3D MODELING OF THE LONG-TERM BEHAVIOR OF A LARGE GEOLOGICAL REPOSITORY FOR HLW AND ILW-LL NUCLEAR WASTE, CONSIDERING HEAT, GAS, AND RADIONUCLIDE RELEASE AND TRANSPORT – OPTIMIZATIONS THAT ALLOW FOR DETAILED LARGE-SCALE MODELING

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ABSTRACT

Deep geological repositories for radioactive waste are currently being planned in several countries. France envisages the disposal of high-level and intermediate-level long-lived waste in the low-permeable Callovo-Oxfordian clay rock, with the objective of retarding the radioactive substances from entering the biosphere.

To assess the long-term safety and performance of the repository, we use numerical modeling to incorporate the relevant nonlinear and coupled thermo-hydraulic flow and transport processes, the impact of construction, and parametric uncertainty. However, addressing all these aspects in a single, large numerical model with a sufficient level of detail poses a challenge with respect to computation.

In the study presented here, we developed a model concept for simulations of a large repository with special regard to computational feasibility, using a modified version of TOUGH2-MP EOS7R accounting for hydrogen instead of air. The model concept involves a set of computing-time-reducing optimization measures, such as suitable geometrical simplifications and skilful discretization techniques.

The simulations performed demonstrate the effectiveness of the developed optimization measures, allowing for reasonable computation times and providing novel, comprehensive insight into the long-term comportment of thermo-hydraulic flow and transport processes within the entire repository and host rock.

BACKGROUND & SCOPE

The French national radioactive waste management agency (Andra) plans the disposal of high-level waste (HLW) and intermediate-level long-lived waste (ILW-LL) in a deep geological repository. The construction and operation of the repository will alter the natural conditions and properties of the affected host rock. Moreover, the generation and release of heat and gas by the stored waste, which will continue for several thousand years, will persistently influence the evolution of the physical state inside the repository and potentially decrease the retention capability of the engineered barriers and host rock for the radionuclides released by the waste. The involved processes take place on different spatial scales—from the decimeter scale of a waste package to the kilometer scale of the entire repository—and over the large time scale of several hundred thousand years.

The current repository concept (Andra, 2006) consists of several thousand horizontal tunnels for waste emplacement and additional tunnels and shafts for access, logistics, and ventilation during construction and operation of the repository. The entire repository encompasses a horizontal area of several kilometers in width and length (Figure 1). The repository is designed such that after its closure (i.e., after all waste has been emplaced and all tunnels and shafts have been backfilled and sealed), no human supervision will be required. To evaluate feasibility Andra has conducted many research programs assessing the performance and safety of the envisaged repository concept, aiming at addressing all relevant phenomenological and technical aspects during operation and post-operation.

