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Comparing modelling approaches for a generic nuclear waste repository in salt

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ABSTRACT

This paper contains a comparison of five modelling approaches for a simplified nuclear waste repository in a domal salt formation. It is the result of a four-year collaboration between five international teams on Task F of the DECOVALEX-2023 project on performance assessment modelling. The primary objectives of Task F are to build confidence in the models, methods, and software used for performance assessment (PA) of deep geologic nuclear waste repositories, and/or to bring to the fore additional research and development needed to improve PA methodologies. This work demonstrates how these objectives are accomplished through staged development and comparison of the models and methods used by participating teams in their PA frameworks. Participating teams made a wide range of model assumptions, ranging from compartmentalized networks to full 3D models of the salt formation and repository. Despite differences in the modelling strategies, all models indicate that salt compaction and diffusion of radionuclides in brine are key processes in the repository. For the isothermal spent nuclear fuel and vitrified waste scenario with multiple early failures considered, all models indicate little of the disposed radionuclides will migrate beyond the repository seal over the 100,000-year simulations. In general, the model output quantities have the largest differences over the short term and near the waste. Disparities between the models are believed to be due to differing simplifications from the conceptual model.

1. Introduction

Disposal of spent nuclear fuel and radioactive waste remains an open challenge in most countries. The present work is focused on comparison of computational methods for assessing performance of a simplified, generic nuclear waste repository in a domal salt geological formation to further the goal of safe, long-term disposal of radioactive waste.

Performance Assessment (PA) is a decision-management tool that provides information from quantitative evaluations of the behaviour of a complex system. PA involves evaluating the level of confidence (considering identified uncertainties) in the estimated performance of the system and seeks to provide reasonable assurance that the system will meet applicable safety standards. In the context of nuclear waste disposal, the complex system is a geological repository for nuclear waste, which consists of the waste forms, the engineered barrier system within the repository, and the geological natural barrier system surrounding the repository. PA is used in an iterative fashion to support site selection, site characterization, and repository design, and to inform data collection and model development throughout the lifetime of a repository program.

At any iteration, the first steps of the PA process for nuclear waste disposal are to establish the assessment context, part of which is to develop performance measures and conceptual models of the repository system from knowledge of the natural and engineered system

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components (Fig. 1). One or more computational models appropriate for forward simulation of the system and calculation of performance measures is developed. Then performance measures are calculated, uncertainty and sensitivity analysis are performed, and results are synthesized.

PA models are not predictive forward models, but rather illustrations of plausible outcomes under realistic, but conservative assumptions. There are multiple justifiable ways of constructing PA models to investigate evolution of a given system which will lead to different results, and differences compound when coupled processes are present. Moreover, calibration of PA models is limited by the timescale and size of a repository, and so uncertainties are large.

DECOVALEX is an international cooperative project focused on modelling challenges of importance to radioactive waste disposal. This paper is the result of a DECOVALEX-2023 (https://decovalex.org/) task that is focused on comparison of the models and methods used in post-closure PA of deep geologic repositories, in the present case a salt dome. This task is about international experts learning from each other different approaches for constructing PA models in domal salt and illustrates how and why differences in key modelling output occur. This project also strives to give a high-level view on whether these differences are likely to be significant from a safety perspective: are the models collectively robust in support of likely key safety arguments, such as indicating sufficiently low release from the repository?

The objectives have been accomplished through a staged comparison of the models and methods used by the five participating teams, shown in Table 1, for deterministic simulation(s) of models for the defined reference case scenario.[2] This is an unusual DECOVALEX task in that it consists of model comparison only, and there is no component of interpreting new field or laboratory data. The task specification has been updated continuously since the initiation of the project in 2020 as complexity has been added and removed as the design of the generic disposal system was refined. The final version contains the complete specification for creation of deterministic crystalline and salt reference cases.[2] A comparison of models developed by five international teams for the salt reference case is the focus of the present work.

Forward modelling requires information characterizing the repository system and its subsystems. For the present code comparison, it is assumed that sufficient geological and engineering data are available to develop a suitable PA model and that key features, events, and processes (FEPs) and their associated uncertainties have been identified for uncertainty quantification and sensitivity assessment.

Conceptual models describe the key FEPs affecting performance measures and their interactions. Each participating team works from a common data set provided in the task specification[2] to develop their own conceptual and computational models for evolution of the repository system. The interpretation of the simulation results is focused on performance measures indicative of the ability of the disposal system to isolate radionuclides in the subsurface through containment and retardation. Performance measures include those related to the overall performance of the repository system and those related to the performance of individual components of the engineered or natural system, such as resaturation and radionuclide transport from one component of the system to another.

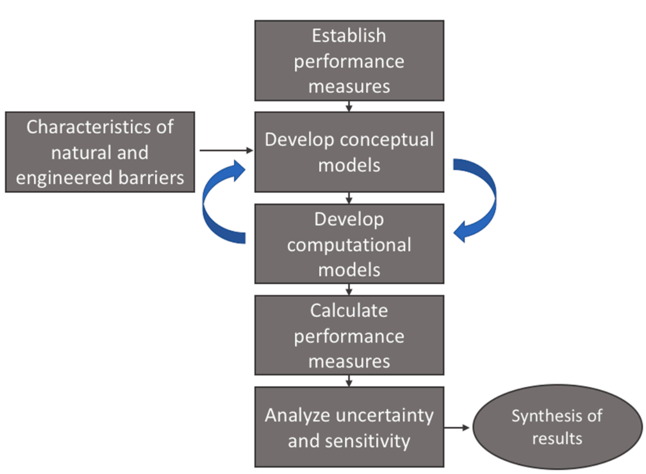

Fig. 1. The performance assessment process (modified from[1]).

Table 1
Participating teams in Task F2.

Abbreviation of team	Team
BASE (Germany)	The Federal Office for the Safety of Nuclear Waste Management (Bundesamt für die Sicherheit der nuklearen Entsorgung)
COVRA (The Netherlands)	Central Organisation for Radioactive Waste (Centrale Organisatie Voor Radioactief Afval)
DOE (USA)	US Department of Energy/Sandia National Laboratories
GRS (Germany)	Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH
Quintessa (UK)	Quintessa Ltd

A schematic for the development of PA models is shown in Fig. 1. This project focused on the second two blocks of iteratively developing tractable conceptual and computational models with an appropriate level of complexity for probabilistic sensitivity analysis and uncertainty quantification. The initial model focused on repository flow, then radionuclide transport, and finally salt creep-closure was added. Each team developed their own forward model(s) and calculated performance measures of the conceptual model at each iteration.

2. Methodology

The salt reference scenario2,3 has been developed collaboratively since the initiation of the project. The specifications were revised to add and remove levels of complexity to create a PA case that is relevant and accessible to all five participating teams. The model represents a valuable output for the radioactive waste community as it is a publicly available domal salt PA conceptual model that contains realistic data for many of the key FEPs, and is amenable to a wide variety of modelling approaches.

The base case focuses on a disturbed (or alternative) scenario for a salt repository. Multiple performance assessments (e.g., PROSA, RESUS, KOMTESS, ISIBEL and VSG)[4–9] have calculated no significant radiological consequences via liquid-phase transport within 1000,000 years for undisturbed disposal in salt formations because of salt's very low permeability and moisture content. The conceptual model is a simplified scenario that has pessimistic assumptions about the engineered barriers: First, the shaft seals fail 1000 years after repository closure, allowing an influx of brine from overlying aquifers down the shafts and into the repository. Second, the vitrified glass begins dissolving at the start of the simulation and the spent nuclear fuel (SNF) containers simultaneously fail at 500 years. Heat generation from radionuclide decay and radiolysis, and their impact on creep closure, are omitted from the model. The full description of the base case model in the task specification[2] is publicly available, and very briefly summarized here.

2.1. Geological setting and repository structure

The geological model is a generic geological cross section of a salt dome developed for the RESUS project[9] that has been simplified to six homogeneous geologic units as shown in Fig. 2a. It is assumed that the salt dome geometry extends 9 km perpendicular to the plane of the cross section. The repository is mined at a depth of 850 m below the ground surface.

