Simulations of Water Flow in Relation to a Steady Criticality in an Unsaturated Alluvial Repository

Spent Fuel and Waste Disposition

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APPENDIX E

NFCSC DOCUMENT COVER SHEET[1]

Name/Title of Deliverable/Milestone/Revision No.	M3SF-23OR010304052 GDSA- PFLOTRAN Modeling and Integration ORNL Annual Progress Report
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Quality Rigor Level for Deliverable/Milestone[2]	☐ QRL-1 ☐ Nuclear Data	☐ QRL-2	☐ QRL-3	☒ QRL-4 Lab QA Program[3]

This deliverable was prepared in accordance with Oak Ridge National Laboratory *(Participant/National Laboratory Name)*
QA program which meets the requirements of

☒ DOE Order 414.1 ☐ NQA-1 ☐ Other

This Deliverable was subjected to:

☒ Technical Review ☐ Peer Review

Technical Review (TR)	**Peer Review (PR)**
Review Documentation Provided	**Review Documentation Provided**
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Name and Signature of Reviewers

Technical Reviewer — Scott Painter
Technical Reviewer — Alex Shaw
Added by Riley Cumberland

NOTE 1: *Appendix E should be filled out and submitted with the deliverable. Or, if the PICS:NE system permits, completely enter all applicable information in the PICS:NE Deliverable Form. The requirement is to ensure that all applicable information is entered either in the PICS:NE system or by using the NFCSC Document Cover Sheet.*

- *In some cases there may be a milestone where an item is being fabricated, maintenance is being performed on a facility, or a document is being issued through a formal document control process where it specifically calls out a formal review of the document. In these cases, documentation (e.g., inspection report, maintenance request, work planning package documentation or the documented review of the issued document through the document control process) of the completion of the activity, along with the Document Cover Sheet, is sufficient to demonstrate achieving the milestone.*

NOTE 2: *If QRL 1, 2, or 3 is not assigned, then the QRL 4 box must be checked, and the work is understood to be performed using laboratory QA requirements. This includes any deliverable developed in conformance with the respective National Laboratory / Participant, DOE or NNSA-approved QA Program.*

NOTE 3: *If the lab has an NQA-1 program and the work to be conducted requires an NQA-1 program, then the QRL-1 box must be checked in the work Package and on the Appendix E cover sheet and the work must be performed in accordance with the Lab's NQA-1 program. The QRL-4 box should not be checked.*

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SUMMARY

Oak Ridge National Laboratory (ORNL) is examining the conditions under which a criticality event could be ruled out for large packages placed in an unsaturated alluvial repository. This work specifically examines the water level in a stylized waste package that is assumed (1) to fail on the top, and (2) to empty as water is driven away—not by boiling—but by fluid flow phenomena driven by thermal gradients.

This analysis uses the PFLOTRAN code package. Specifically, this year's work includes examination of the heat rate at which water is driven away for various percolation rates using the same assumptions listed in the 2022 annual report.

The STANDARDS (formerly UNF-ST&DARDS) package has predicted dual-purpose canister (DPC) neutron multiplication factors (k-effectives) ranging above 1.1 (unitless) with failed components. The DPC designs were not created with the intent to use for disposal purposes. Emplacing such packages may be worth consideration if it can be shown that criticality is either extremely unlikely or of very low consequence to the repository's safety case. This work aims to help establish hydrologic boundary conditions for a highly hypothetical, highly stylized subsurface criticality event. The approach to critical is assumed to be slow, producing steady heating rates under a few kilowatts.

For a DPC containing capillary media, the simulated power required for dry-out was proportional to the percolation rate but was unaffected by the size of a large breech on top of the DPC. Results for single cases with no capillary media in the DPC suggest that higher infiltration rates may be required in those cases to cause flooding.

Bounding mechanisms and assumptions must be identified and characterized further by performing additional perturbations to various input parameters to demonstrate robustness of the results. This might be accomplished by examining responses to power pulses to determine the system transfer function required to enable a reduced order feedback model.

