Detailed Gas Generation and Transport Modelling at the Room and Repository Scale

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The NWMO has undertaken a postclosure safety assessment of a conceptual deep geological repository for used nuclear fuel at a hypothetical sedimentary rock site in the Michigan Basin in Ontario. The assessment includes a Disruptive Scenario where container failure 10,000 years post-closure exposes steel components of the containers to groundwater. The migration of gas generated by steel corrosion processes is assessed through simulations conducted with the T2GGM code at the placement-room and repository scales. The model results indicate: 1) that room resaturation (in the absence of gas generation) is 90 percent complete by 10,000 years, 2) pore pressure in the host rock never exceeds 80 percent of the lithostatic stress, and 3) gas transport is primarily in gaseous (as opposed to dissolved) form and is substantially confined to the engineered sealing materials and excavation-damaged zone. The different scale models were linked through a manual iterative process, where gas flows calculated using the Room-Scale Model were provided to the Repository-Scale Model. End-of-room boundary conditions on the Room-Scale Model were adjusted based on Repository-Scale Model results and the process repeated until sufficient congruence was attained. Recent T2GGM code developments have included the capability to link different scale models explicitly. Preliminary results are presented that illustrate the advantages of this approach.

I. INTRODUCTION

The postclosure safety assessment, supported in part by the work presented here, considered a conceptual deep geological repository for used nuclear fuel at a hypothetical sedimentary rock site in the Michigan Basin in Ontario[1]. The conceptual design can hold 12,778 containers at a repository depth of 500 m. One of the Disruptive Scenarios considered in the safety assessment is the "All Containers Fail" case whereby the copper cladding of the containers is breached by some unknown mechanism at 10,000 years postclosure, resulting in the exposure of the interior steel container components to groundwater that has migrated into the sealing materials from the surrounding geosphere. Corrosion of the steel ensues, with attendant hydrogen gas generation. The fate of this gas, as it migrates through the repository sealing materials, excavation-damaged zone (EDZ), and the surrounding host rock can affect both the internal repository pressure and the transport of volatile radionuclides.

Detailed gas generation and transport modelling was conducted using T2GGM[2], a numeric code that assesses the coupled behavior of gas generation, temperature and multiphase (gas and water) transport. T2GGM integrates a Gas Generation Model (GGM) with the TOUGH2 simulator[3].

There is a mismatch between the scales of models required to provide data necessary to support the safety assessment. Gas transport to the biosphere through the sealing materials in the tunnels and shafts is considered in dose calculations[4]. Such transport represents the collected corrosion-generated gas from 275 placement rooms, within each of which are 50 containers. Placement rooms are organized in panels and attach to five cross-cut drifts. Those cross-cut drifts connect to the main access tunnels and perimeter drifts, which in turn connect to the shafts. However, gas generation is a localized process that depends upon conditions within the placement room sealing materials adjacent to each container. It is not computationally feasible to simulate gas generation and transport with full geometric fidelity at the repository scale.

Consequently, a more tractable two-model approach has been developed. A Room-Scale model simulates gas generation within one placement room, and calculates gas flow leaving the room into cross-cut and perimeter drifts. Gas behavior within each placement room is assumed sufficiently similar for Room-Scale results to be representative of gas behavior in all placement rooms. Gas transport results are scaled to represent entire panels, with the scaled results specified as an injected gas flux into the Repository-Scale Model. The Repository-Scale model consists of a single access tunnel connecting two shafts, with gas injection points corresponding to locations where drift panels connect to the tunnels.

Although conceptually attractive, the two-model approach is complicated by the necessity of ensuring the congruence of pressures and saturations between the exit point of the Room-Scale Model and the injection points of the Repository-Scale Model. Boundary pressures affect pressures within the placement rooms and flow rates from the rooms. A manual iterative approach has been used with multiple simulations required before sufficiently similar pressure and saturations are obtained.

Implementation of, and results from, the Room- and Repository-Scale models are described in Sections II and III respectively. Section IV presents a modified version of T2GGM that supports explicit coupling of the two model scales in a single simulation, enforcing model boundary congruence and eliminating the multiple manual iterations required for separate models. The conceptual design, implementation and verification, and preliminary results are described.