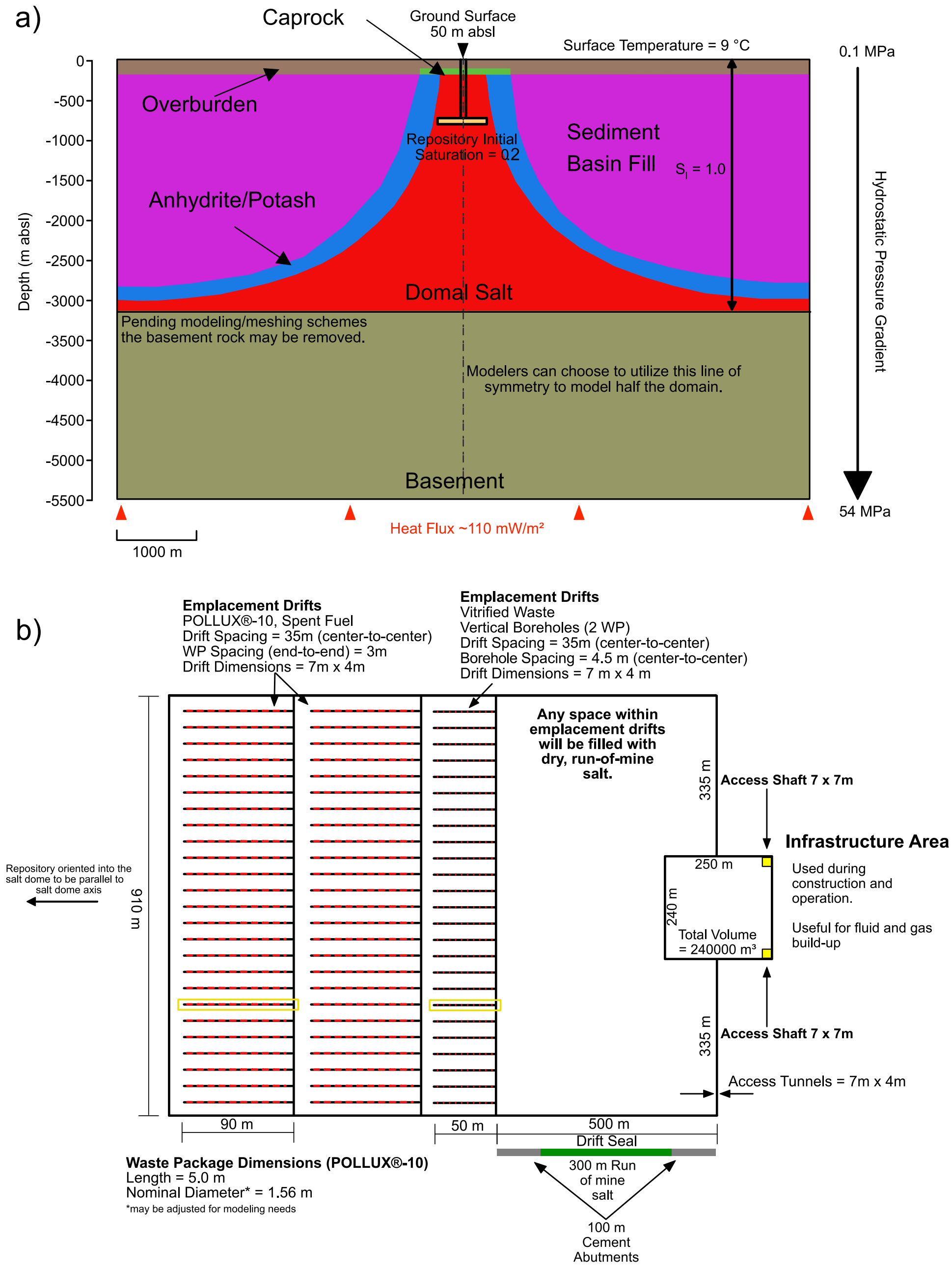

Fig. 2. a) Geological cross-section with model units for the generic salt reference case. The model units are simplified from 9. The repository location and initial model conditions are shown. b) Schematic of the waste repository in the generic salt dome. Quantities of interest (QOI) to be compared are in the highlighted areas. The drift seal is shown in green, while the lower shafts, SNF, and vitrified waste drifts are highlighted in yellow.

Fig. 2b shows that within the repository there are three sets of 25 emplacement drifts. For the SNF waste, POLLUX-10 containers are placed end-to-end in two of the sets of 25 emplacement drifts that are 90 m long with 10 containers per drift for a total of 500 containers. The vitrified waste emplacement area consists of one set of 25 emplacement drifts. Each 45-m-long drift contains 10 vertical boreholes with two waste canisters per borehole. The boreholes are backfilled with sand and have a salt plug seal at the top. This configuration results in a total of 500 vitrified waste canisters. The repository is not representative of any repository configuration under consideration but represents a hypothetical waste repository with mixed radioactive waste types and realistic engineered barriers.

The waste areas are isolated from the infrastructure area and shafts connecting the repository to the surface by two seals that consist of 300 m of run-of-mine salt between two concrete abutments, as shown in Fig. 2b. The infrastructure area is filled with gravel to accommodate fluid influx from the surface or gas generated by the waste (though this FEP is not currently considered). All other waste and non-waste areas are backfilled with run-of-mine salt. The shaft is a layered sequence of gravel, sealing elements, and concrete, but is modelled as homogenous in the base case because it was shown in separate work[10] that a high level of complexity was not necessary in the conceptual model.

2.2. Flow and transport modelling

Simulations are run for 100,000 years. The initial condition of the repository is 10 % porosity and 20 % saturated with brine; variably saturated single-phase flow (frequently called Richards' flow) is assumed in the base case. This is likely to be an unrealistically high initial saturation but was necessary for numerical stability in some models. The impact of this assumption will be investigated using a variant in Section 4.3.1.

In the present study, comparisons are made of two ideal (non-reacting, non-adsorbing, and non-decaying) tracers. The SNF Tracer is only in the SNF fuel and is representative of the instant release fraction of ^{129}I from the POLLUX-10 containers when they breach at 500 years. The VW Tracer is only in the vitrified waste (VW) and represents the ^{99}Tc that is slowly released as the glass dissolves. Radionuclides are in the conceptual model;[2] however, the tracer simulation results are the focus of this study because they satisfy the need to compare the models as simply as possible and comparison of radioactive contaminants resulted in similar observations. Additionally, the tracers will tend to overestimate transport of radionuclides and provide information about the origin of contaminants in the repository, as the SNF Tracer is only in the SNF and the VW Tracer is only in the vitrified waste.

2.3. Salt closure model

Drift convergence and resulting changes in porosity are modelled based on Gorleben data[9] as implemented in the GRS LOPOS[11,12] software. This approach is considered state-of-the-art as it has been used in Germany for many years for different salt formations like the Gorleben salt dome, Asse, Morsleben and others, and validated by measurements as well as by detailed finite-element salt creep computations. Salt creep begins at the start of the simulation according to the LOPOS equations or to tabular data from LOPOS, both of which are given in the task specification.[2] Closure is rapid because the initial water saturation is 20 % and wet salt creep is faster than dry. It is assumed that the run-of-mine salt backfill permeability returns to intact salt permeability once the drifts have fully closed. A Kozeny-Carmen type equation for permeability as a function of porosity is provided.[2]

3. Calculation and modelling approaches

Each team's computational approach is discussed in more detail in the Appendices of the final report.[13] Software used, and how each team handled key features and processes are briefly summarized in Table 2 and Table 3. Schematics of each team's model are shown in Fig. 3.

3.1. Comparison of modelling approaches

Detailed information on individual team models is available in 13, the DECOVALEX task final report, and only the differing assumptions that are believed to drive Quantities of Interest (QOIs) are discussed here. Every team uses all parameter values given in the task specification,[2] as far as possible in their software and model concept[13] (e.g. repository dimensions, diffusion coefficients, initial and final permeability and porosity, relative permeabilities).

As can be seen in Table 2 and Table 3 all teams have different conceptual models, software capabilities, and make different simplifying assumptions from the model in the task specification. This results in different features and events in the models and higher or lower fidelity representations of some aspects of the models. Simplifying assumptions made by all teams were to omit discretization of both the individual SNF waste canisters and the vertical emplacement boreholes for the VW containers. All teams also utilized the half-symmetry of the domain to reduce computational overhead.

Each team's model invokes simplifications in some places to capture complexity in others. In particular, the fully-coupled, salt closure model from the GRS software LOPOS was challenging to reproduce in PFLOTRAN and COMSOL. Fig. 3a shows that the COVRA model is a 1D model for the shaft coupled to a 2D model of the repository by a shared boundary condition. Differences in the rate and coupling of salt compaction to other processes is believed to be influential in flow modelling of the reference case, as discussed in Section 4.

3.1.1. Spent Nuclear Fuel and Vitrified waste drift modelling

BASE, COVRA, and DOE mesh the combined drift/container region into multiple grid cells and use average properties for the buffer and SNF container in the drifts. Quintessa homogenises the drifts into several, larger compartments in their model. GRS lumps the waste drifts into two compartments for computational efficiency. It is unlikely that these simplifications will cause differences between the models as all teams make similar assumptions, and containment provided by the SNF waste form and the vitrified waste canister and overpack are neglected in the conceptual model. However, all teams' homogenization of the drift and waste containers may indicate increased migration of radionuclides inside the drift as compared with a fully resolved model. DOE is the only model that includes influx of liquid from the geosphere, as geosphere influx was not explicitly included in the task specification, but is a consequence of DOE meshing the surrounding geosphere in their model.

3.1.2. Creep closure modelling

Table 4 shows an overview of porosity evolution by creep closure in the teams' models. They can be grouped into three model types: fully-coupled compaction according to the task specification for GRS and Quintessa, simplified compaction for BASE and COVRA, and only changing permeability for DOE. As will be seen in the next section, the three levels of fidelity in the models results in three distinct sets of outcomes for porosity compaction and fluid flow.

3.1.3. Diffusion modelling

Diffusion is found to be an important mechanism for transport of radionuclides in all the models. The diffusivity assumptions of each team are shown in Table 5. Diffusion coefficients are linked to porosity, so differences in porosity evolution (Table 4) mean that the models have different effective diffusivity during the simulation. In particular, the BASE, GRS, and Quintessa models have the effective diffusivity as a function only of the current porosity, while COVRA assumes that the effective diffusivity depends on the initial porosity times the changing porosity. Porosity does not change in the DOE model, so effective diffusivity remains at the high initial value throughout the simulation.

Diffusive transport in the simulations will be determined by a combination of the numerical dispersion and diffusion resulting from the effective diffusion in the model. Numerical dispersion may be larger than physical diffusion and dominate diffusive transport. BASE was the only team to conduct a numerical convergence study and ensure their results are independent of grid resolution[14]. Thus, differences in effective diffusivity and numerical dispersion are both potential sources of discrepancies between the teams' models.

Table 2
Features in teams' model.

Feature	BASE	COVRA	DOE	GRS	Quintessa
Software	PFLOTRAN[14]	COMSOL	PFLOTRAN[14]	LOPOS[11]	QPAC
Dimensionality	3D	1D/2D	3D	1D	3D
Includes host rock?	No	No	Yes	No	No
Numerical Method	Finite Volume	Finite Element	Finite Volume	Finite Difference	Finite Volume
Includes overburden?	No	No	Yes	No	No
Continuous or compartments model?	Continuous	Continuous	Continuous	Compartment	Continuous

Table 3
Processes in teams' model.

