GDSA – Modeling and Integration – ORNL: PFLOTRAN Modeling 2022 Progress Report

Spent Fuel and Waste Disposition

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APPENDIX E

NFCSC DOCUMENT COVER SHEET[1]

Name/Title of Deliverable/Milestone/Revision No. ____N/A______________________________

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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]

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SUMMARY

This report summarizes work done at Oak Ridge National Laboratory (ORNL) related to post-closure criticality consequence analysis of dual-purpose canister (DPC) direct disposal in unsaturated alluvium. PFLOTRAN software was used to model the behavior of a breached DPC with low water infiltration rates and unsaturated conditions in alluvial deposits such that a low-power criticality event occurs with a focus on thermal hydrological constraints on criticality timing and power output. This summary describes initial exploration of those thermal hydrological processes and of the long-term average power output from a criticality event that could be sustained without driving water out of the DPC package and thereby terminating the criticality event. The objectives are (1) to identify, for different groundwater infiltration rates, the time at which the DPC fills with water sufficiently to potentially initiate criticality; (2) to bound the power output that could be produced by a criticality event that would thermally drive water out of the package at various percolation rates; and (3) provide an estimate of how the size of a package breach affects the water infiltration and therefore the possibility timing of criticality.

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ACKNOWLEDGMENTS

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REVISION HISTORY

Revision	Changes Made
0	Initial issue

ACRONYMS

DPC	dual-purpose canister
ORNL	Oak Ridge National Laboratory
PWR	pressurized water reactor
SNF	spent nuclear fuel

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GDSA MODELING AND INTEGRATION: ORNL

1. INTRODUCTION

Thousands of dual-purpose canisters (DPCs) designed for storage and transportation are presently loaded with spent fuel at independent spent fuel storage installations at reactor sites. These DPCs were not specifically designed for direct geologic disposal, and it is possible that some already loaded DPCs could achieve criticality over the repository performance assessment time frame if water (i.e., moderator) were to infiltrate the canister and poison plates are degraded[1]. There could be cost and safety benefits of direct disposal of spent nuclear fuel (SNF) in existing DPCs as opposed to cutting open loaded DPCs and repackaging the SNF for disposal; however, to implement direct disposal of DPCs, the prominent challenge of mitigating the potential for post-closure criticality must be evaluated.

For a waste package criticality to occur, a neutron moderator (e.g., water) would have to enter a breached waste package and neutron poisons must become degraded. The criticality could continue if sufficient water is retained, and no other reconfiguration occurs. Low water infiltration rates and unsaturated conditions in alluvial deposits could diminish the probability that enough water would be available to fill a breached canister such that a criticality event occurs, but these particulars may not necessarily eliminate the possibility [2–4]. This summary describes initial exploration of those thermal hydrological processes and of the long-term average power output from a criticality event that could be sustained without driving water out of the package and thereby terminating the criticality event. This work builds on the conceptual model developed in a recent study [5]. The objectives are (1) to identify, for different groundwater infiltration rates, the time at which the DPC fills with water sufficiently to potentially initiate criticality; (2) to bound the power output that could be produced by a criticality event that would thermally drive water out of the package at various percolation rates; and (3) provide an estimate of how the size of a package breach affects the water infiltration and therefore the possibility timing of criticality.

2. MODEL SETUP

2.1 Assumptions and Conditions

Numerous assumptions were made in this work. This evaluation is being made principally to obtain direction for further work. For this work, a square waste package geometry 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 in two cases where 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. Backfill and host medium were 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/year).

Criticality power is treated as an input. 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. We are simply concerned with the high-level behavior and simulation steps needed to model ground water reacting to a stylized criticality event which initiates when the upper face of the DPC is assumed to disappear, and water ingresses.

2.2 Representative Dual-Purpose Canister

The water flow 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 [6]. PFLOTRAN solves a system of generally nonlinear partial differential equations describing multiphase, multicomponent and multiscale reactive flow and transport in porous materials. In the recent past, convergence issues were encountered when modeling the complex environment and long timescales of a DPC emplaced in a geologic repository, but PFLOTRAN capabilities have matured, and convergence issues have been sorted out.

The portion of the problem domain surrounding the waste package is shown in Figure 1. This is located at a depth of 250 m. 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 a square cross section, which is 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 actual DPCs. Using boundary conditions, the single package is treated as being in an array of similar packages. 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. 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.