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EXPLORATORY SIMULATIONS OF WATER FLOW IN RELATION TO A STEADY CRITICALITY IN AN UNSATURATED ALLUVIAL REPOSITORY

1. INTRODUCTION

Oak Ridge National Laboratory (ORNL) is examining the conditions under which a criticality event could be ruled out for large packages placed in an unsaturated alluvial repository. This work specifically examines the water level in a stylized waste package that is assumed (1) to fail on the top, and (2) to empty as water is driven away—not by boiling—but by fluid flow phenomena driven by thermal gradients.

This analysis uses the PFLOTRAN code package (Hammond et al. 2014). Specifically, this year's work includes examination of the heat rate at which water is driven away for various percolation rates using the same assumptions listed in last year's report (Painter et al., 2022).

The STANDARDS (formerly UNF-ST&DARDS) package has predicted dual-purpose canister (DPC) neutron multiplication factors (k-effectives) ranging above 1.1 (unitless) when considering component failure (Shaw et al. 2022, p. 235). Emplacing such packages may be worth consideration if it can be shown that criticality is either extremely unlikely or of very low consequence to the repository safety case. This work aims to help establish hydrologic boundary conditions for a highly hypothetical, highly stylized subsurface criticality event where the criticality is steady in power level.

The existing literature has documented several scenarios under which to consider the possibility of DPC criticality (Price et al, 2019a; Price et al. 2019b; Painter et al., 2019; Furtney et al. 2021). Broadly speaking, they can be categorized using the following parameters

- Dynamic behavior: pulse/cyclical/slow transient
- Hydrologic environment: saturated/unsaturated

This report examines the results of DPC criticality in an unsaturated alluvial repository, with slow transient dynamic behavior. Criticality is not modeled, so this is not a multiphysics simulation in that regard. In such cases, the approach to critical allows feedback mechanisms such as water movement to act before power can increase to levels exceeding kilowatts. The authors have not yet found assurance that this assumption is justified in all cases.

A key assumption in this analysis is the water transfer properties both inside and outside the DPC. In the stylized scenario considered, the upper boundary of the DPC is assumed to be open. This allows water to enter and collect in the DPC. It is assumed that because of the slow entry rate of water, the approach to critical is controlled, and the water is driven away in a slow manner. Presumably, the water will return, and this work examines the initiating conditions in such a cycle. Other sources of reactivity insertion, such as collapsing of absorber panels, are not considered. The various hydrological parameters are fixed, as in last year's report.

The status of cylindrical mesh development for the problem domain late in the fiscal year is noted. Although the mesh was developed, PFLOTRAN convergence was not achieved.

2. MODEL AND ASSUMPTIONS

2.1 Assumptions

Numerous assumptions were made in this work and are identical to those made in the last FY report. This evaluation is being made principally to obtain direction for further work. In this effort, a waste package geometry of a square prism was assumed for expeditiousness. The waste package is modeled with its longest side aligned horizontally. The side of the DPC facing upward was assumed to be completely breached except for cases in which the size of the breach was reduced to 50% to measure its effect. Furthermore, the internals of the DPC are modeled uniformly as a core material without resolving individual fuel assemblies. The waste package's outer shell was assigned a very low permeability to prevent water from flowing through it. The backfill and host medium are assumed to be the same material with the same density. The unsaturated alluvium repository is assumed to be infiltrated by water percolating from above at rates given in volume per area per time (mm/yr).

Fission power is treated as an input. Fission (because of criticality) is considered to begin when the package fills with water, and the power levels considered here should be justified by case-specific calculations. It is far beyond the scope of this work to evaluate the critical power level or the initiating conditions.

The key objective in this work is to determine the high-level behavior and simulation steps needed to model groundwater reacting to a stylized criticality event which initiates when the upper face of the DPC is assumed to disappear and water ingresses with backfill media falling into the canister in many cases. This media was given no credit in terms of preventing criticality.

2.2 Representative Dual-Purpose Canister

The waterflow and saturation calculations are performed using the open-source package PFLOTRAN, a massively parallel subsurface flow and reactive transport code which simulates chemical reactions occurring within the flow (Hammond et al. 2014). PFLOTRAN solves a system of generally nonlinear partial differential equations describing multiphase, multicomponent, and multiscale reactive flow and transport in porous materials.