Process	BASE	COVRA	DOE	GRS	Quintessa
Repository resaturation	Richards' equation	Richards' equation followed by diffusive transport	Richards' equation	Darcy equation	Richards' equation (multi-phase flow as variant)
Solubility limits?	Yes	No	No	Yes	Yes
Inflow from the geosphere?	No	No	Intact salt included	No	Geosphere inflow can be modelled (only used as variant)
Maximum Fluid Pressure	Hydrostatic	Hydrostatic	Hydrostatic	Lithostatic	Hydrostatic (but configurable)
Salt creep?	Yes	Yes	No	Yes	Yes

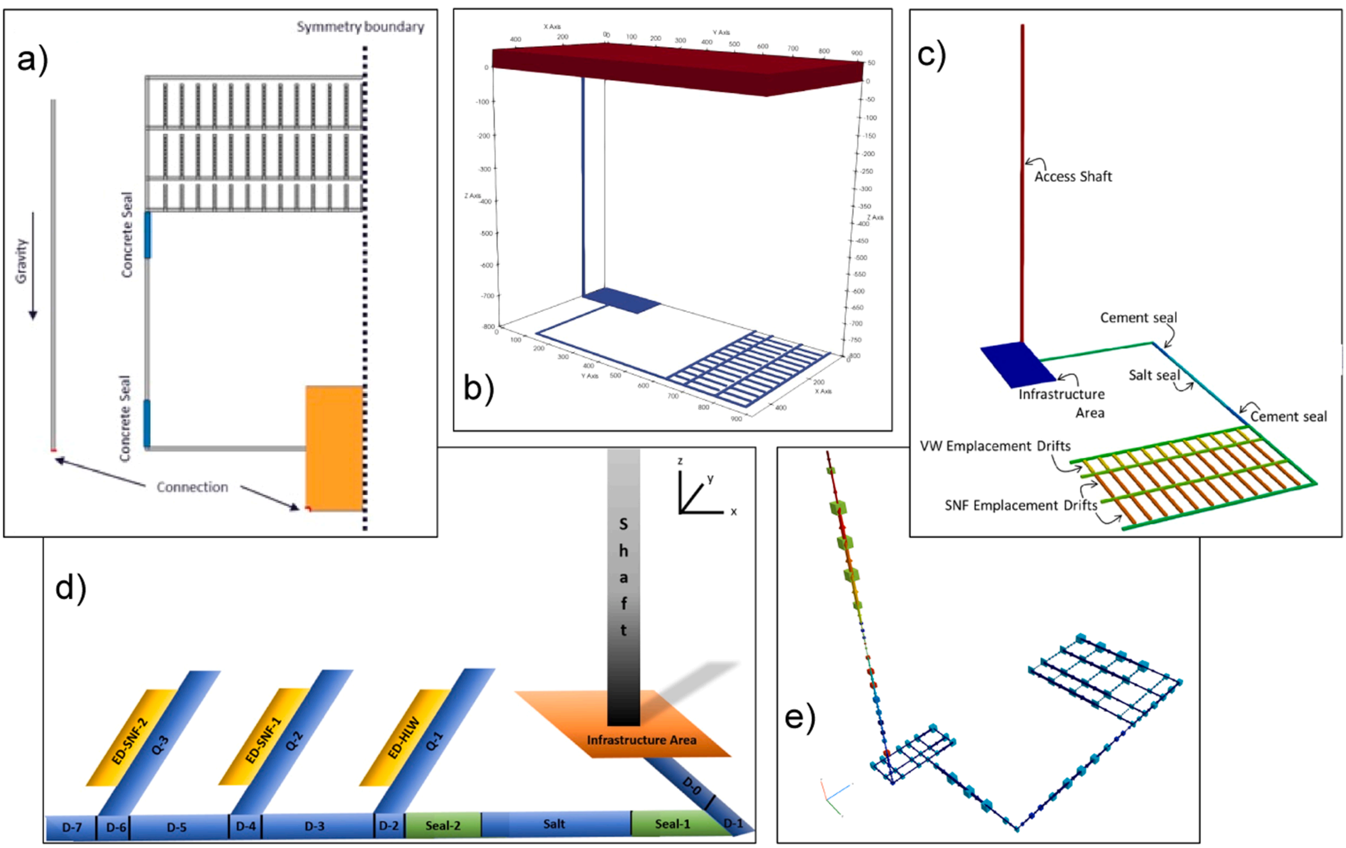

Fig. 3. Team computational models. a) COVRA, b) DOE, c) BASE d) GRS e) Quintessa.

Table 4
Porosity evolution in teams' models.

Question	BASE	COVRA	DOE	GRS	Quintessa
Using the provided compaction?	No, prescribed porosity reduction	No, exponential decay of porosity	No, simple stepped approach to reduce permeability	Yes	Yes
What variables is it coupled to?	Pressure and saturation	Pressure only	N/A	Pressure and saturation	Pressure and saturation
One way or two-way coupling?	One-way (porosity impacts saturation and pressure)	Two-way	N/A	Two-way	Two-way
Is convergence parameterization different between repository areas?	Yes, Two models: one for the seal, another for all other areas	No, but convergence rate varies locally	N/A	Yes	Yes
Does permeability vary with porosity?	Yes, according to task specification	Yes, according to task specification	No, permeability was stepped down	Yes, according to task specification	Yes, according to task specification

4. Results

Comparison of the QOIs between the individual models focuses on two parts of the repository: QOIs in the disposal drifts and QOIs related to the safety function of the repository seals. The first group serves to demonstrate similarities and differences in how the radionuclides are initially released into the repository, while the second explores radionuclide transport towards the shaft to the surface. Model outputs are compared in the example SNF drift and in the example VW drift. Both are highlighted yellow in Fig. 2b. As the SNF and VW have

Table 5
Diffusion modelling in teams' models.

Question	BASE	COVRA	DOE	GRS	Quintessa
Were the effective diffusion coefficients used as described in the task specifications?	Yes	Yes	Yes	Yes	Yes
Are the diffusion coefficients coupled to porosity?	Yes	Yes	Yes, but porosity is fixed in the simulation	Yes	Yes
Does the model have numerical dispersion associated with advection?	Yes	Yes	Yes	Yes, from coupling between regions, but not within regions	Yes

fundamentally different release mechanisms it is necessary to consider both. The third point of comparison is the salt in the repository seals, shown in green on the bottom right of Fig. 2b. The final point of comparison is one of the lower shafts (yellow squares on the right of Fig. 2b.)

QOIs in the disposal drifts and seal salt are further broken down into three subsets: local evolution of porosity, flow quantities, and radionuclide transport quantities. This additional breakdown is necessary because porosity evolution drives changes in fluid saturation and flow, which in turn may drive radionuclide transport. The transport QOI are mass and mass transport rate of the SNF and VW Tracers at the locations of interest.

The final QOI is fluid flow through the lower shaft. This QOI is used to demonstrate the direction of the driving forces between the surface and the repository. Transport quantities are not investigated in the shaft, as no team's model shows significant radionuclides or tracers in the shaft at any time in the simulation.

4.1. Porosity evolution and fluid flow

4.1.1. Porosity evolution during compaction

The porosity evolution in the SNF drift and seal salt are shown in Fig. 4. Porosity evolution in the VW waste drift is similar to the SNF drift and is not shown. The GRS model was used to create the porosity evolution curve in the task specification. Porosity in the SNF and seal salt are reduced to around 2 % by 10 years for the BASE, GRS, and Quintessa models and by 50 years for COVRA. This is due to the 20 % initial water saturation and resulting rapid salt compaction.

The porosity evolution curves reflect the differing compaction assumptions made by each team. GRS and Quintessa, with fully coupled compaction models, have very similar curves as well as the highest rate of compaction. Both the BASE and COVRA models are calibrated to the LOPOS model. BASE uses a prescribed porosity reduction forward-coupled to liquid saturation and pressure (see Fig. 4). This approach results in a salt compaction curve that is similar in shape and timing in the seal salt, but slower in the SNF drift. The coupling technique used by COVRA also results in a compaction curve of similar shape, but is the slowest compaction rate of the four compaction models due to challenges in coupling pressure for the rapid creep closure. Finally, DOE does not explicitly include porosity reduction in their model and is not shown.

4.1.2. Resaturation of the repository

Fig. 5 shows the liquid saturation in the SNF drift and seal salt. As anticipated, in the BASE, COVRA, GRS, and Quintessa models, as the porosity decreases the liquid saturation increases in a clear inverse relationship. This is because there is little external force in the conceptual model to drive changes in liquid saturation via flow. The DOE model re-saturates much later due to having influx only from the geosphere and shaft seal failure.

Pressure is not shown because in the specified creep closure model,[2] creep and pressure are coupled so that the pore pressure evolves from atmospheric at the start of the simulations towards hydrostatic or lithostatic pressure at full closure of the repository. However, lithostatic pressure is not approached during the 100,000 year simulations.

In the seal salt, the BASE and COVRA models both reach a maximum saturation, and then experience a drop in saturation after compaction has slowed. The BASE model also shows this trend in the SNF drift. During rapid compaction the non-compacting concrete plugs at either end of the seal salt (see Fig. 2b) don't fully re-saturate with liquid. Subsequently the concrete plugs draw water from the salt to re-equilibrate the repository. This occurs on different timescales for the two models. Different grid refinements were considered in the BASE model, but the same result is obtained, so the difference in timing does not appear to be a grid-related numerical artefact.