II. ROOM-SCALE MODEL

The Room-Scale Model considers hydrogen gas generation from corrosion processes and two-phase flow within a single geometrically simplified placement room. It also considers thermal loading from the container, heat transport by conduction and convection, and consequent thermal effects on gas generation and gas and groundwater flow.

II.A. Gas Generation Model

The non-isothermal container corrosion model includes four corrosion processes[2], each of which occurs under different conditions that are anticipated to occur throughout the evolution of conditions in each placement room: 1) Dry Air Oxidation, 2) Aerobic Unsaturated Corrosion, 3) Anaerobic Unsaturated Corrosion, and 4) Anaerobic Saturated Corrosion. Each of these corrosion processes has its own temperature-dependent corrosion rate expression.

Available oxygen to support 1) and 2) is consumed rapidly, with the result that anaerobic corrosion processes dominate in the time periods of interest. These processes lead to the generation of hydrogen gas (H_2). Unsaturated anaerobic corrosion occurs prior to complete room resaturation provided that relative humidity exceeds a threshold (60%). Saturated anaerobic corrosion commences once the container is in contact with liquid groundwater. Processes are not necessarily sequential, for example, saturated corrosion processes may generate sufficient gas to raise room pressures above hydrostatic, forcing groundwater to leave the room, and causing a transition back to unsaturated conditions.

Calculated gas generation rates are based on active corrosion processes, temperature, surface area and thickness of container steel components. At each time step, TOUGH2 simulation results are averaged over sealing components adjacent to each container to provide temperature, saturation, and pressure data to the GGM. Calculated gas generation rates are then applied as gas source terms into the adjacent sealing materials.

II.B Model and Assumptions

The Room-Scale Model describes a placement room located in the middle of a central repository panel. The model assumes symmetry and describes half the room, the room entry and seal, and the associated portion of cross-cut drift (Figure 1 and 2). The 50 containers to be placed in the room are combined into 10 container elements, each of which has the metal surface area, mass and thermal load of five containers. Vertically the model includes the geologic column from 1000 metres below the room to ground surface 500 metres above. This large extent is not shown in the figures but was required to accurately simulate the thermal response of the system to the container heat source.

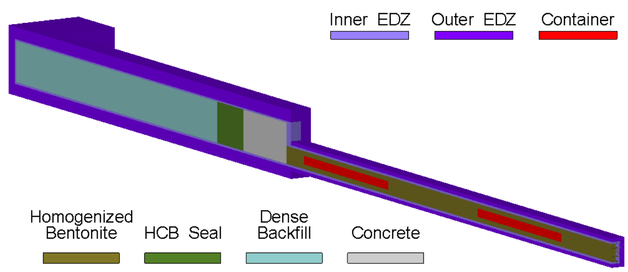

Fig. 1. Detail of Room-Scale Model showing sealing materials and EDZ in room entry and first 10 containers (2 container elements).

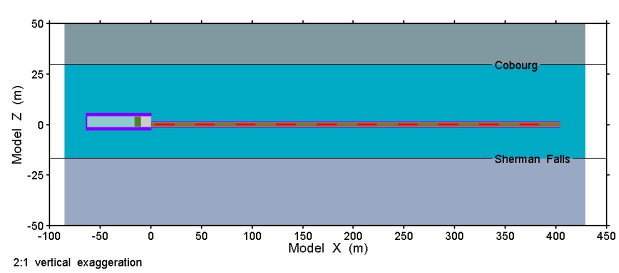

Fig. 2. Vertical Section through placement room of Room-Scale Model

Initial conditions in the geosphere included: no initial gas saturation, hydrostatic pressure profile, and a specified geothermal gradient. Prior to container placement, the 60-year operational period was simulated with air at atmospheric pressure in the tunnel and room. This served to develop a pressure and saturation gradient through the EDZ and adjacent geosphere. At closure, sealing materials were initialized at specified saturations and atmospheric pressure. Performance was simulated to 1 Ma postclosure, with gas generation processes commencing at container failure at 10,000 a. During the gas generation phase, elements at the end of the cross-cut drift portion of the grid were given extremely large volumes and set at specified pressures and gas saturations. Gas flow into these elements was extracted for use as input to the Repository-Scale Model.