The portion of the problem domain surrounding the waste package is shown in Figure 1. It is based upon previous years' work (Painter, 2021) This is located at a depth of 250 m. Because the assumed geologic medium is considered uniform from surface to water table, depth is not of great importance. The model domain includes a single waste package (blue + green) positioned in a backfilled emplacement drift (red) in a repository situated in unsaturated alluvium (orange). To simplify calculations, the waste package and drift are both approximated as having square cross sections: 1.77 m × 1.77 m for the DPC, and 4.00 m × 4.00 m for the emplacement drift. These dimensions are similar to the range of dimensions for actual DPCs, as animated in Figure 2. Using boundary conditions, the single package is treated as being in an array of similar packages, for convenience. The centerline-to-centerline drift spacing is 40 m. The waste packages are 5 m long and are spaced at 40 m along the drift by means of reflective boundary conditions. By symmetry, only half of the waste package and 20 m of the drift are modeled, with no-flow boundary conditions assumed on the north, south, east, and west, implying no crossflow. In addition to the waste package internals, a shell/overpack with a thickness of 0.1 m is included in the mesh. The model domain extends from the land surface to the water table in the vertical direction, with the DPC far enough below the surface and far enough above the water table to avoid interaction with either. Top flow conditions were set to Dirichlet saturation condition for stability, and bottom flow was set to a 1 atmosphere hydrostatic pressure, corresponding to the top of the water table.

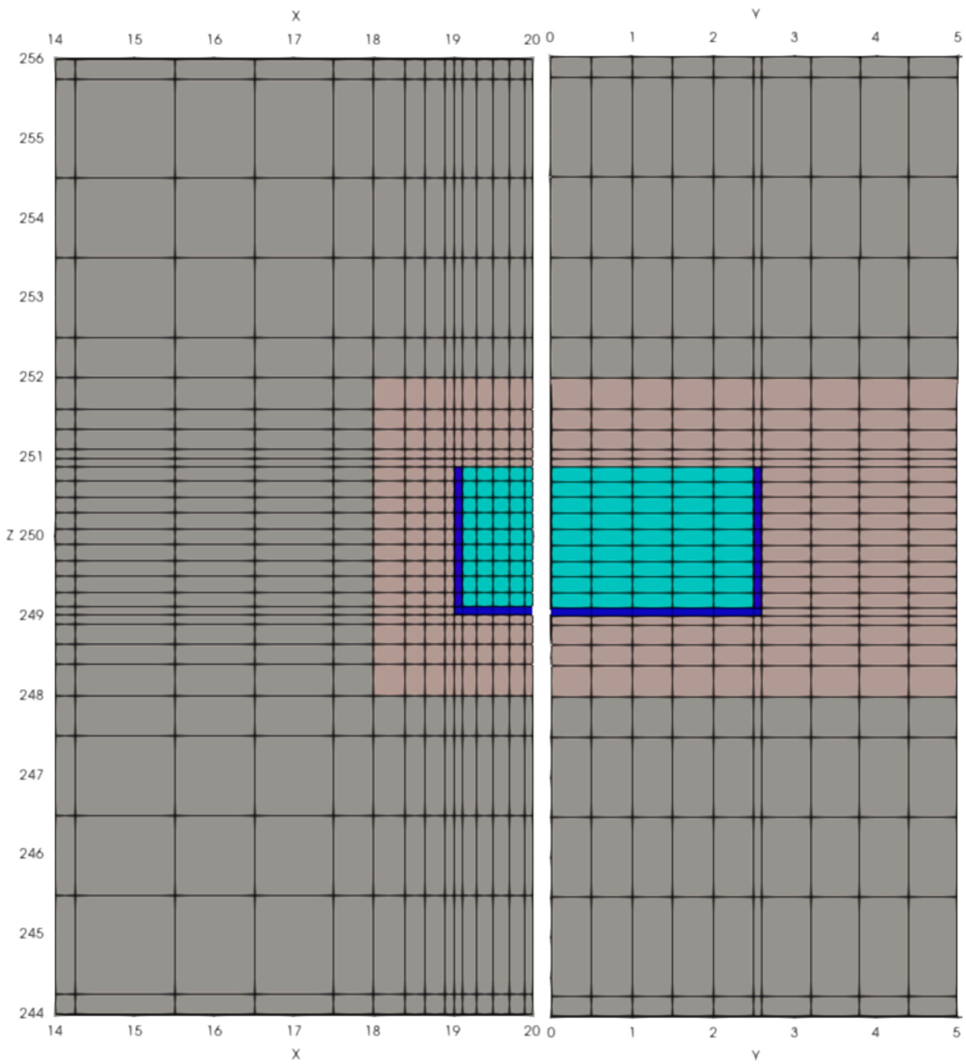

Figure 1. Details from a computational mesh showing backfilled drift (pink), host formation (grey), waste package internals (aqua), and waste package shell (blue). Left image is a vertical cross section perpendicular to the drift, and right image is a vertical cross section along the drift centerline.