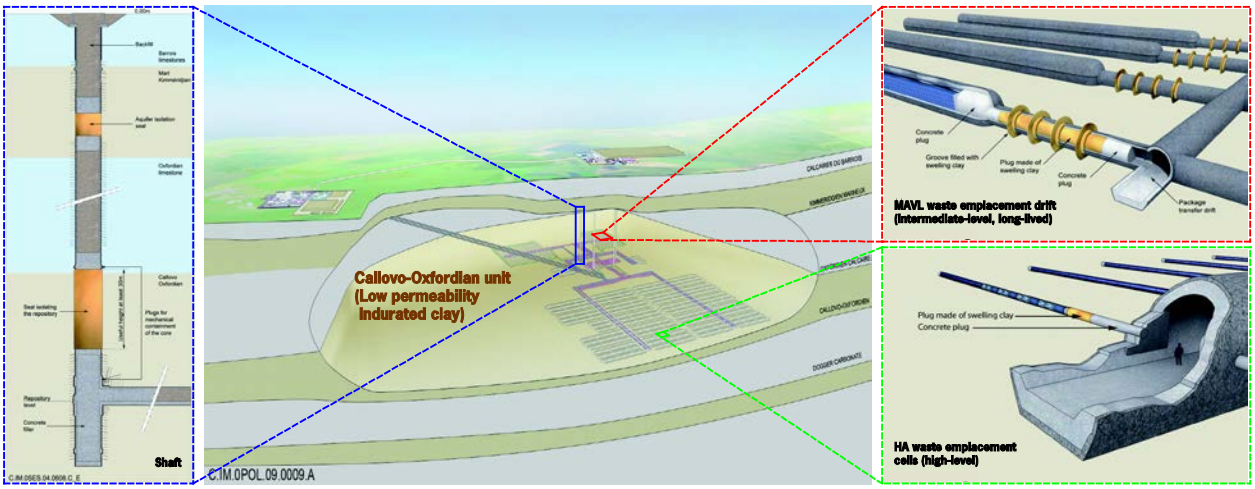

Figure 1. General repository architecture concept with emplacement tunnels for HLW & ILW-LL waste packages, tunnels and shafts for access, logistics, and ventilation, Andra (2006).

In the context of these programs, the objective of the study presented here is to model the thermo-hydraulic behavior inside the entire repository and the ambient host rock, as well as the migration of mobilized radionuclides within a time-frame of 1 million years. The model should represent all relevant details with a single integrated model mesh of the entire repository domain. Important phenomenological aspects to be considered are (i) the depressurisation and desaturation of the excavation damaged zone (EDZ), and the adjacent intact host rock, as a result of tunnel ventilation in the operational phase, with a re-saturation by pore water from the host rock and repressurisation in the post-operational phase; (ii) the appearance, migration, and disappearance of a gas phase due to waste-type-specific release of gaseous substances, mainly hydrogen; (iii) the decay-heat induced temperature increase leading to a pressure increase resulting from heat expansion of fluids and solids; and (iv) the mobilization of the radionuclide species ^{14}C and ^{129}I due to the degradation and corrosion of the waste packages and their migration under advection, diffusion, retardation, and decay.

The modeling requirements are to provide an adequate spatial representation of all repository components, considering the arrangement of the more than 10 different waste types, the waste-type-specific source terms of heat, gas, and radionuclides, respecting cooling times and early canister failure, and the spatial and temporal schedule of tunnel excavation, emplacement, and backfilling during construction and operational phases. Given these complex processes, the huge number of constructional elements, and the large range in scale—from the kilometer scale of the overall repository site to the decimeter scale of a single waste canister—an adequate and still manageable model representation poses a challenging task with respect to setup and its numerical computation on a medium-sized Linux-cluster.

Standard TOUGH2-MP (Pruess et al., 1999, Zhang et al., 2008) enables consideration of the above processes using equation-of-state module EOS7R. For the study presented here, some modifications were implemented: (a) hydrogen instead of air as primary gaseous component; (b) temperature-dependent diffusion of the dissolved components in the liquid phase[1]; (c) a break of the radionuclide decay chain to represent two individual radionuclides; and (d) fully mass conservative source-terms[2].

In a previous study on the maximum pressures and hydrogen transfer in the entire repository, spatial discretization of the entire repository site

[1] Andra heating experiments showed a factor of ~5 in diffusivity increase for dissolved components in fully saturated argillite heated from 22° C to 80°C, Andra (2009).

[2] With the exception of MOP(12)=2 (rigorous step rate) in standard TOUGH2, the implemented routines for transient source terms in the original TOUGH2/-MP source code do not guarantee a numerically exact input of the specified quantities

was implemented using the approach of *Subdivision, Multiplication, and Connection* (Poller et al., 2009, 2011, Enssle et al., 2011) in which symmetrical and repetitive subareas of the repository were discretized using a single mesh with effective properties representing the aggregated area. To form the mesh of the entire repository, several aggregated sub-area meshes were attached to each other. The approach allows for a massive reduction of the mesh size (i.e., the number of gridblocks and connections) and of the corresponding order of the Jacobian matrix solved by TOUGH2-MP, but nevertheless preserves a relatively fine mesh discretization at the locations of interest and does not compromise the robustness of the solution.

The simplifications used there are appropriate when maximum pressures or cumulated fluxes are of interest. However, in the study presented here, a straightforward adoption of this approach is not feasible, since radionuclide transport processes are to be studied in detail and resolved in time. Hence, we develop a new concept of the geometrical model, with special regard to radionuclide transport on a detailed temporal scale over the entire repository site, as well as to the computational feasibility of this approach.