II.C. Results

The primary variables for T2GGM calculations are gas pressure, liquid saturation, and temperature. Liquid pressure within a model element is determined from gas pressure by adding the capillary pressure at the calculated liquid saturation. Capillary pressure is defined on a material basis as a negative or suction pressure; liquid pressure is always less than or equal to gas pressure. Capillary pressures in the Ordovician host rocks and bentonite sealing materials can be very high, as shown in Figure 3.

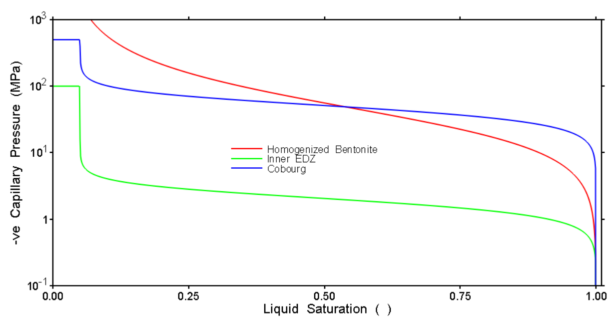

Fig. 3. Capillary Pressure Curves for Placement Room Bentonite (Homogenized Bentonite), Repository Inner EDZ, and the Cobourg Formation

The saturation-averaged pressure, or pore-pressure, represents the pressure seen by the formation from a geomechanical stress perspective. Excessive pressure can induce fracturing within the intact rock if the pore pressure exceeds the local minimum stress. The geosphere under consideration is assumed to be in a compressive stress regime with the minimum stress being the vertical lithostatic stress induced by the weight of rock and overburden material. A target acceptance criterion has been set where pore pressure in the intact rock should not exceed 80% of the lithostatic stress.

Average room and intact rock pressures, room liquid saturations and gas flow rates for the final simulations are shown in Figure 4. Room resaturation is nearly complete at 10,000 a, when gas generation commences, although room gas pressure is still low. Pressure rises rapidly after the start of gas generation, reaching a maximum that is controlled by the specified fixed liquid pressure at the drift boundary. Pore pressures in the intact rock are well below the target stress criterion. Initial gas generation serves to pressurize the room, however once the maximum is reached, gas exits the room into the drift. The relatively high rate of initial gas generation is due to the average room liquid saturation exceeding the specified threshold (0.9) for the onset of Anaerobic Saturated Corrosion with its attendant higher corrosion rates. As pressures increase, expelling liquid, the saturations reduce slightly below the threshold, reverting to Anaerobic Unsaturated Corrosion. Subsequently, saturation crosses the threshold again at approximately 90 ka and Anaerobic Saturated Corrosion resumes. Gas generation ceases at 400 ka when all steel has been consumed by corrosion reactions.

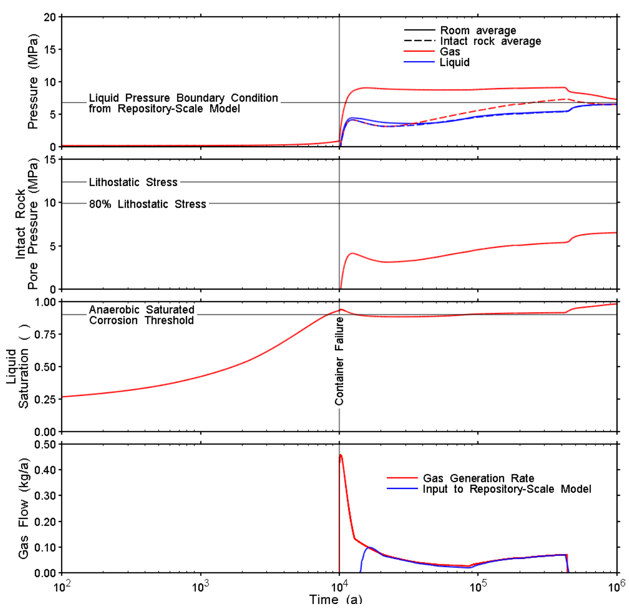

Fig. 4. Summary results for Room-Scale Model

Distribution of hydrogen in gas- and dissolved-phase within the model is shown in Figure 5. Note that the single room results are scaled to reflect the total of all 275 placement rooms in the repository. Gas phase hydrogen is largely restricted to the sealing materials and EDZ. Dissolved phase mass within the host rock increases with the majority of hydrogen mass remaining in the system being found in dissolved phase beyond 550 ka.