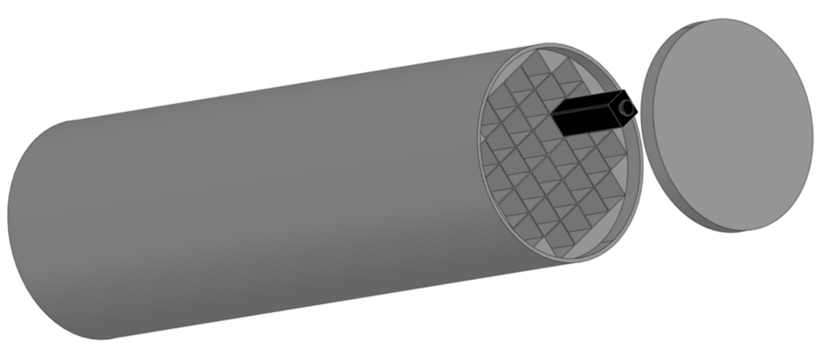

Figure 2. Animation of a DPC without overpack having a single fuel assembly and lid removed. Produced by Abiodun Adeniyi

This initial calculation in PFLOTRAN assumes that after breech and sufficient cooling, the canister will be filled with fresh water, whereas the neutron absorber materials (panels) and coated carbon steel structural components will be quickly degraded and transported away from the system. In this stylized scenario, the stainless-steel structural components maintain functional integrity after the assumed canister breach. The canister is assumed to be loaded with 37 pressurized water reactor (PWR) assemblies with a total decay heat of about 2.9 kW at the time of repository closure. Decay heats were obtained from ORIGEN results for a stylized PWR assembly. The canister decay heat decreases to only 280 W at 9,000 years post-closure—the time of waste package breach as assumed in this work.

An example assumed heat production curve is shown in Figure 3. The "decay heat" case is from SCALE/ORIGEN's decay heat output for 37 PWR assemblies, and the "decay heat + criticality" case accounts for a constant and continual 100 W power criticality following package breech, as an assumption. The time of criticality shown here corresponds to the time the canister first becomes fully saturated with water. Individual fuel assemblies and package internals are not specifically modeled.

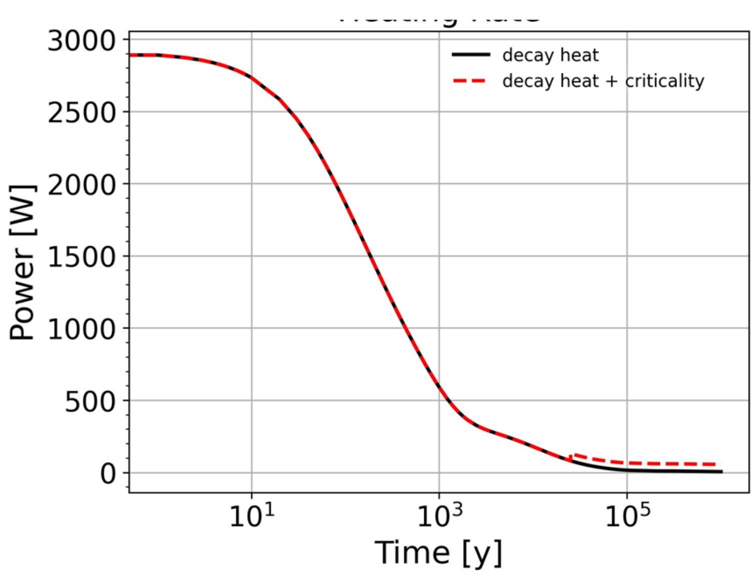

Figure 3. Heat production of emplaced DPC canisters vs. time.