The modeling concept, its parameterization, and the mesh optimization techniques are explained in the following section (Modeling Concept). Examples of physical results, and an assessment of the performance and benefits of the optimized modeling approach, are given in the results section below, followed by our conclusions.

MODELING CONCEPT

Physical & Numerical Model

The numerical TOUGH2-MP model is based on the equation-of-state module EOS7R considering all relevant implemented processes, including abovementioned code modifications (a) to (d), concerning two-phase flow and transport of mass and heat components. We modeled the radionuclide species ^{14}C in the chemical form of methane (and hence highly volatile[3]), and ^{129}I in the chemical form of hydroiodic acid (and hence perfectly soluble, i.e. with virtually no volatile fraction). Decay products and chemical reactions were not considered.

Parameterization

The model domain represents the host rock in its full vertical depth of ~150 m between the cap rock and bed rock, and has a lateral extent extending sufficiently beyond the horizontal dimensions of the repository, in order to minimize the influences of lateral no-flow boundaries. The surface area (footprint) of the domain totals ~3×5 km^2. The top and bottom boundaries were time-invariant and fixed at the values corresponding to the naturally occurring conditions of pressure[4], temperature, concentration, and 100% water saturation.

The overall simulation was split into seven phases. The first phase concerned the simulation of the natural conditions for initialization of the model. Phases 2 to 6 concerned the operational phase with excavation, ventilation, waste emplacement, and backfilling/sealing. In total, they lasted 100 years and represented the planned chronogram by Andra. Phase 7 concerned the post-operational phase, lasting between 100 and 1 million years.

Reference material properties were assigned according to Enssle et al. (2011). Selected reference transport properties are given in Table 1.

Table 1. Selected reference transport parameters.

Parameter	H_2	^{14}C	^{129}I
D_{gas} [m^2/s]	9.5E-5	1.3E-4	-
D_{liq} [m^2/s]	6.0E-9	4.9E-11	4.9E-11
Inv. Henry's const. [1/Pa]	1.4E-10	3.0E-10	1E+50
Half life [a]	-	5.7E+3	1.6E+7

$D_{gas/liq}$ = diffusion coefficient in the gas or liquid phase.

Source terms for hydrogen, heat, and radionuclide release were assigned, and accounted for the various expected waste types, as well as for

[3] Dissolution is considered according to Henry's law yet allowing for solute transport of ^{14}C.

[4] At the top boundary pressure decreased linearly by ~3 bar over the entire simulation time of 1 million years reflecting the expected evolution of the regional hydraulic state

the corresponding cooling times, emplacement dates, and the possibility of early canister failure.

Discretisation & Mesh Optimization

From physical and numerical perspectives, the domain discretization must be sufficiently fine to reflect all relevant geometrical features and to ensure a numerically robust solution, minimizing numerical diffusion. Conversely, from the computational point of view, the discretization needs to be sufficiently coarse in order to produce a computable solution within a reasonable execution time and without exceeding memory requirements. The reconciliation of these conflicting requirements is a steady issue in numerical modeling, especially when creating mesh designs.

In view of the given large and spatially heterogeneous repository domain, as well as the physical complexity, (e.g., nonlinear capillarity, relative permeability, sharp contrasts in permeability), model-mesh simplifications and optimizations were inevitable. A set of measures including topological simplifications and a methodology (to which we refer as the *embedded meshing approach*) was developed, exploiting the meshing flexibilities inherent to the finite volume method in TOUGH2/-MP[5].

Topological Simplifications

(S1) All tunnels and shafts, including their concrete lining and EDZs, are represented by squared or rectangular instead of circular cross sections respecting the real cross-sectional area[6]—see Figure 2 for illustration.

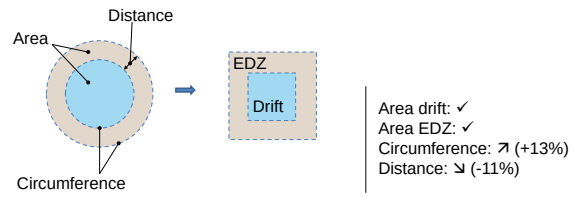

Figure 2. Transition from circular to squared cross-sectional shape of tunnels and shafts.

(S2) Parallel tunnels are represented by a single tunnel with an equivalent cross-sectional area, (Figure 3).