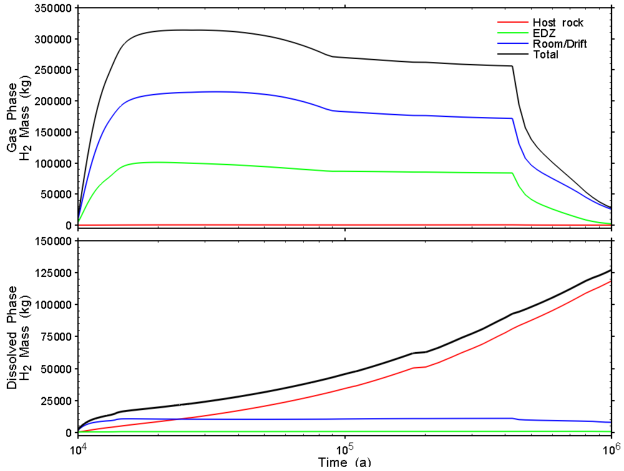

Fig. 5. Room-Scale Model gas allocation (scaled for full repository)

III. REPOSITORY-SCALE MODEL

The Repository-Scale Model considers the transport of gas and water, without thermal effects, along the main drifts and shaft of the repository, to estimate the amount of gas reaching the biosphere. Gas is injected into the main drift. The gas injection rate is calculated by multiplying the gas flow out of the Room-Scale Model cross-cut drift by the number of rooms in a single panel.

III.A Model and Assumptions

The Repository-Scale Model consists of a single drift connecting two shafts (Figure 6). Horizontal symmetry is assumed, with the model describing half the drift and shafts. The model extends vertically from 100 m below the repository to 300 m above the repository.

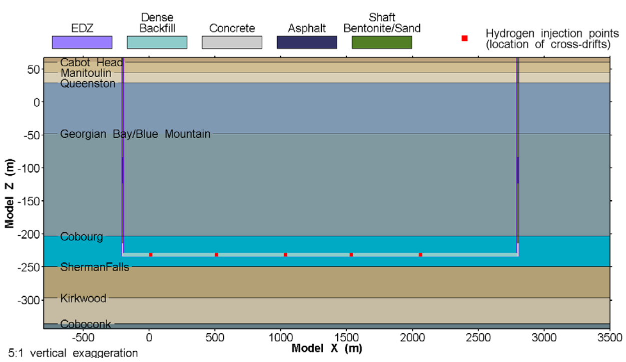

Fig. 6. Vertical Section through Repository-Scale Model

Pressure boundary conditions are defined at the top and bottom of the model, with the top pressure set based on a site-scale flow model[1] and the bottom pressure is a calculated hydrostatic pressure. The geosphere initial conditions are hydrostatic pressure and full water saturation.

As in the Room-Scale Model, an operational period of 60 years was simulated with atmospheric pressure and full gas saturation in the drift and shaft to develop representative pressure and saturation conditions in the EDZ and geosphere. Simulations presented here assume closure at 60 a, with sealing materials at atmospheric pressure and 80% water saturation. Performance was simulated to 1 Ma postclosure.

Gas is injected into the model at five locations, corresponding to intersections of the main access tunnel and the cross-cut drifts (Figure 6). The gas source term is calculated from results of the Room-Scale Model, multiplying the gas flow exiting a single room (i.e., from the end of the cross-cut drift segment) by the average number of rooms in each panel. This source term ignores the migration and accumulation of gas in the cross-cut drifts so that all gas leaving the Room-Scale Model is assumed to immediately reach the main access tunnel.

III.B. Results

Figure 7 shows average pressures, average saturations and gas flow for the Repository-Scale Model. Average pressures and saturations in the tunnel are determined from results in the sealing material of the main tunnel at the intersection with the cross-drifts (where gas is injected). Flow results shown in Figure 7 illustrate the amount of gas leaving the shaft at the top of the model. The onset of the Anaerobic Saturated Corrosion (see third panel of Figure 4) is responsible for the change in slope that occurs just prior to 100,000 years. As the permeable Guelph formation that lies almost 300 metres above the top of the repository has a much lower gas-entry pressure than the shaft sealing materials, the rising hydrogen gas is expected to exit the shafts and enter the Guelph formation.