This work used PFLOTRAN's *general mode*, which includes mass and energy conservation equations for water as liquid and vapor, as well as air as gas and dissolved in liquid. The specific phenomenon of interest in this study is the thermally driven flow of fluid away from the interior of a DPC. This type of flow is driven by the temperature, internal energy, and enthalpy terms in the energy conservation equations.

3. SWEEP OF PERCOLATION RATES

The *percolation rate* is defined as the volume of water passing a unit area per unit of time and is a measure of the speed at which water percolates through the medium. Percolation rate is measured in cm or mm per year. In cases considered thus far, percolation rates considered are 2 mm/year and 5 mm/year. Repository siting often prefers the absence of surface water, but no repository location is defined presently. As a case study, some percolation rates for the Mojave Desert (Prudic 1994, Stonestrom et al. 2003) were reviewed. Depending upon rainfall and runoff patterns, values encountered were in the range of mm per year to over ten cm per year, changing with the presence of surface water, location, and other parameters. Absent irrigation or the presence of a river channel, the southwest tends to have very low deep percolation rates (Stonestrom et al. 2003). Because this sampling of literature is small, it does not necessarily bound the range of percolation rates encountered at all possible locations.

Noting that the range of rates may change according to context such as location, rainfall, runoff, and soil permeability, this work focuses on lower rates, corresponding to arid regions with no surface water sources such as rivers or irrigation. This section sweeps the percolation rate from 1 mm/year to 10 mm/year. Section 7 of this report begins to examine the implications of higher percolation rates.

The time-to-saturation of the DPC containing a porous matrix with capillary action for various percolation rates is shown in Figure 4below. The corresponding DPC powers to remove the water are shown in Figure 5. For the range considered, the power necessary to drive off the water is roughly linear with the infiltration rate. As the infiltration rate increases, the time at which the potential criticality event is initiated is closer to the time of breach where the DPC internal temperatures and decay heats are much higher. The DPC internal temperature post-breach decreases upon water ingress if no criticality is assumed to occur.

With a 1 mm/yr. percolation rate, the DPC does not saturate with liquid post breach within the 100,000 years for which decay heats are available for the current analysis (see Figure 6). Therefore, the 1mm/yr. case is not included in Figure 4 or Figure 5.

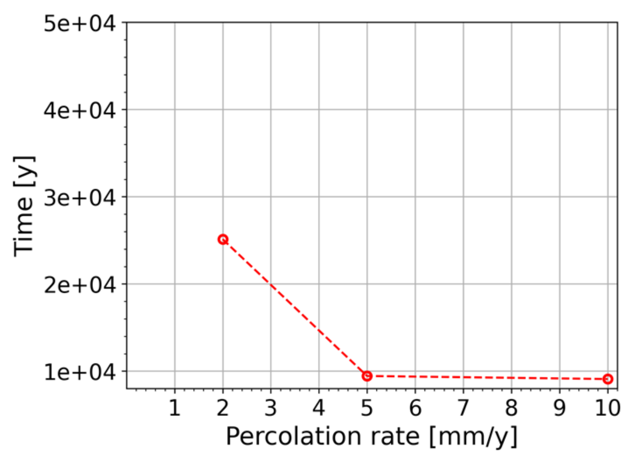

Figure 4. Time to saturate the DPC (breech at 9000 years).

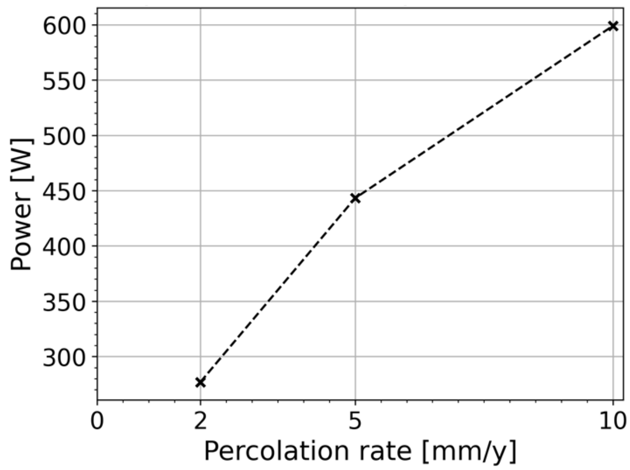

Figure 5. Minimum total heat from criticality and decay to drive away water.