4.1.3. Fluid flow in the drifts and seal

As the liquid saturation increases due to compaction in the BASE, COVRA, GRS, and Quintessa models, pressure begins to build in the SNF drift and seal salt, creating flow of liquid out of the drift (Fig. 6a). There is a clear correlation between the peak flow rate of liquid and the SNF drift approaching or reaching full resaturation in the BASE, GRS, and Quintessa models while the COVRA model has peak liquid flow rate during the resaturation process. Liquid flow rate out of the SNF drift peaks with a very similar timing and magnitude for the GRS and Quintessa models due to their similar compaction curves. It makes intuitive sense that the two models with the most rapid reduction in porosity have the highest and earliest peak in liquid flow rate. The BASE and COVRA models have lower peak liquid flow rates that occur at later

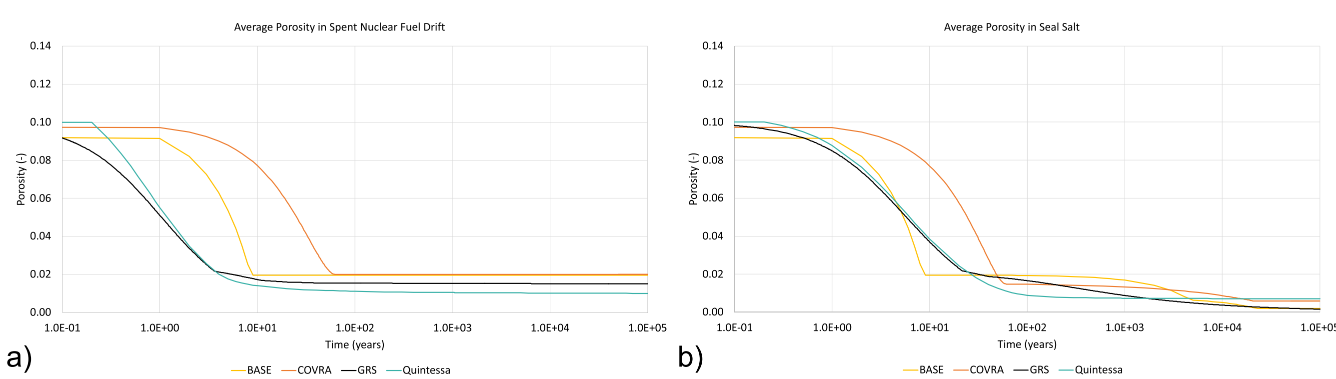

Fig. 4. Porosity evolution a) for the example SNF drift and b) for the repository seal.

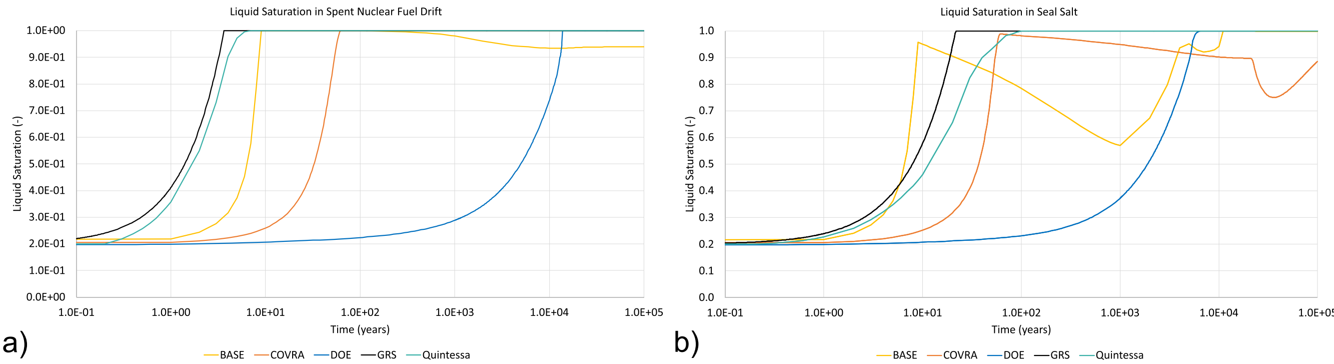

Fig. 5. Average liquid saturation a) for the example SNF drift. b) for the repository seal.

time. On the scale of the 100,000-year simulations, the timing of the peak flow out of the SNF drift is remarkably similar between these four models. The DOE model resaturation process is driven by fundamentally different physical mechanisms than the other four models as this model has no decrease in porosity over time. The DOE model shows a spike in liquid flow out of the SNF drift lasting around 1000 years after full saturation is reached at 14,000 years.

Fig. 6b and c show liquid flow rates from the cement abutments on the repository side into the seal salt, and flow rates from the seal salt into the cement abutment on the side of the seal salt closest to the infrastructure and shafts to the surface, respectively. The BASE, COVRA, and Quintessa models all show a very similar trend in liquid flow rates out of the seal salt. As the salt compacts, the liquid saturation increases, and the liquid is pushed out of the seal salt in both directions. In the BASE and COVRA models the peak flow rate occurs when the salt is nearly fully saturated. In the Quintessa model the peak flow rates occur earlier during compaction at 7 years and there is a secondary peak at 40 years when the salt becomes fully saturated. The double peak is localized to the interface and occurs because of the contrasting relative permeability and capillary pressure curves on either side of the interface and the monotonically decreasing porosity and permeability of the salt during compaction. The GRS model shows a similar trend, but has a reversal of flow when the seal salt is fully saturated at 50 years. Due to the compartmentalized structure of the LOPOS model, once the inner repository is fully saturated there is no more pore space available, and flow can never again be directed to the inner repository. In this model, the flip in flow direction corresponds to resaturation of seal salt, as it is the last part of the inner repository to reach full resaturation.

The GRS, BASE, Quintessa, and DOE models all show a late-time reversal of flow direction after full saturation (see inset in Fig. 6b-c). The DOE model does not have compaction so the flow of liquid out of the salt seal is much lower and delayed relative to the other models. However, it follows a similar trend to the GRS model.

After 15,000 years there is little or no advective force driving repository liquid towards the shaft in any model. The BASE and DOE model have flow towards the waste (negative) after 22,000 and 5500 years, respectively (see inset on Fig. 6b). For the BASE model the flow into the repository persists for the rest of the simulation. In the DOE model there is an additional flow reversal at 15,000 years. The COVRA, DOE, and Quintessa models have flow out of the salt seal towards the shaft on the order of 1 $\times 10^{-3}$ m^3/yr or lower after 15,000 years (see inset on Fig. 6c).

In all the models there is hydraulic decoupling of the ‘inner’ and ‘outer’ repository with the seal functioning as a highly effective hydraulic barrier between them. ‘Inner’ and ‘outer’ are separated by the repository seal salt, with the waste side being ‘inner’.

4.1.4. Fluid flow in the shaft

The final flow QOI is liquid flow observed within the lower shaft 25 m above the infrastructure area (see Fig. 2b). Only fluid flow is compared because none of the five models indicate the presence of tracers at this location or at any location further up the shaft. As can be seen in Fig. 7, the dominant direction of flow in every model is flow of liquid from the surface downwards into the repository due to the step change in permeability at 1000 years.

In all the models, prior to the failure of the shaft seal, flow through the lower shaft is negative and too small to be visible on the scale of Fig. 7. All models have a sharp decrease in flow rate once the gravel-filled infrastructure area is saturated. The GRS model shows the lowest and longest pulse of water from the surface while the DOE model shows the largest and briefest water pulse, likely because the lack of compaction in this model means that flow within the repository is less restricted.

Recall from Section 3.1 that the COVRA model consists of two coupled sub-models. The COVRA shaft model (solid orange line) is used until 2620 years, when the shaft is nearly fully saturated. The negative values of the flow rate into the repository (orange dashed line) are shown for times greater than 2620 years. This results in three distinct peaks in flow rate, but like the other models, inflow declines to a very low rate at late time.

The BASE, DOE, and Quintessa models predict that after 6000 to 15,000 years there is a reversal of the flow direction and a small amount of flow upwards towards the surface, due to the lithostatic pressure being higher than hydrostatic pressure, thus allowing some residual compaction to occur as brine flows very slowly out of the facility. This indicates there is a small driving force that could push radionuclides further up the shaft, if there were any present after 100,000 years.

4.2. Transport of tracers

4.2.1. Transport out of disposal drifts

Fig. 8a-d show the mass and transport rates of the SNF and VW Tracer in their respective disposal drifts. The GRS software LOPOS does not calculate mass in the waste compartment in their model, so is not shown.

At 500 years, the POLLUX-10 containers in the SNF drift all breach simultaneously. The trend of declining mass of the SNF Tracer in all the models is remarkably consistent (Fig. 8a). This is in large part because the peak flow rate of water in all the models with compaction occurs long before the containers breach, by which time the liquid flow rate is very low in every model (see Fig. 6). Fig. 8c shows the SNF Tracer transport out of the drift for the five teams. In all the models, transport begins when the containers breach, followed by a rapid decline as the mass of SNF Tracer decreases. In the BASE, GRS, and Quintessa models, there is a clear trend that the model with the highest fluid flow rate has the highest transport rate of the SNF Tracer. More detailed analysis by the individual teams in the final report[13] indicates that the BASE, GRS, and Quintessa models have some advection but have