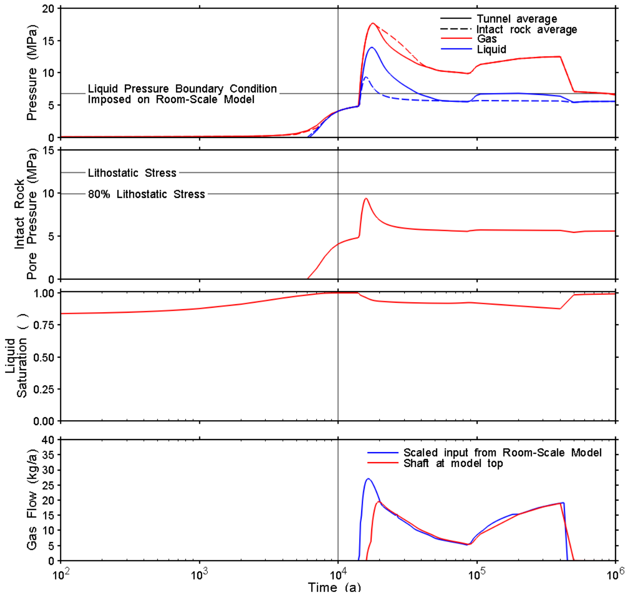

Fig. 7. Summary results for Repository-Scale Model

As shown in the second panel of Figure 7, pore pressure within the intact rock adjacent to the tunnels reaches a maximum of 9.6 MPa at 15,700 years, and does not exceed the target acceptance criteria of 80% of lithostatic stress over the 1 Ma simulation period, indicating that the pressure from gas generation is insufficient to fracture the rock. While accounting for model and data uncertainties that could result in higher pressures, the conservatism associated with this case, where all containers fail at 10,000 years, provides confidence that rock damage will not occur.

Figure 8 describes the distribution of gas- and dissolved-phase hydrogen within the model. Hydrogen is moving primarily in gaseous form, with dissolved hydrogen accounting for approximately 0.01% of hydrogen transport. Gas is found mostly within the sealing materials in the repository tunnels and shafts, with some gas found within the EDZ, and very little gas within the host rock. Compared to the hydrogen mass presented in Figure 5, it is evident that most hydrogen, dissolved or gas phase, remains associated with the placement rooms.

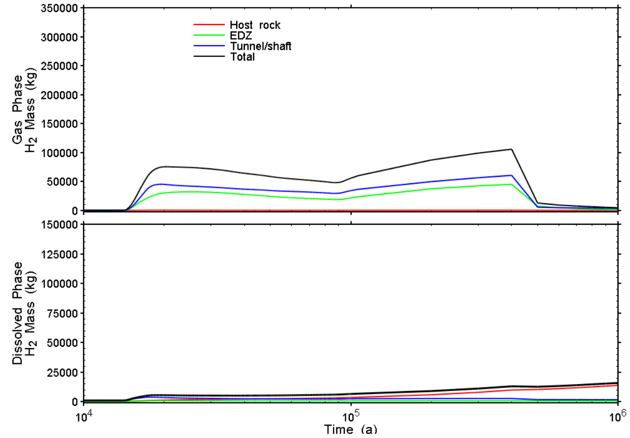

Fig. 8. Hydrogen allocation results for Repository-Scale Model

IV. MODEL LINKING

Neither the pressures nor the saturations in the Repository Scale tunnels shown in Figure 6 are constant. On average, the liquid pressure is close to the specified Room-Scale Model boundary pressure over the time interval where gas generation occurs. However, the pressure peak apparent immediately after the start of gas generation is likely higher than would occur in a fully-coupled system, where the increase in pressure above that of the gas source would reduce the flow rate, thus moderating the magnitude of the peak. This is an unavoidable consequence of the lack of coupling between the models. Improvements could be made with time-varying pressures, but the trial-and-error nature of the iterative approach is time consuming, especially when the multi-day model execution times are considered.