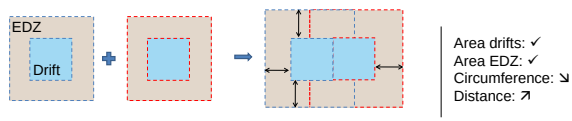

Figure 3. Aggregation of two parallel drifts with adaption of geometrical properties.

(S3) Inclined ramps are represented by horizontal drifts and vertical shafts with combined equivalent lengths.

(S4) The spatial arrangement of the waste emplacement zones and the locations of the shafts and tunnels are slightly shifted in order to gain a higher degree of symmetry.

(S5) Meshing algorithms for regular gridblock meshes such as MESHMAKER (Pruess et al., 1999) extend the cell size of a gridblock over the entire plane of the model mesh. Hence, small gridblock sizes—from the topological perspective needed only at certain locations—lead to a needless fine discretization at distant locations. In the study presented here, such configurations result especially from the discretization of annulus shapes, such as the EDZs. To avoid these, the concerned gridblocks are adapted to have nonrectangular cuboidal shapes, removing the comparatively small corner gridblocks (see Figure 4). These new gridblocks do not strictly satisfy the Voronoi criterion that postulates orthogonality of the connection between the centres of adjacent gridblocks and their common interface.

Further, the definition of the effect of gravity in these connections is ambiguous. The concerned connections occur, however, only at the annular space of the EDZs and thus enter the computation of circular fluxes within these materials

[5] In the finite volume method in TOUGH2 space is discretized by gridblocks and connections between adjacent gridblocks. Normally, the arrangement and properties of the gridblocks and their connections are chosen in a geometrically realistic fashion; however, the user is free to modify the geometrical arrangement and properties such as (for example) to increase the volume of a certain gridblock.

[6] The entailed increase in circumference and reduction of radial distance is less than 13% and 11%, respectively, and was neglected, yet this could be corrected for if sensitive.

only. These fluxes are of negligible magnitude compared to the axial and radial fluxes, where the mesh conforms to the Voronoi criterion as well as to gravity orientation; thus, the impact of the simplification on the simulation results is estimated to be minor.

(S6) Certain small-scale components are up-scaled to larger components with equivalent properties. This is, for example, applied to some components within the interior of a waste emplacement tunnel, e.g., the ILW-LL primary waste packages and the waste containers, or the EDZs and the concrete lining of the tunnels and shafts.

Incorporating these simplification measures, we generate the actual mesh of the entire model domain by following the process outlined in the following section.

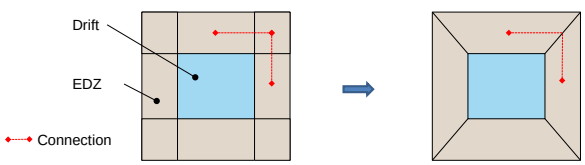

Figure 4 Modification of rectilinear gridblocks. Left: drift cross section discretized with nine rectangular gridblocks. Right: same drift configuration composed of five geometrically adapted gridblocks.

Embedded Meshing Approach

As a starting point, the entire model domain (i.e., the host rock including all waste emplacement zones, as well as the cap rock and bedrock) are discretized in a straightforward way with gridblocks of rectangular cuboidal shape, using MESHMAKER (Pruess et al., 1999). This mesh is referred to as the *global mesh*.

Tunnels and shafts, including their concrete linings and EDZs, are embedded into the global mesh with gridblocks having (a) a non-rectangular cuboidal shape (per the simplification discussed in S5) and (b) a rectangular cross section (cf. S1). This includes all ILW-LL emplacement tunnels.

The representation of the thousands of HLW emplacement cells is implemented by aggregation[7]. This means that several adjacent identical emplacement cells of the same geometry and waste-type are assembled into one aggregated emplacement cell with adapted geometry and properties. The adaptation is performed radially, and the axial length kept constant. The aggregation factor f equals the number of assembled emplacement cells[8].