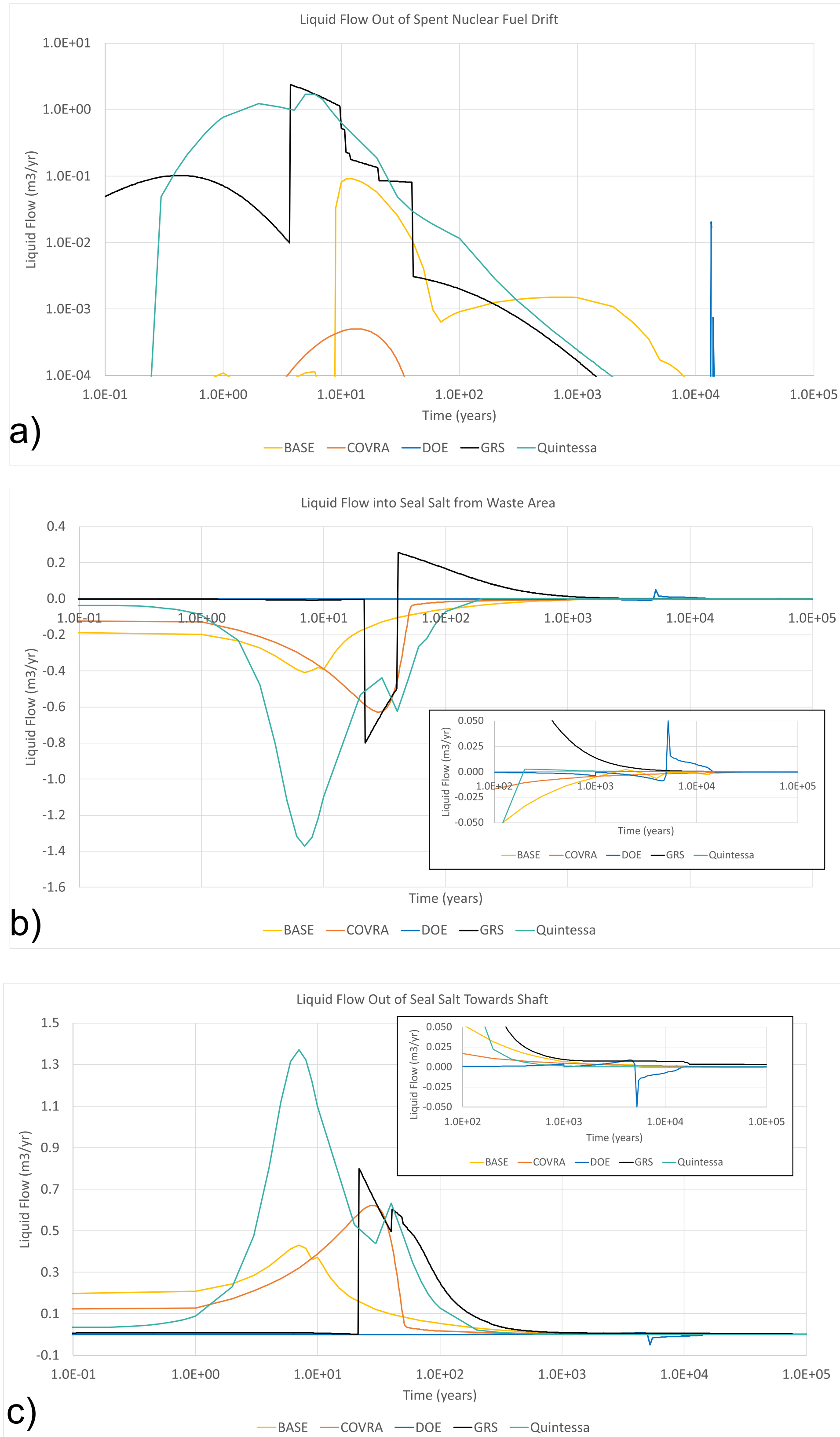

Fig. 6. Liquid flow rates in the repository a) for the example SNF drift, b) between the salt and concrete abutment connecting to the waste area, and c) between the salt and concrete abutment connecting to the infrastructure area and shaft. Positive flow is defined as flow out of the drift towards the shaft.

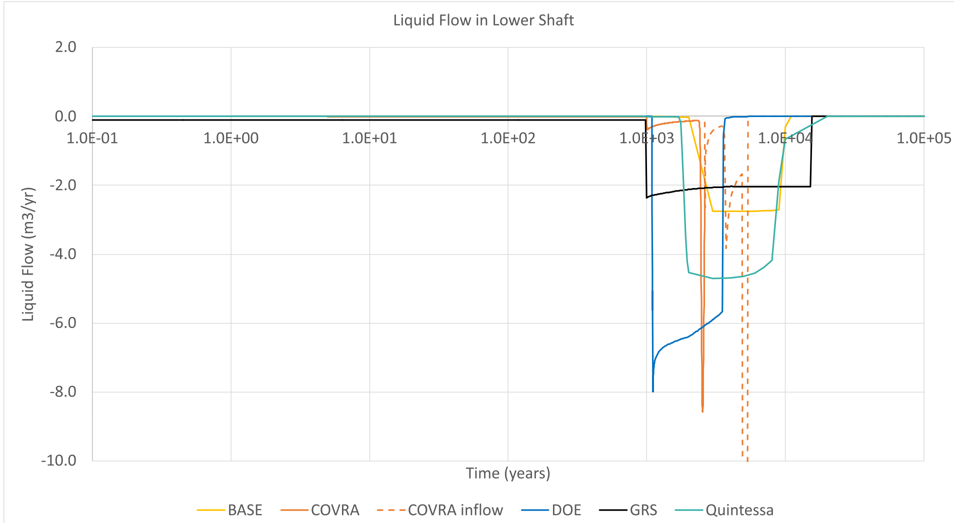

Fig. 7. Liquid flow rates in the lower shaft. Negative flow is defined as flow from the surface down into the repository.

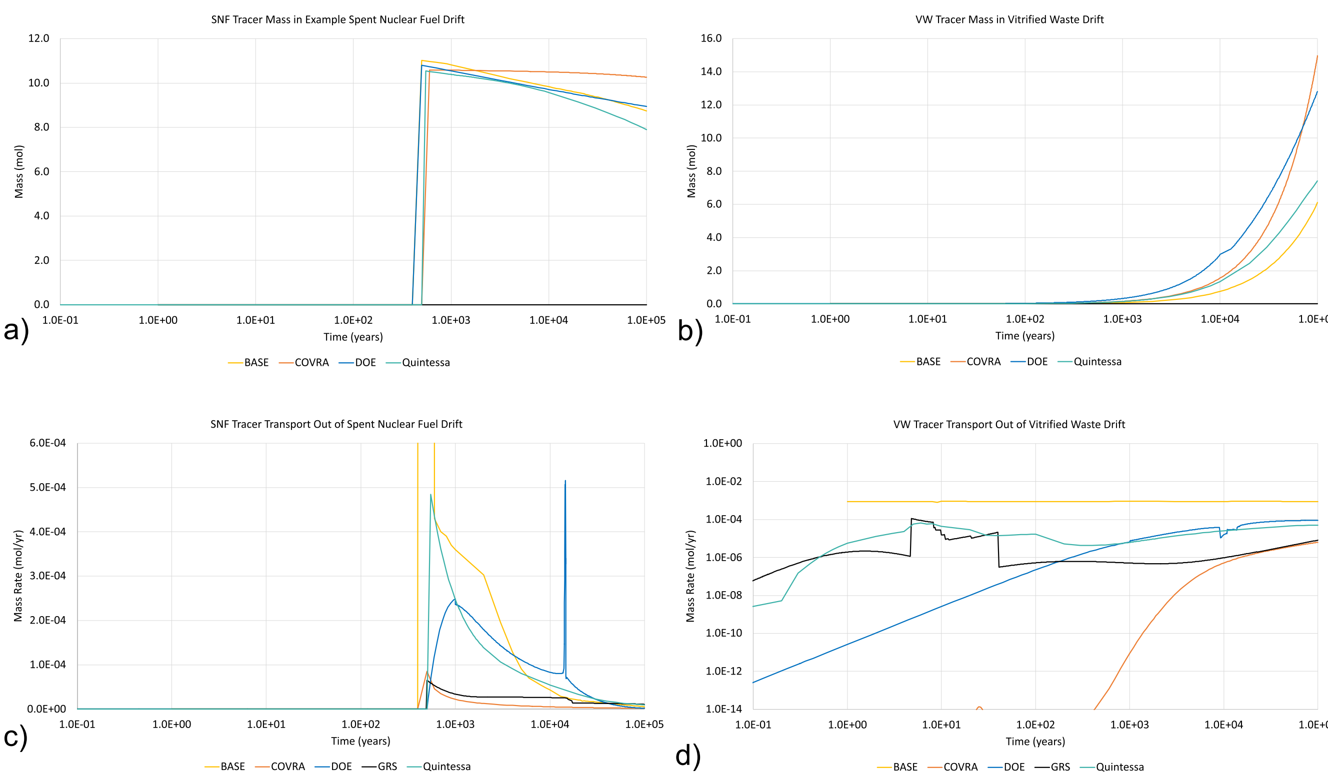

Fig. 8. SNF and VW Tracer transport quantities in the drifts. a) SNF Tracer mass in the drift. b) VW Tracer mass in the drift. c) SNF Tracer transport rate out of the drift. d) VW Tracer transport rate out of the drift. GRS mass is not shown as the LOPOS software does not output this quantity for this model. Positive is defined as transport out of the repository and towards the shaft.

diffusion-dominated transport of the SNF Tracer. The liquid flow rate in the COVRA model at the time of container breach is very low and in the DOE model the liquid is flowing **into** the SNF drift, so SNF Tracer transport is diffusive in these models. Transport of the SNF Tracer by diffusion in the DOE models is in between the other models because of the competing effects of resauturation and diffusion. In the DOE model effective diffusivity depends on the high initial salt porosity which increases tracer diffusion, but diffusivity also depends on saturation, and all other models are saturated before the SNF containers fail and before there is significant VW Tracer present, while the DOE model does not resaturate until after 10,000 years (Fig. 5).

The vitrified glass waste begins to dissolve at a slow, constant dissolution rate from the start of the simulation. Fig. 8b shows there is very little VW Tracer in the drift until 1000 years and the mass increases uniformly with time in all the simulations. It takes 10,000 years to accumulate more than 2 mol of the VW Tracer in the vitrified waste drift in every model. By this time all the models predict fluid flow rates of less than 0.01 m^3/year out of the drift (not shown, but similar to Fig. 6a). The VW Tracer transport rates are similarly low and relatively constant in time, as shown on Fig. 8d. Thus, unlike the SNF Tracer, transport of the VW Tracer out of the vitrified waste drift is diffusion-dominated in every model.

4.2.2. Transport into the seal

Fig. 9a-d shows the transport quantities for the SNF and VW Tracers in the seal salt. There is high variability in the breakthrough time of the tracers in the seal salt. Comparison of subplots a) and b) of Fig. 9 reveals that in all the models the VW Tracer appears earlier than the SNF Tracer. This makes intuitive sense as the vitrified waste drift containing the VW Tracer is closer to the seal than the SNF drift (see Fig. 2b) and VW is gradually released from the start of the simulation (see Fig. 8a).

The appearance of tracers in the seal does not appear to have correlation with fluid flow rate, as all models except GRS have very slow or negative fluid flow into the seal salt at the time of the tracers' appearance (see Fig. 6). In the GRS model the VW Tracer arrival coincides with the reversal of the liquid flow direction from negative to positive. Thus, transport of the VW Tracer may have an advective component in the GRS model, though it too is believed to be largely diffusive.[13] This indicates that, for these models the transport regime into the seal salt for the tracers must be diffusive.