Coupling of the different model scales would resolve this issue. However, as mentioned previously, a complete repository model with 275 placement rooms is not feasible computationally. What was required was an approach similar to the manual process, where flows from a single room are scaled and distributed, but where room boundary pressures and saturations are continuously adjusted in response to simulated tunnel responses.

IV.A. Approach

The TOUGH2 code architecture lends itself to this sort of approach. Multiple models can be defined and executed simultaneously. Models can be linked by defining special-purpose connections, but there is no intrinsic capability to scale flows to suit conceptual models such as that described in this paper, where one Room-Scale Model represents many actual rooms.

Modifications were made to the T2GGM code to allow for explicit linking and flow scaling for different scales of models. Multiple models execute simultaneously, with flow calculations from one model dependent upon pressure and saturations calculated at boundary calculation points in the other. Flows are scaled (if necessary) and used as input at boundary calculation points.

IV.B. Implementation and Verification

To implement this approach, we define the following:

- Pressure Nodes (PNs) – these are groups of grid blocks with similar material properties for which average pressures and saturations are calculated at the end of each time step. There may be more than one PN defined. For example, separate PNs could be used to account for EDZ and sealing materials. At the end of each time step, average pressures and saturations are calculated for each group of nodes. These nodes occur within the Repository Scale sub model.

- Flow Nodes (FNs) - these are associated with large-volume grid blocks (e.g. boundary-condition nodes) at the end of the gas-generating Room Scale sub-model. They are grouped by material properties similarly to PNs. At the start of each time step, pressures and saturations for FNs will be set to the average values of the associated PNs from the previous time step.

- Flow Connections (FCs) – these connections calculate flows from the gas generation model into the FNs. They are similarly grouped by material properties. Total flows calculated at the end of each time step will be scaled and applied at PN locations at the beginning of the next time step.

A new TOUGH2 input block, MLINK, is defined, where PNs, FNs and FCs are read, as well as scaling factors and control flags.

Figure 9 is a schematic of a simplified verification representation of two linked models, with source and destination sub-models (analogous to, but not otherwise similar to the Room- and Repository-Scale Models, respectively). The linked sub-models have two material types: a low-permeability rock and a higher-permeability tunnel. A gas injection node at one end of the source sub-model provides a constant source of gas at a rate of 0.1 kg/s. Flow from the source sub-model is calculated at connections attached to the identified flow nodes. The calculated flows are injected into the destination sub-model at the seven identified pressure nodes. No further flow scaling is applied. Boundary nodes at each end of the destination sub-model tunnel are set to zero pressure to force flow out of the model.

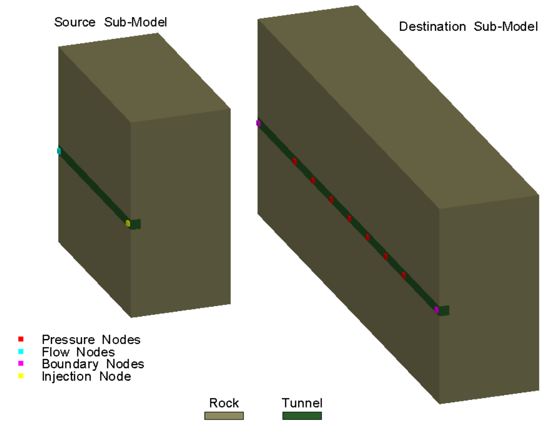

Fig. 9. Model-linking verification model

The simulated pressure response within the model domain at 100 a is shown in Figure 10. Visually, the results are as expected with primarily the high-permeability tunnels being affected. Peak pressure is at the injection point in the source sub-model and pressure dissipates towards the boundaries in the destination sub-model tunnel.