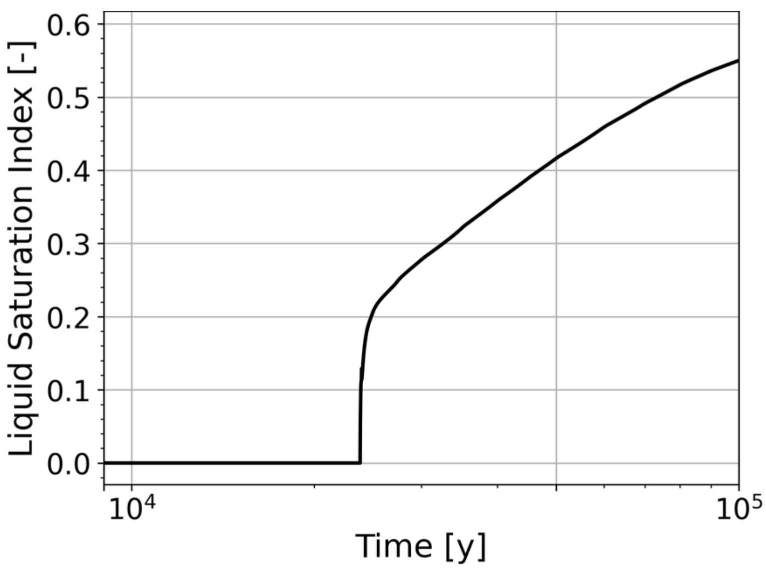

Figure 6. Liquid saturation index plot for 1 mm/yr. percolation rate assuming 100% of the DPC cap is breached (breech at 9000 years).

4. BREECH SIZE

Package breech size was considered a parameter of interest in last year's study. In this year's work, the power required to drive off water under assumed conditions was computed for two percolation rates and two breech sizes, as shown in Table 1. Although the time-to-saturation was dependent upon breech size, the total power to drive away water was independent of large breech size. Lack of sensitivity to the breech size is because water exits the DPC in the vapor phase and the rate-limiting process is the evaporation rate not the resistance to vapor movement. For the conditions considered, time-to-saturation following a breech was decreased by approximately 40% when breech size doubled.

Table 1. Fill time and power to drive away water for various breech sizes

Percolation rate [mm/y]	Fraction breached [%]	Time after breech for DPC to saturate [y]	Bounding power [W]
2	100	16,120	276.86
2	50	28,890	276.00
5	100	440	443.17
5	50	680	443.00

5. MESH DEVELOPMENT

Some work to develop a cylindrical DPC geometry using an unstructured mesh has occurred using Cubit. Figure 7 shows the mesh snapshot with the different regions delineated. However, the postclosure case did not converge beyond 5 years after several attempts using the unstructured mesh with the following solver options: enabling the Newton trust solver, mesh refinements in and around the DPC, and smaller timesteps for the Newton iterations. Therefore, the existing PFLOTRAN rectangular mesh was used with the work to remain within the schedule.