All models predict monotonically increasing SNF Tracer mass and transport into the seal with time (see Fig. 9c), but at different rates. Numerical dispersion and diffusivity/porosity coupling are believed to drive some of the differences between the models. For the COVRA model, transport into the seal salt is always below 1 $\times 10^{-14}$ mol/yr so it is not visible on Fig. 9c, though the SNF Tracer mass accumulates enough to be visible on Fig. 9d just before 100,000 years.

In the COVRA and DOE models, VW Tracer mass and transport rates (see Fig. 9b and d) into the seal salt from the waste area curves are similar in shape, but earlier in time than the SNF Tracer curves. Fig. 9b) shows that for the BASE, GRS, and Quintessa models, the VW Tracer mass initially increases rapidly after breakthrough and then approaches a plateau. In the GRS and Quintessa model transport rates of the VW Tracer into the seal salt (Fig. 9d) decrease after breakthrough and then increase again after 50,000 years. The BASE model shows a more complex, but apparently similar trend. This may be caused by the gradual VW Tracer release or may be a late-time trend that is only observable when the VW Tracer arrives at the seal earlier in the simulation.

The BASE, COVRA, and DOE models do not show transport rates above 10^{-14} mol/yr of either tracer out of the seal salt towards the shaft during the 100,000-year simulation (not shown). The Quintessa model shows a small amount of VW Tracer transport between 1 $\times 10^{-14}$ to 1 $\times 10^{-13}$ mol/yr the last 10,000 years of the simulation, while the GRS model has the highest transport rate through the salt seal, increasing to a maximum of 3.8 $\times 10^{-7}$ mol/yr at the end of the simulation for the SNF Tracer and a relatively flat VW Tracer transport rate below 2.3 $\times 10^{-8}$ mol/yr from 100 to 100,000 years. These low transport rates of the tracers indicate that, in every model, the salt and concrete abutments in the repository seal provide containment and keep the radionuclides from migrating through the seal towards the infrastructure area and the shaft for the duration of the 100,000-year simulation. However, transport rates of the tracers out of the seal are increasing at 100,000 years.

4.3. Variants

We explore a small sub-set of model variants for two reasons; first to investigate the consequences of plausible differences in the model setup; and second to test that the model responses are reasonable with major changes and hence gain understanding (and hopefully confidence) that the models are generally appropriate for the analysis end-points.

4.3.1. Initial saturation and compaction rate

This variant is prompted by the importance of the compaction rate as a driver for fluid flow. The initial liquid saturation of the repository was 20 %, however this is unrealistically high and, because moisturised salt compacts more quickly than dry salt, resulted in rapid compaction of the salt in the base case.

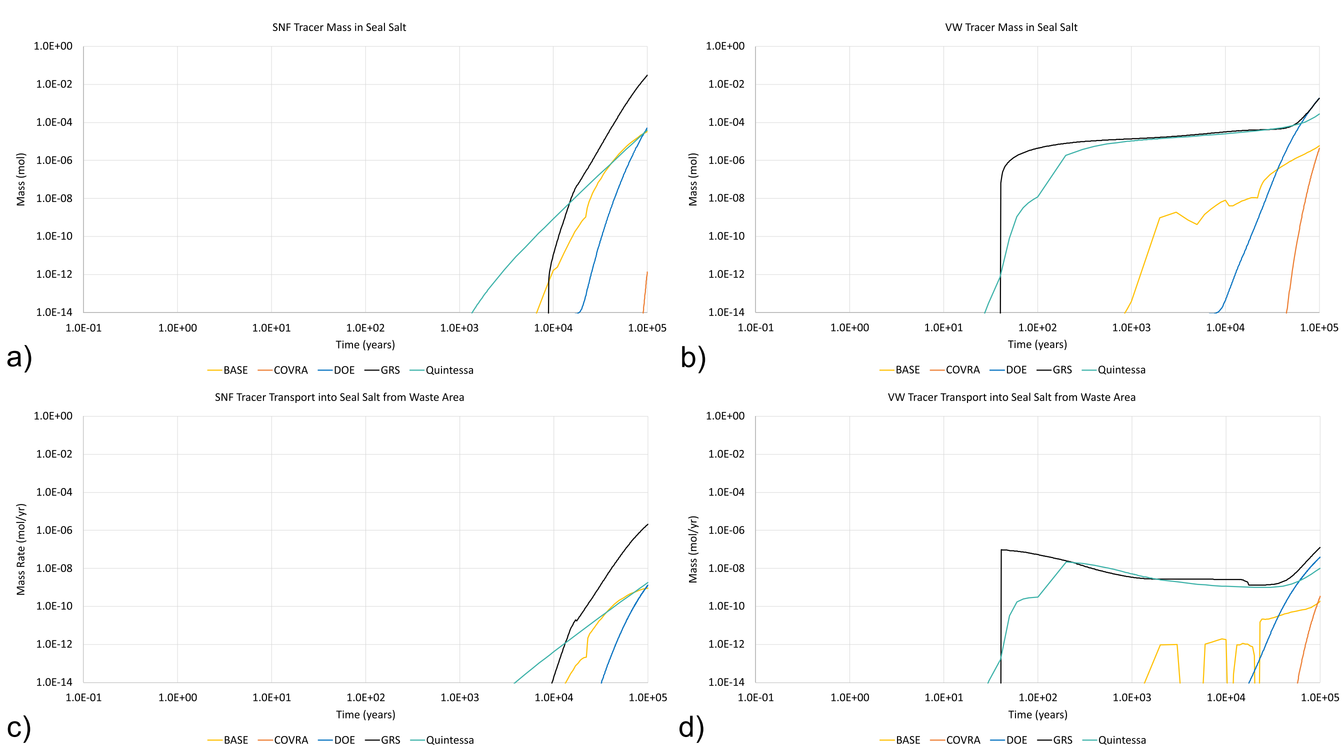

Fig. 9. SNF and VW Tracer transport quantities the salt in the repository seal. a) SNF Tracer mass. b) VW Tracer mass c) SNF Tracer transport rate between the salt and drifts connecting to the waste area. d) VW Tracer transport rate between the salt and drifts connecting to the waste area. Positive is defined as transport towards the shaft.

In this variant the initial saturation is set to the residual saturation of the crushed salt backfill, which is 3 %. The salt convergence parameters are also changed to reflect the reduced water content. The GRS and Quintessa teams chose to participate in this variant. Recall that GRS and Quintessa both have fully-coupled compaction and as a result, had similar porosity decline curves (Fig. 4).

4.3.1.1. Porosity and fluid flow. Fig. 10 shows the porosity and liquid saturation in the SNF drift for the GRS and Quintessa base case and low initial saturation/slow compaction variant. These quantities are not shown for the vitrified waste drift or the seal salt as the trends are similar. Fig. 10a and b show that the shapes of the porosity and liquid saturation curves are very similar to those in the base case (in log-time). In the low saturation/slow compaction variant the onset of creep-closure is delayed until nearly 100 years (instead of less than 1 year), and porosity does not drop to less than 2 % until after 10,000 years (instead of before 50 years).

Fig. 10 shows that, like the base-case (Fig. 4 and Fig. 6a), there is a clear inverse relationship between porosity and liquid saturation. Again, this is because saturation increases primarily due to the decreasing pore space until full saturation is reached. The models also have a peak in fluid flow out of the model corresponding to the time of full saturation. However, because drift closure is so much slower, the peak flow rates are four orders of magnitude lower than in the base case (not shown).

Fig. 10b also shows the resaturation curve from the DOE base case model that has resaturation driven only by influx from the geosphere and the rest of the repository. The DOE base case model reaches full saturation at nearly the same time as the GRS variant model, indicating that in the low initial saturation/slow compaction variant, influx of water from the geosphere could become a more important physical mechanism for driving fluid flow in the repository.

The trend for flow through the seal salt in the GRS and Quintessa models is fundamentally different for the low initial saturation/slow compaction case compared to the base case. It appears that, rather than fluid being squeezed out of both ends of the seal salt as it compacts and saturates, after resaturation around 10,000 years, fluid is pushed through the seal at a slow rate from the infrastructure area towards the waste (not shown). The rate for the Quintessa model is higher than in the GRS model, but always less than 0.5 m^3/yr.

Both the GRS and Quintessa models have a delay in the pulse of water flowing down the shaft into the infrastructure area (not shown) in the low saturation/slow compaction variant as compared with the base case, but the maximum flow rates are very similar.