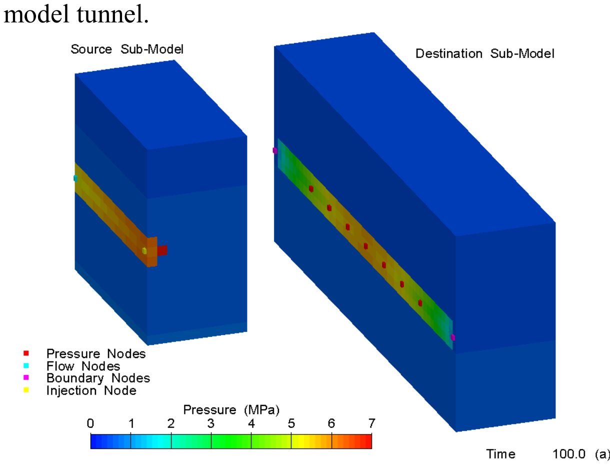

Fig. 10. Pressure distribution at 100 a

The time history of pressures and flows shown in Figure 11 verifies correct operation of the model. The post-processed average pressure at pressure nodes (dashed blue line) is identical to the average pressure applied at the flow node (red line). Flow out the designated flow node rapidly equilibrates with the injection rate, and cumulative flow out the destination sub-model boundary nodes reflects the factor of seven multiplier implied by the seven pressure nodes.

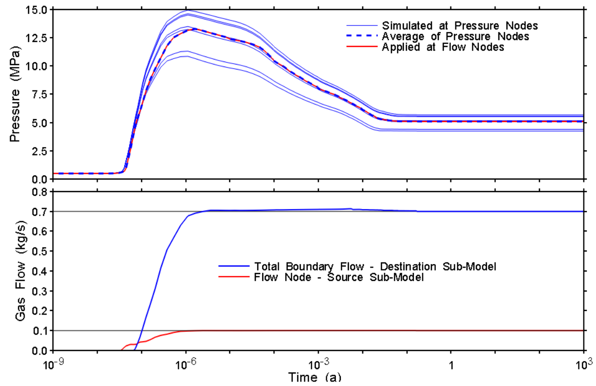

Fig. 11. Verification model pressure and flow results

IV.C. Preliminary Results

The model linking capability was applied to a single combined Room- and Repository-Scale Model. Discretizations of both sub-models were simplified but still reflect the general configuration and property assignments shown in Figures 1, 2, and 6, with the exception of the Outer EDZ material type. Examination of the separate model results had shown that the presence of the outer EDZ was not significant from a gas transport perspective. Additionally, as shown in Figure 12, the Room-Scale sub-model does not include the cross-drift segment; instead, gas flow rates are calculated at the end of the dense backfill room seal.

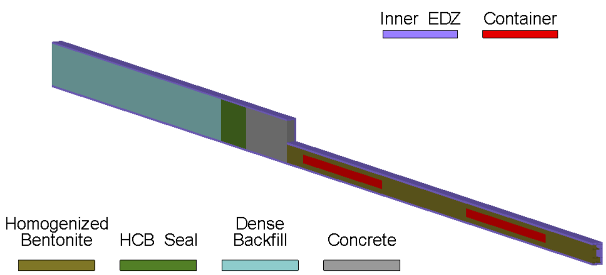

Fig. 12. Room-Scale sub-model property assignment

The model was executed without linking the sub-models for the 10,000 a pre-failure period. Linking and gas generation were simulated from 10,000 a to 1 Ma. During this phase, the volumes of the gas injection nodes in the Repository-Scale sub-model were adjusted to include the porosity available for storage in the associated cross-cut and perimeter drifts.

Summary results of the linked Room-Scale and Repository-Scale sub-models are shown in Figure 13. In contrast to the individual model results, average gas pressures in the placement room and repository tunnels are almost identical post-failure, with the exception of a several-thousand-year period immediately post-failure where room pressures exceed repository tunnel pressures. Differences in liquid and pore-pressures are due to a combination of differences in liquid saturations and different capillary pressure functions for the different sealing materials.

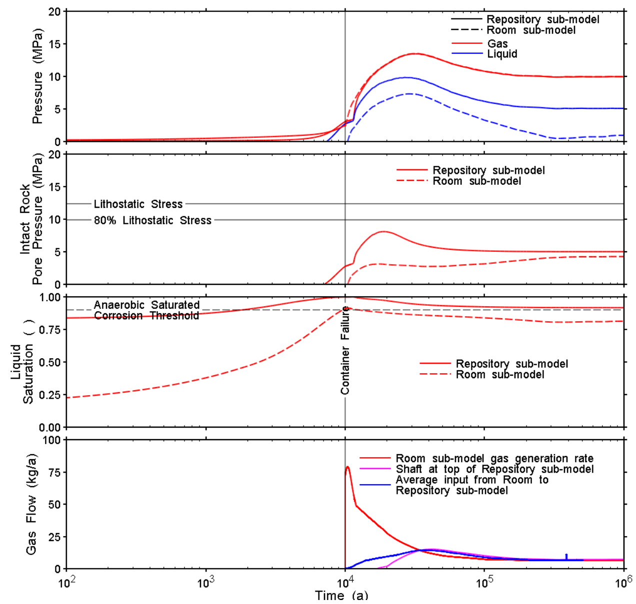

Fig. 13. Linked model results.

