertical cross-section through the centre of the HLW repository in Nördlich Lägern, comprising the entire Mesozoic layer stack, (b) simulation of tracer transport from the repository structures towards the top and base of the CRZ.

The dose-relevant radionuclide for the HLW repository is ^{129}I and the corresponding performance indicator is called TF_{I-129} . A source strength, which represents in a simplified manner the release rates applied in the safety assessment calculations (see Nagra 2024j), is used in the numerical simulations to ensure representative estimates of the expected maximum tracer fluxes. For ^{129}I , it is assumed that 10% of the total inventory of radionuclide are released instantaneously after canister breaching (see Nagra 2024l for further details). The total tracer flux, TF_{I-129} in [Bq/a], is calculated as the sum of tracer fluxes passing the base of the Malm and top of the Keuper aquifers. For this, the transients of the local tracer flux $F(y, z_{\text{top/base CRZ}}, t)$ in [Bq/(a·m)] at top / base CRZ are extracted from the 2-D model. The total tracer flux TF_{I-129} released from the CRZ into the aquifer systems is calculated by spatial integration of the tracer profiles $F(y, z_{\text{top CRZ}}, t)$ and $F(y, z_{\text{base CRZ}}, t)$ along the lateral extent w of the model and multiplication with the decay factor:

$$TF_{I-129}(t) = \left[\int_0^w \left(F(y, z_{\text{top CRZ}}, t) + F(y, z_{\text{base CRZ}}, t) \right) dy \right] \cdot e^{-\lambda \cdot t}$$

in [Bq/a], where λ represents the decay time of ^{129}I ($\lambda_{I-129} = 4.41 \cdot 10^{-8} \text{ a}^{-1}$).

E.2.1 Derivation of the performance index NTF

The dimensionless performance index NTF_{I-129} is derived by conversion and normalization of TF_{I-129} :

$$NTF_{I-129}(t) = \frac{TF_{I-129}(t) \left[\frac{Bq}{a} \right] \times BCDF \left[\frac{Sv}{Bq} \right] \times 1000}{0.1 \left[\frac{mSv}{a} \right]}$$

where

$$BCDF = 6,32 \cdot 10^{-13} \left[\frac{Sv}{Bq} \right]$$

represents the biosphere conversion factor for the present-day climate and the normalization factor 0.1 mSv/a corresponds to the regulatory dose limit.

The performance index NTF_{I-129} is defined in such a way that a value greater than one indicates a CRZ that is deemed unacceptable with respect to the regulatory dose limit. Lower index values imply an increasingly favourable performance of the CRZ. The evaluation scale in Tab. E-1 is adopted for the for assessment of the performance of the CRZ of the HLW repository as a transport barrier.

Tab. E-1: Evaluation scale for assessing the performance of the CRZ of the HLW repository with the dimensionless performance index $NTFCRZ, I-129$

Quality level	Performance index
Very favourable	$NTF_{I-129} < 0.001$
Favourable	$0.001 \leq NTF_{I-129} < 0.01$
Less favourable	$0.01 \leq NTF_{I-129} < 0.1$
Unfavourable	$0.1 \leq NTF_{I-129} < 1$
Unacceptable	$NTF_{I-129} \geq 1$