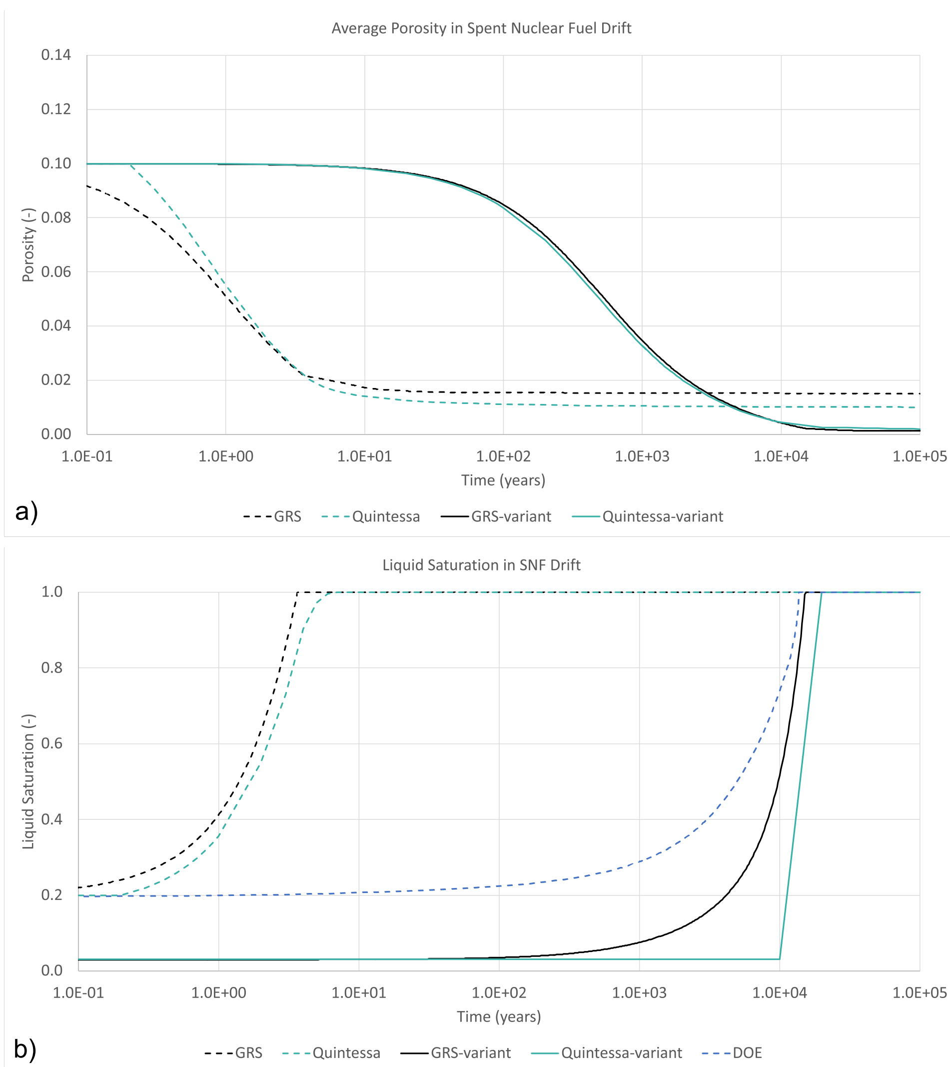

Fig. 10. Porosity and saturation QOI for the SNF drift for the base (dashed lines) and low initial saturation/slow compaction (solid lines) case. a) Average porosity. b) Average liquid saturation. The DOE base case is shown in b) to demonstrate that it re-saturates via influx from the geosphere on the same timescale as the GRS and Quintessa variant cases.

4.3.1.2. Tracer transport. Transport rates of the SNF and VW Tracers out of their respective disposal drifts are shown in Fig. 11a-b for the base case and low initial saturation/slow compaction models. Fig. 11a shows that for the SNF drift, in both models the low initial saturation/slow compaction variant has a maximum transport rate of the SNF Tracer after container failure at 500 years, though in the GRS model the maximum SNF Tracer transport rate is significantly higher than in the base case, and in the Quintessa model the maximum is significantly lower. The SNF Tracer transport rate in both teams' models then decreases to below the base case after 10,000 years and finally increases again at the peak in liquid flow corresponding to full liquid saturation of the SNF drift at around 15,000 years. Thus, SNF Tracer transport in the disposal drift has a significant advective component, as opposed to diffusion-dominated transport of the SNF Tracer in the SNF drift observed in the base case.

Fig. 11b shows that, in the vitrified waste drift, transport of the VW Tracer has a conceptually consistent trend in the base case and the low initial saturation/slow compaction variant models, though transport in the variant case is slower for the first 1000 years in both teams' models. This indicates that the transport of the VW Tracer is diffusion-dominated for both teams' low initial saturation/slow compaction models, as was the case for the base case models.

Fig. 12 shows the transport rate of the SNF Tracer in the seal salt is diffusion dominated in the low initial saturation/slow compaction model. The GRS model shows arrival of the SNF Tracer via diffusive transport earlier than in the base case. Transport from the repository side declines sharply as the seal closes to 2 % porosity around 10,000 years then resumes transport into the seal salt via diffusion in the GRS model, around the same time it appears in the Quintessa model. For the GRS model, the SNF tracer diffusion out of the seal salt (not shown for brevity) is broadly similar to the base case, but for the Quintessa model, the SNF Tracer transport out of the seal towards the shaft is higher than in the base case.

The VW tracer transport through the seal salt for the low initial saturation/slow compaction variant is very similar to the transport of the SNF Tracer and is not shown. This represents a different outcome than the base case, where the VW Tracer arrived an order of magnitude in time earlier than the SNF Tracer and showed a more complex trend in the rate of transport into the seal salt from the waste area (see Fig. 8).

4.3.1.3. Summary. The results of the low initial saturation/slow compaction variant suggest that this compaction regime fundamentally

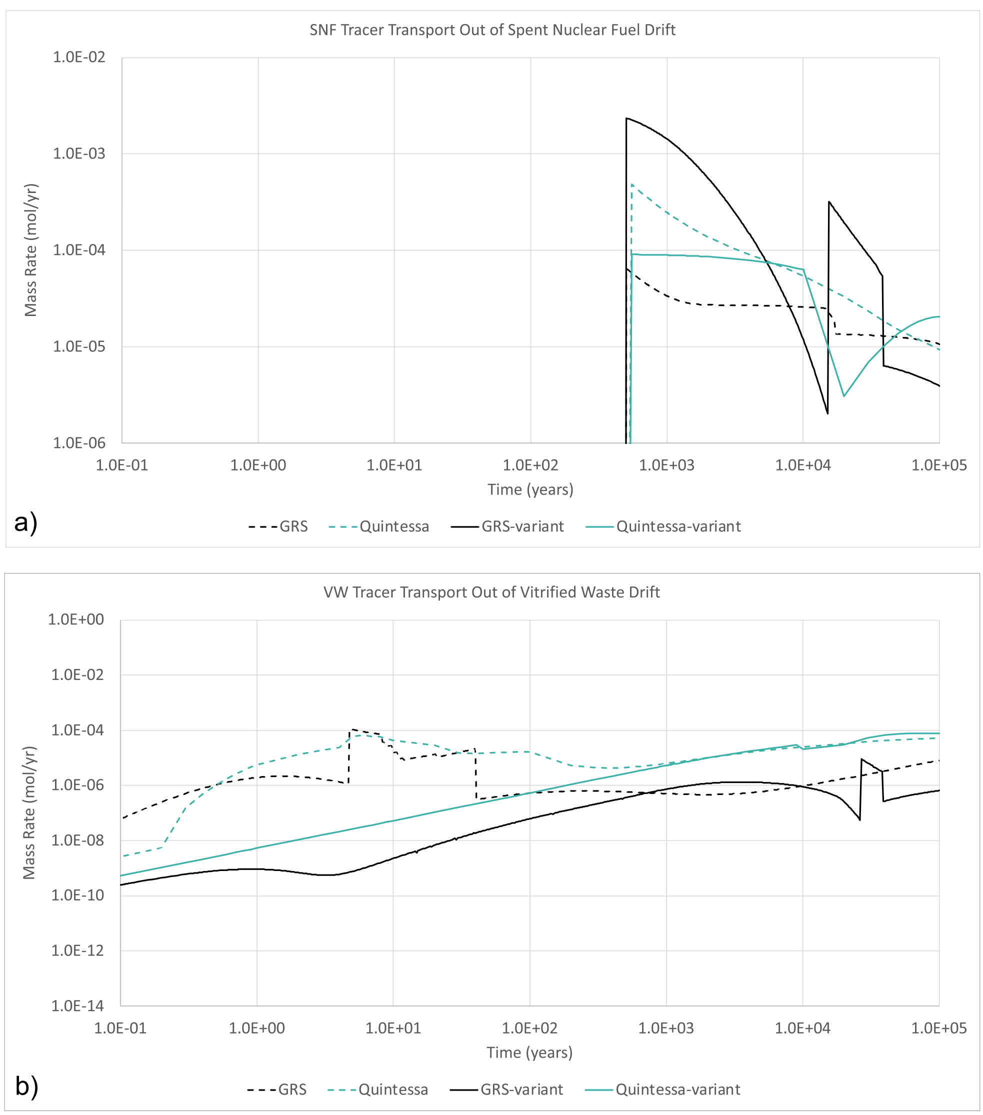

Fig. 11. Transport rate of tracers out of the disposal drifts for the base (dashed lines) and for the low initial saturation/slow compaction (solid lines) case. a) SNF Tracer transport rate out of the SNF drift. b) VW Tracer transport rate out of the vitrified waste drift. Positive transport is defined as flow out of the drift towards the shaft.

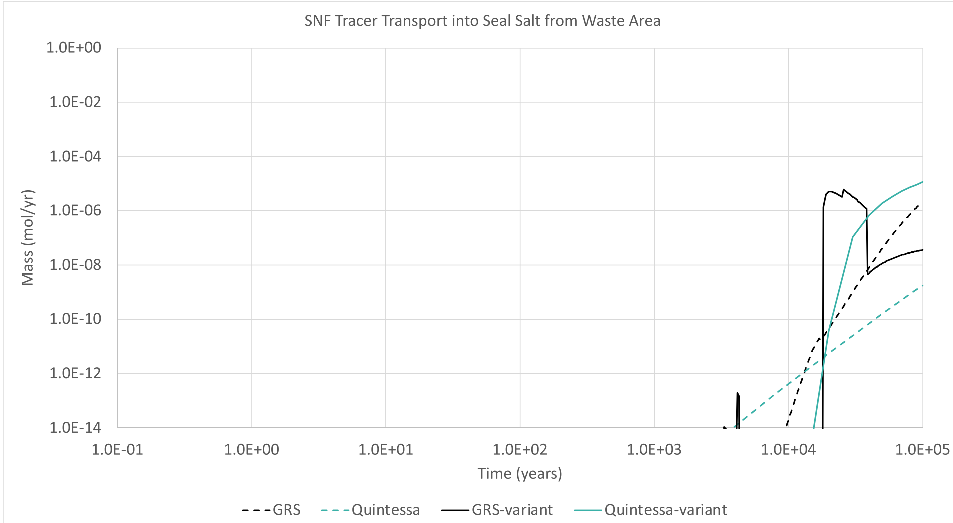

Fig. 12. SNF Tracer transport rate between the salt and concrete abutment connecting to the waste area for the base (dashed lines) and low initial saturation/slow compaction (solid lines) case. VW tracer transport is similar.

changes the fluid flow and tracer transport in the repository, causing advective transport out of the SNF drift. Both tracers clearly have diffusion-dominated transport into the seal because of the low flow rates, and the VW Tracer transport into the seal salt occurs orders of magnitude later in time than in the base case.