The consequences for an aggregated HLW emplacement cell are as follows:

- Its extensive quantities (such as the ones listed below) are multiplied by f:
  - volume of gridblocks
  - interface areas
  - source terms
- Its intensive quantities or properties remain unchanged, such as:
  - distances between gridblocks
  - material properties
  - state variables, i.e., pressure, saturation, and temperature

Each aggregated emplacement cell is discretized with an axi-symmetric submesh (MESHMAKER 2D-R-Z grid). This submesh contains the engineered components of the HLW emplacement cell, the EDZ, and the near-field host rock in a radius of ~ 1.2 m (Figures 5 and 6). The outer, surrounding host rock is represented by brick-shaped gridblocks in the global mesh to which the submesh (the aggregated emplacement cell) is connected. The embedding of each of the submeshes into the global mesh is carried out as follows:

(A) Each submesh is connected to the global mesh at its radial average location. The average location is the location of the emplacement cell situated at the center of the set of emplacement cells assembled together (cf. Figure 6, position "(f+1)/2"). The global mesh is constructed such that this location coincides with the centers of several specific gridblocks to which the corresponding sub-mesh gridblocks are connected.

[7] This approach partially adopts the previously developed approach of *Subdivision, Multiplication, and Connection* (Poller et al., 2009).

[8] In the model mesh presented here, the aggregation factor was chosen to be around 10.

(B) The volumes of the global mesh gridblocks that are intersected by the sub-mesh are adjusted by subtracting the volume of the intersecting sub-mesh (see Figure 5).

(C) All gridblocks on the mantle of the sub-mesh are connected to the corresponding (intersecting) gridblocks of the global mesh (see Figure 5). The connection lengths are the distance between the center of the mantle gridblock to the mantle (*d1*) and the distance between the mantle and the center of the corresponding gridblock in the global mesh, i.e., the mantle radius of the submesh (*d2*) (Figure 6).

An illustration of the entire repository mesh created with the embedded meshing approach is given in Figure 7. The complete mesh consists of some 250,000 gridblocks and around 700,000 connections. With "conventional" mesh generation, i.e., without topological simplifications, aggregation of HLW emplacement cells and their representation by axi-symmetric gridblocks, the mesh size would reach some tens of millions of gridblocks and connections, and the corresponding Jacobian matrix would have been correspondingly large and possibly beyond the solution capabilities of practically all but the largest clusters and/or supercomputers.

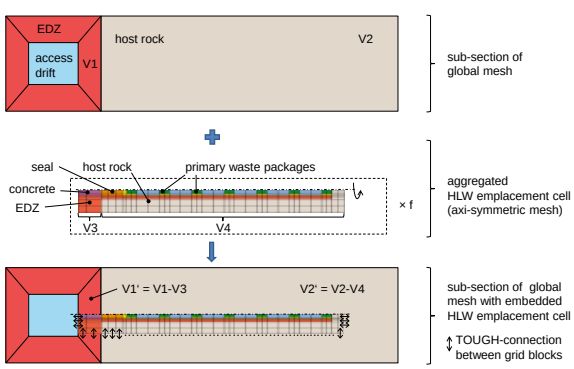

Figure 5. Aggregation and embedding of HLW emplacement cells to global mesh (cross-sectional view along a HLW emplacement cell). Top: gridblocks of the global mesh. Middle: gridblocks of the axi-symmetric submesh. Bottom: gridblocks of the global mesh with embedded axi-symmetric sub-mesh.

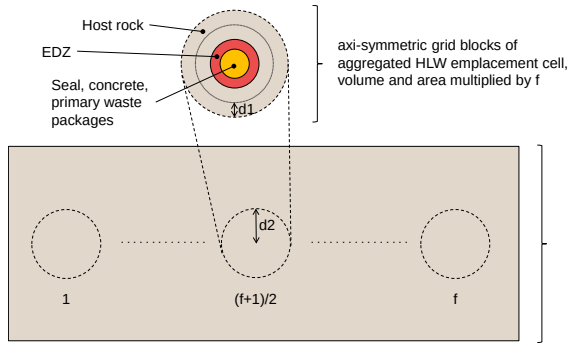

Figure 6. Aggregation and embedding of HLW emplacement cells to global mesh (cross-sectional view along an access drift).