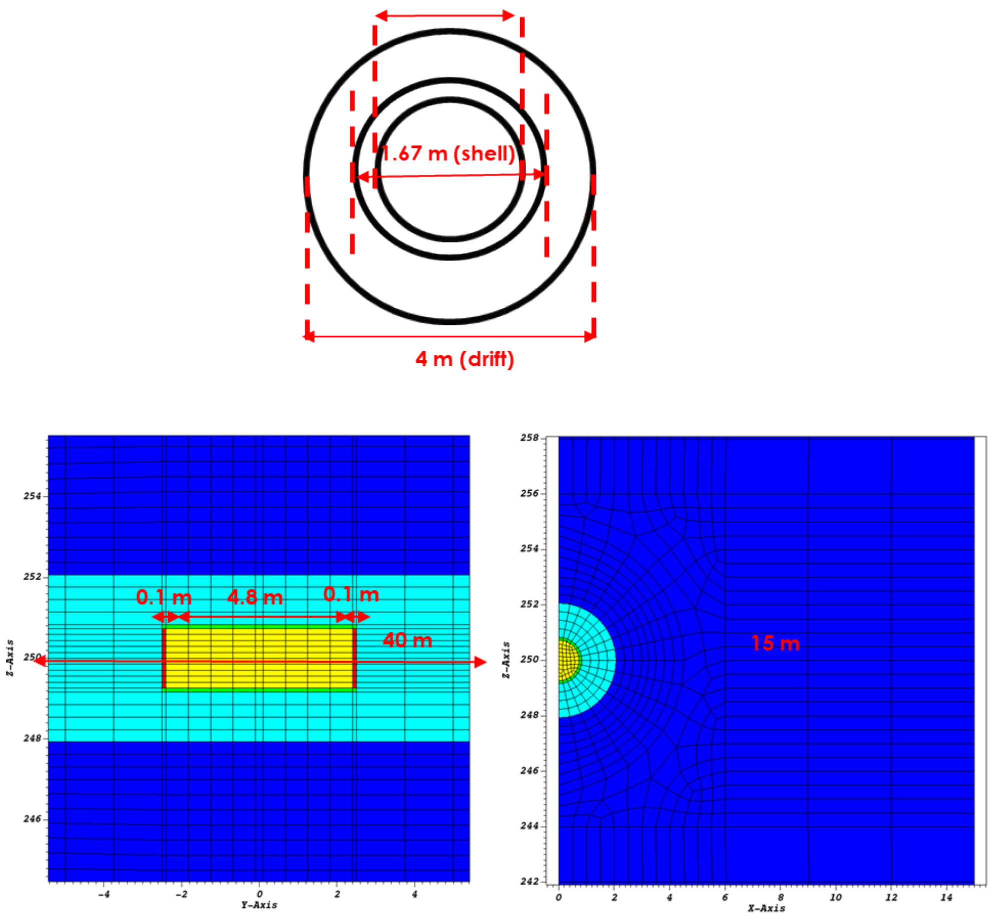

Figure 7. Unstructured mesh snapshot developed in Cubit for the cylindrical DPC geometry. The mesh is clipped in the vertical direction.

6. ZERO DPC CAPILLARY ACTION

The behavior of voids within the DPC is addressed in the FY22 report. In preceding scenarios, it was assumed that media with capillary action had entered the DPC, so capillary action occurred both within and outside the DPC.

In some cases, the DPC may not be full of fine debris, with little capillary suction occurring within the DPC. Thus, an alternative case with no ingress of capillary media is evaluated with PFLOTRAN. Permeability was increased to 2×10^{-9} m^2 from the baseline of 1×10^{-13} m^2. This reflects the highest value of roughly 2,000 Darcys (Alsafi 2017) for a bed of multi-millimeter sized glass beads, which very roughly corresponds to fuel rods. Clearly, fuel rods would have an even higher permeability than glass beads and may be more precisely quantified in the future.

This case was modeled using a DPC with a modified porosity and a maximum capillary suction pressure of 0 Pa within the DPC, but with capillary action maintained outside the DPC. In that case, with a 2 mm/year infiltration rate, a capillary barrier formed at the top of the DPC and no water pooled within the DPC, as shown in Figure 8.

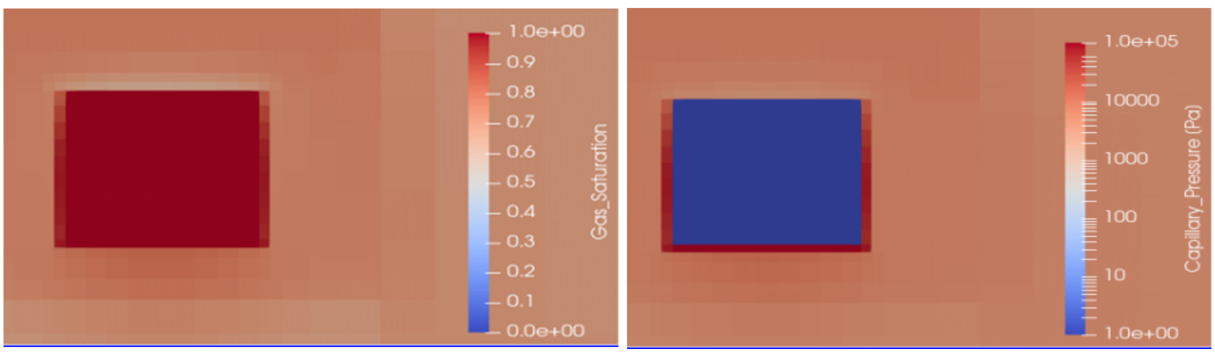

Figure 8. (Left): gas saturation at end of simulation (91,000 years post breach) with 2 mm/yr. infiltration rate, and zero capillary pressure within the DPC; (Right) capillary pressure distribution (note: 0 evaluates to 1.0 in the log-scale colormap)