4.3.2. *Time of shaft seal failure*

The failure of the shaft seal at 1000 years appears to have relatively little impact on fluid flow or radionuclide transport in the base case scenario. This is believed to be because salt compaction is largely complete in the models with compaction prior to shaft failure and the repository was nearly at equilibrium when the shaft seal failed. Moreover, the tracers have not yet reached the seal salt. To test this hypothesis two variants were simulated by DOE, GRS, and Quintessa. The first variant has earlier failure of the shaft seal at 100 years, while compaction is underway and the second is later failure at 10,000 years, when there are tracers in the seal salt.

Due to the decoupling of the inner and outer repository by the repository seal, early or late shaft seal failure results in essentially no changes in flow or transport rates in the waste disposal drifts and only small changes in the seal salt and are not shown. The only significant difference in transport is that the VW Tracer diffusion rate in the DOE model is lower for the late shaft seal failure variant (not shown for brevity).

Hence, for this conceptual model, with rapid salt compaction and the repository seal operating as designed, shaft seal failure at 100, 1000, or 10,000 years does not appear to have a significant impact on flow and transport rates in the inner repository where the waste is located.

5. Discussion

Fig. 4 through Fig. 9 show a comparison of the porosity, saturation, fluid flow rates, and transport rates in the repository models. In some of the QOI, there is a great deal of difference between the models, but in other areas there is good agreement.

In every model there is hydraulic decoupling of the inner (from the waste drifts to the seal salt) and outer (from the seal salt to the shaft) repository, with the seal functioning as a highly effective hydraulic barrier between them. Flow and transport in the inner repository are driven by salt convergence and are impacted very little by the shaft seal failure. Flow in the outer repository is driven by shaft seal failure, which floods the large pore space of the gravel-filled infrastructure area. There is minimal radionuclide transport in the outer repository in any model.

5.1. *Importance of salt compaction*

The largest differences between the models are in quantities related to liquid saturation and flow and are most pronounced at early time, before 1000 years, as shown in Fig. 5 and Fig. 6. These differences are believed to be driven largely by the difference in creep-closure modelling between the teams and the resultant rate of reduction of porosity, which in turn depend on the assumptions in the compaction models (Table 4). The DOE model has the slowest resaturation and generally lower liquid flow rates because there is no reduction in porosity in their model; however this is somewhat counteracted by influx from the geosphere, a much slower process. The low initial saturation/slow compaction variant showed fundamental changes to the flow and transport regimes and highlighted the pessimistic assumptions made in the base case. These differences in liquid flow QOI reflect the **importance of implementing a high-fidelity salt compaction mechanism** in this salt conceptual model to study performance of the repository.

5.2. *Importance of diffusive transport*

The large differences in the short-term flow field have relatively little impact on the transport of the SNF and VW Tracers out of the SNF and vitrified waste drifts, respectively. This is believed to be because in the models with compaction there is no SNF Tracer in the SNF drift, and very little VW Tracer in the vitrified waste drift until after salt compaction is nearly complete. As can be seen by comparing Fig. 6 and Fig. 8, the liquid flow rates out of the waste drifts are very small when the SNF containers fail at 500 years and when the VW Tracer mass begins to accumulate to significant quantities after 1000 years. Similarly, in all the models the tracers appear in the salt seal when there is little or no fluid advection as a driving force, as shown in Fig. 9. Consequently, transport of both tracers out of the waste drifts and though the seal salt is believed to be largely diffusive in all models.

Though the differences in diffusive transport are generally smaller than the fluid flow differences, this indicates that **diffusion, or effective diffusivity, is a key physical mechanism** that impacts long-term transport of radionuclides in the repository. Diffusivity is closely linked to the salt creep-closure mechanism via porosity reduction and the coupling between porosity and effective diffusivity. Moreover, diffusion in the models will be impacted by numerical dispersion.

5.3. System performance implications

Finally, the three QOIs related to potential for the release of radionuclides out of the repository are transport rates of the SNF and VW Tracers from the seal salt towards the shaft, and liquid flow in the shaft. These three QOIs show a remarkable degree of agreement across all the models. Fig. 9 shows that little or no tracer is transported past the seal salt in any model during the simulations, though rates are increasing at 100,000 years. Fig. 7 shows that large flow rates through the shaft are limited to a pulse of water downward into the repository at the time of shaft seal failure. Due to the decoupling of the inner and outer repository by the highly effective repository seal, none of the models predicts significant migration of radionuclide tracers into the outer repository.

Differing simulation results inside the repository for these five plausible repository models demonstrate the need to use multiple lines of argument to create a robust safety case for nuclear waste disposal. For the parameters used and the FEPs and model scenarios considered in the task specification,[2] the simplified disposal system in the conceptual model indicates radionuclide containment during the simulated period of 100,000 years.

This result is similar to the expected and alternative scenario of the generic case of Bertrams.[9] In those scenarios, the release of radionuclides within their assessment period is negligibly small, the diffusive transport rates are very low, and the transport distances are long. A significant discharge of radionuclides from the repository into the overburden occurs only at times greater than one million years.[4,9]

6. Conclusions and future work

6.1. Summary and conclusions

The salt performance assessment task of DECOVALEX-2023 is a comparison of the models and methods for a simplified post-closure performance assessment model of a deep geologic repository in domal salt host rock. Five international teams participated in the code comparison: BASE, COVRA, DOE, GRS, and Quintessa.

All teams made simplifying assumptions in their models relative to the conceptual model in the task specification.[2] All teams made the simplification of not meshing individual SNF containers or vitrified waste canisters in the boreholes. The other most common simplifications are reducing dimensionality and simplifying the salt creep-closure model.

Despite differences in the modelling strategies, all models indicate that salt compaction and radionuclide diffusion are key physical processes in the repository. However, there are significant differences in the details of fluid flow and tracer transport, while the models agree that tracer discharge past the seal is very small up to 100,000 years. The repository models are all decoupled into an inner and outer repository by the repository seals that effectively contain the radionuclides in the inner repository.

For the four models that include a reduction in porosity because of creep-closure (BASE, COVRA, GRS, and Quintessa), flow in the inner repository is driven by salt compaction for the first few hundred years and the timing of the liquid flow and flow rates are determined in large part by rate of the porosity reduction. The DOE team applied resaturation of the inner repository by influx of fluid from the geosphere, which is a much slower process. Liquid flow in the outer repository is driven by the influx of surface water caused by the shaft seal failure in every model and for all variants considered.

The QOIs related to radionuclide transport that are compared are the SNF Tracer (present only in the SNF) and the VW Tracer (present only in the vitrified waste). Transport of both tracers is largely diffusive in every model. The rate of tracer diffusion is determined by a combination of the effective diffusion coefficients, how they depend on the reduction in porosity, and numerical dispersion. The last two are different for every model. Tracer transport takes place on different timescales in the models, though the trends are qualitatively similar. The SNF and VW Tracers have very different tracer transport behaviour in the base case, due to the different release mechanisms from the waste forms and their interaction with the fast pore space closure in response to the high initial fluid saturation of 20 %.

Two variant cases are also considered to test the impact of the high initial saturation and resulting rapid creep-closure of the salt, and the timing of the shaft seal failure. The low initial saturation/slow compaction case results show the time it takes to resaturate the drifts is increased by orders of magnitude, and the models give differing predictions on the impact on tracer transport. This comparison highlights the importance of considering uncertainty in both initial conditions and parameters in the creep-closure model in future stochastic simulation cases. The early and late shaft failure cases demonstrate that, though the timing of the shaft seal failure had a large impact on flow in the outer repository, the inner repository is relatively unaffected. This highlights the importance of the seal salt and concrete abutments as the primary barrier between the waste drifts and parts of the repository closer to the surface, and indicates the importance of further investigating assumptions around the effectiveness of the seal including the increase in our knowledge base about the mechanical behaviour of salt backfill in combination with concrete seals.

6.2. Future work

A further four years of research has been approved for DECOVALEX-2027. The future round includes physics that are believed to be important to repository performance that were left out of the current conceptual model. These may include heating of the repository due to heat generated by the waste, gas generation, and full two-phase flow modelling. Sensitivity analysis and uncertainty quantification will be an integral part of the next four years of work, with a particular emphasis on sensitivity to initial conditions, salt compaction models, effective diffusivity, and understanding the interaction of numerical dispersion and physical diffusion.

CRediT authorship contribution statement

Carl Rudolf Dietl: Writing – review & editing, Formal analysis, Conceptualization. **Tanja Frank:** Writing – review & editing, Formal analysis, Data curation, Conceptualization. **Steven Benbow:** Writing – review & editing, Formal analysis, Conceptualization. **Jodie Stone:** Investigation, Formal analysis. **Alexander Bond:** Writing – review & editing, Project administration, Formal analysis, Conceptualization. **Jens Wolf:** Supervision, Formal analysis. **Fabiano Magri:** Writing – review & editing, Formal analysis, Conceptualization. **Josh Nicholas:** Investigation, Formal analysis. **Ingo Kock:** Writing – review & editing, Supervision. **Jeroen Bartol:** Writing – review & editing, Formal analysis, Conceptualization. **Philip H. Stauffer:** Writing – review & editing, Formal analysis, Conceptualization. **Dirk-Alexander Becker:** Writing – review & editing, Formal analysis, Conceptualization. **Emily Stein:** Writing – review & editing, Project administration, Methodology, Funding acquisition, Data curation, Conceptualization. **Rick Jayne:** Writing – original draft, Project administration, Formal analysis, Data curation, Conceptualization. **Tara LaForce:** Writing – original draft, Supervision, Project administration, Formal analysis, Conceptualization. **Marek Pekala:** Writing – review & editing, Formal analysis, Conceptualization.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper

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Data availability

The complete conceptual model is available in the task specification, which is report SAND2023–04005R at osti.gov.

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