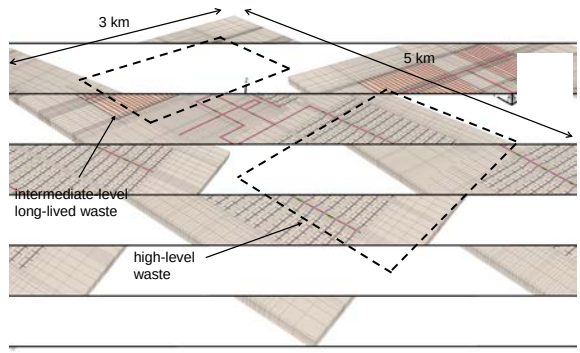

Figure 7. Entire repository mesh representing the planned layout; all gridblocks above the repository level are blanked.

RESULTS

Simulation Results

Approximately 20 simulation cases with and without radionuclides[9] were conducted. We considered two different layouts of the repository, and single- and two-phase flow. We varied important parameters, such as permeability, diffusion coefficients, gas generation-rates, and saturation-dependent gas generation, adopting the approach by Croisé et al. (2011), which considers the impact of water consumption and saturation-dependent corrosion rate on the hydrogen generation.

The simulation results represent a comprehensive and unprecedented pool of information regarding the transient thermo-hydraulic performance of the repository concept, one that particularly enables thorough insight into the

[9] Simulations without radionuclides used TOUGH2-MP EOS5.

coupled effects resulting from the large system heterogeneity in terms of space, time, and processes. As an example, the simulations demonstrate (and confirm) that all factors influencing hydrogen generation, its migration, and thus the distribution of a gas phase are of great importance for the transfer of ^{14}C. Figure 8 illustrates the ^{14}C transport at the repository level for the cases with and without hydrogen generation.

In contrast to the ^{14}C transport, the transport of ^{129}I shows little sensitivity with respect to the number of phases involved (one- vs. two-phase conditions resulting from gas generation), as is shown on Figure 9.

The different migration behavior of the two radionuclide species is attributed to their oppositional thermo-dynamic properties, with ^{14}C (in the chemical form of CH_4) being highly volatile and hence mainly transported in the gas phase (if present), which preferentially follows higher permeability pathways such as the EDZs around the tunnels. In contrast, ^{129}I, in the chemical form of hydroiodic acid, is very soluble and mainly transported by diffusion in the formation water. Regarding the gaseous convective transport of ^{14}C, only a very small fraction of the totally mobilized mass finally reaches the shafts (~10^{-4} % in the reference case).

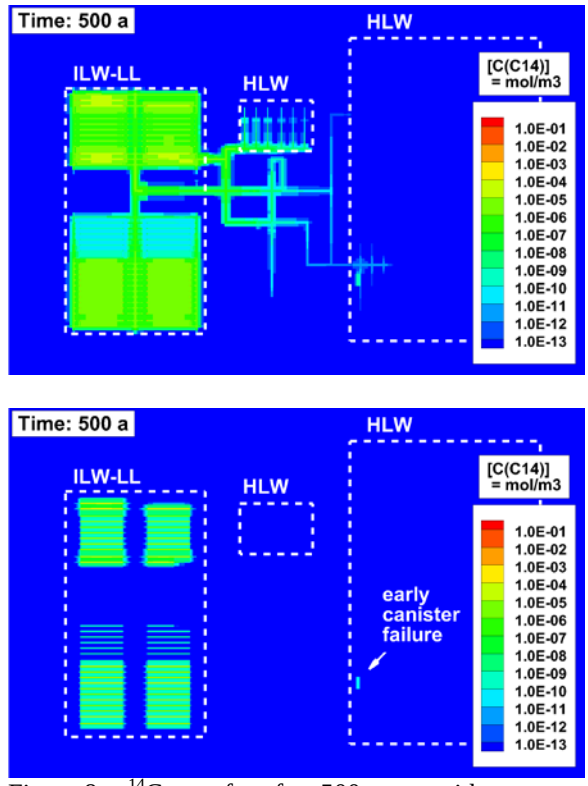

Figure 8. ^{14}C transfer after 500 years with gas generation (top) and without gas generation (bottom)