Gas flow from the Room-Scale sub-model to the Repository-Scale sub-model is earlier in onset, but diminished in magnitude compared to the separate model approach (comparing blue lines in bottom panels of Figures 7 and 13). The earlier start is due to the lower initial pressures at the combined boundary as flow to the boundary starts as soon as room pressure exceeds the boundary pressure. The reduction in peak flow rates is due to the opposite effect – higher boundary pressures reduce the gradient from the room, thus reducing gas flow.

Peak pressures in the Repository-Scale linked sub-model are reduced relative to the individual model for two main reasons: 1) the effect of model linkage on boundary pressures described above, where higher boundary pressures reduce flow rates; and 2) slightly lower liquid saturation in the Room-Scale Model which reduces the amount of initial Anaerobic Saturated Corrosion (compare dashed line in centre panel of Figure 13 to centre panel of Figure 4), and thus the gas generation rate. This latter effect also impacts the longer term pressure profile as Anaerobic Saturated Corrosion never restarts subsequent to the initial peak. Sufficient container mass exists to support Anaerobic Unsaturated Corrosion for the full 1 Ma simulation period. The inclusion of additional storage volume associated with perimeter drifts also mitigates the peak pressure, although this effect is minor.

There are some numeric issues with the explicit nature of the linked model approach. Calculated flow out the end of the room is relatively stable during the period when a pressure differential exists between the Room-Scale and Repository-Scale sub-models. However, as post-failure pressures converge, some oscillations in flow rates start to occur. However, as shown in Figure 14, integrated boundary flow rates converge on, and do not exceed, the integrated gas generation, implying that overall mass balance is not affected and that the average flow is correct. Various approaches for ameliorating the oscillations have been investigated and may be implemented in the future. However, the oscillations do not appear to have significant impact on the primary simulation results of pore pressures and gas flow rates in the shaft.

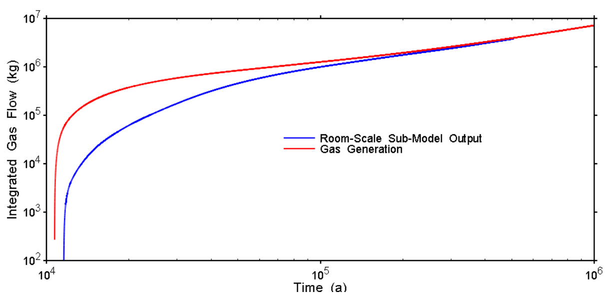

Fig. 14. Integrated gas generation and room outflow

V. SUMMARY AND CONCLUSIONS

Preliminary results from the model linking approach compare well to the separate Room- and Repository-Scale Models and provide a conceptually pleasing congruence in boundary conditions that is lacking in the separate model approach.

Differences in results between the two approaches are minor with the separate models giving a higher peak pressure in the Repository-Scale Model and slightly different average saturation profiles. The lower room-saturation in the combined linked model reduces the amount of gas generated due to Anaerobic Saturated Corrosion and is thus partially responsible for the lower peak pressures in the Repository sub-model. The flow rate response to changing boundary conditions also serves to reduce peak pressures.

Given that most proposed repositories typically contain multiple identical placement rooms attached to a drift or tunnel network, the linked model approach could be useful for evaluating gas generation and transport in other repository designs.

The scenario evaluated here is a Disruptive Scenario, contingent on the highly improbable event of simultaneous failure of copper cladding on all containers after only 10,000 years. As such, it is considered a bounding case. Nonetheless, even under this extreme gas generation scenario, pore pressures in the intact rock do not exceed the target acceptance criterion of 80% of lithostatic stress, indicating that there is virtually no possibility of host rock damage due to gas-generation-induced pressures.

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