7. ZERO DPC CAPILLARY ACTION AND INCREASED INFILTRATION RATE

Although not reflective of any repository design, increasing the infiltration rate to a high value of 115 mm/year resulted in almost immediate flooding upon the stylized package failure. This value corresponds to Table 4 of the 2003 report by Stonestrom et al. The mesh cell used to monitor package water content became saturated at 7 years post breech. Adding 1,300 W of fission power to the model roughly 7 years following the initial influx of water stopped further ingress (Figure 9, left), but it did not remove the water in any appreciable quantity over the course of 100 years. However, it did raise the package temperature to above boiling in a dry region (Figure 9, right). Although this is an interesting simulation, it is difficult to draw any robust conclusion from this single simulation.

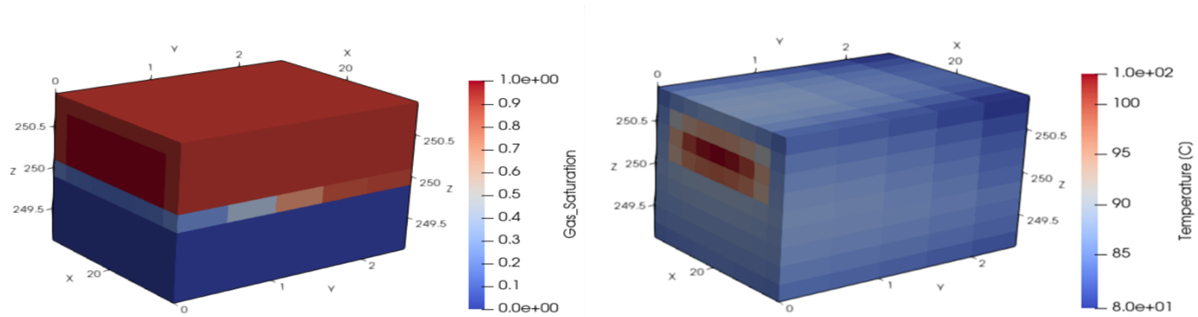

Figure 9. (Left): gas saturation post breach with 120 mm/yr. infiltration rate: half slice viewed from center of square-prismatic DPC and water level held roughly constant with 1,300 W of power; (Right) temperature distribution of same scenario showing higher temperatures in the upper DPC region with non-DPC regions shown only in wire-frame.

8. CONCLUSION

In FY23, ORNL performed a basic analysis to examine the minimum heat required to offset water incursion for various infiltration rates. For a DPC containing capillary media, the simulated power required for dryout was proportional to the percolation rate, but it was unaffected by the size of a large breech on top of the DPC although the breech size did affect the time required for water to pool and initiate criticality. Results using single cases with no capillary media in the DPC suggest that higher infiltration rates are required to flood a DPC. In the future, perturbations to various input parameters should be performed to show robustness of results.

Future activities are as follows:

- Further examinations of numerical behavior could be performed, especially for limiting conditions.
- Dynamic responses to power pulses can be analyzed to determine a transfer function to enable a reduced order feedback model.
- Bounding mechanisms and assumptions should be further identified. For instance, ingress of material surrounding the DPC that supports capillary action has an unclear effect. It appears to encourage water ingress, but at the same time limits the volume fraction of water and may provide some neutron absorption. Furthermore, thermal conductivity establishes the temperature gradient, which drives fluid flow. This range and influence of thermal conductivity remains to be reviewed and sampled.
- Additional dry-out curves can be developed to show steady-state saturation indexes corresponding to various power levels at various infiltration rates for differing capillary curves. These curves might be used to analyze the consequences of slow-burn type events.
- Eventual partial coupling to criticality modeling of specific DPC configurations could be implemented.

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