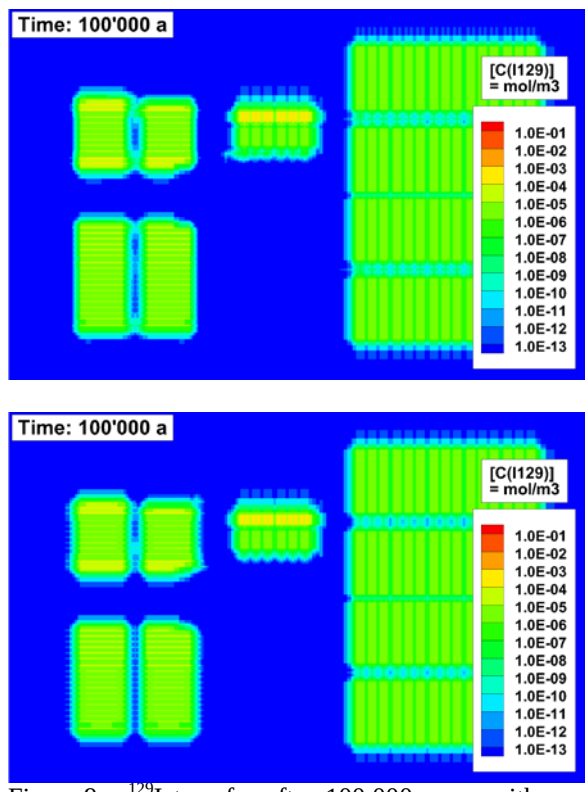

Figure 9. ^{129}I transfer after 100,000 years with gas generation (top) and without gas generation (bottom).

Comprehensive details of the simulation results will be presented in a separate paper (Enssle et al., 2012).

Assessment & Justification of the Approach

Previous large-scale modeling studies using TOUGH2-MP revealed the need for optimization measures to enable computationally feasible two-phase flow and transport simulations. This led to the developments of the embedded meshing approach. Relevant details, such as the corresponding topological simplifications and mesh manipulation measures, were presented above.

The first test simulations in the early stages of this study had extremely large computational demands and led to further mesh optimization measures, such as the upscaling of the HLW components and the EDZs.

The computation times strongly depended on the simulation case and the degree of complexity/nonlinearity of the processes and conditions under study. For single-phase cases, omitting gas generation led to computational times in the range of a few hours, whereas two-phase simulation cases with gas generation exhibited execution times as high as 30 days[10]. These computational times were observed using a parallel system involving six Intel Core2Quad 2.83 GHz machines with eight processors each.

To the extent possible, the results were validated by comparison with previous modeling studies. However, it is important to note that these studies usually involved smaller domains with different assumptions concerning the model boundaries, and often disregarded coupled phenomena.

An assessment of the Péclet numbers corresponding to the major travel paths of the radionuclides suggested that the mesh discretization resulting from the simplified approach described in this paper is sufficiently fine for an accurate computation of the quantities in question.

[10] This computation time was required in a case with reduced hydrogen diffusion in the liquid phase and hence a prolonged presence of the gas phase. With the reference diffusion coefficient, resaturation occurred considerably earlier and a computation time of around 10 days.

CONCLUSION

This study demonstrates the general feasibility of simulating coupled thermo-hydraulic two-phase flow and radionuclide-transfer processes on the scale of an entire repository, while simultaneously accounting for the relevant small-scale details. The simulations revealed that hardware resources are not necessarily the most important factor for successful model simulations. By choosing a suitable model conceptualization, including adequate upscaling, aggregation and mesh embedding techniques, and efficient data handling, we have developed a successful model, that is capable of solving very large problems without the need to resort to very large clusters and/or supercomputers, and which is a good basis for future parametric studies.

The single-phase and two-phase simulations in this study produced a consistent dataset characterizing the repository performance with respect to water, gas, ^{14}C, and ^{129}I transport. We have observed the strong dependency of ^{14}C transport on several parameters, such as permeability, diffusion coefficients, gas generation-rates, and saturation-dependent gas generation. The most important aspect here is the consideration of gas generation, which leads to largely increased transport rates of ^{14}C along the backfilled drifts and shafts by advection in the gas phase. By contrast, the transport of ^{129}I is virtually independent of the gas generation because of its high solubility.

ACKNOWLEDGMENT

This work was funded by Andra, and the modelling presented is based on data provided by Andra. Valuable input was provided by Guillaume Pépin and Jean Croisé. Thanks also to Keni Zhang, who kindly performed test calculations on a supercomputer.

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