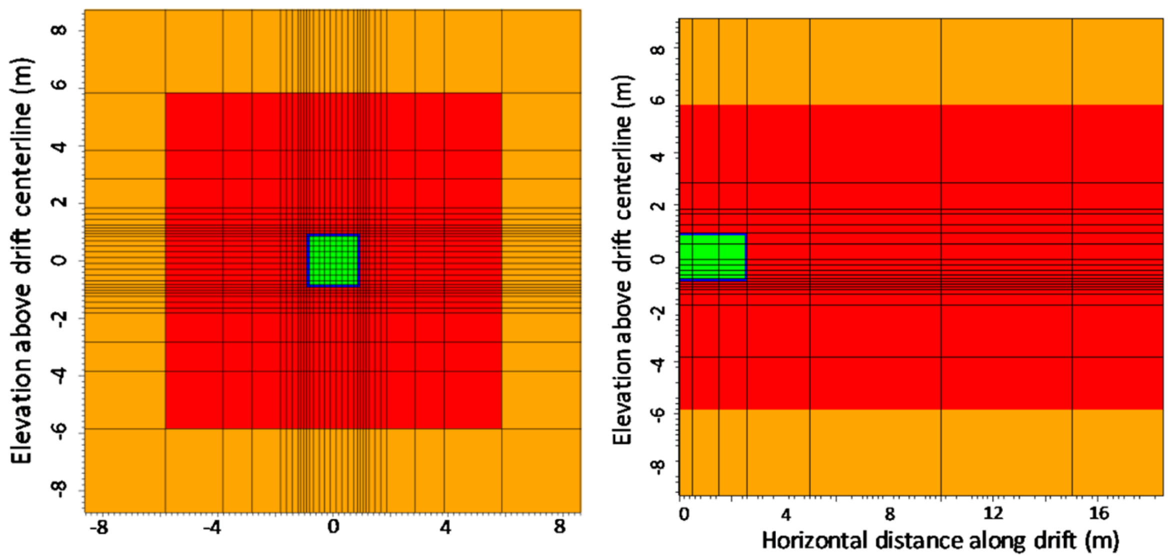

Figure 1. Details from the computational mesh showing backfilled drift (red), host formation (orange), waste package internals (green), and waste package shell (blue). Top image is a vertical cross section perpendicular to the drift, bottom image is a vertical cross section along the drift centerline.

This initial calculation in PFLOTRAN very conservatively assumes that the canister will be flooded with fresh water, whereas the neutron absorber materials (panels) and coated carbon steel structural components will be completely degraded and transported away from the system. In this scenario, it is also considered that the stainless-steel structural components will 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—a time of waste package breach assumed in this work. The assumed heat production curve is shown in Figure 2. The 0 W case is from SCALE/ORIGEN's decay heat output for 37 PWR assemblies, and the 100 W criticality is treated as being constant and continuing, as an assumption because the fission chain reaction is not modeled here in the absence of neutronics coupling. 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.

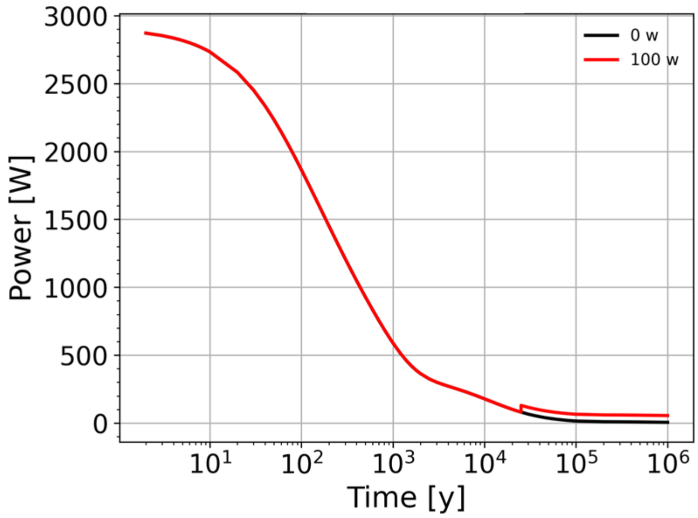

Figure 2. Heat production of emplaced DPC canisters vs. time.

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.

The alluvium host medium for the repository is assumed to have a dry thermal conductivity of 1.0 $W/m^2 \cdot K$ and a wet thermal conductivity of 2.0 $W/m^2 \cdot K$ as in previous work [2]. Backfill material is assumed to have a dry thermal conductivity of 1.0 $W/m^2 \cdot K$ and a wet thermal conductivity of 2.0 $W/m^2 \cdot K$. The authors acknowledge and recognize that these are the same values.

The internals of the waste package use the fuel assembly models listed in the PFLOTRAN documentation. Some discussion of thermal model is included to help define the meanings of the input parameters and the mechanisms modeled. These can be found in the PFLOTRAN documentation.

Thermally driven flow is driven by thermodynamic state points, heat conduction, and heat capacity of the host matrix. In the general (multiphase) mode, mass balance equations are solved for the gas and liquid phases, as well as the energy equation (shown below). Subscript l indicates liquid, subscript g indicates gas, t stands for time, stands for T temperature, Q stands for other heat generation, κ stands for thermal conductivity, ρ stands for density, $C_p$stands for heat capacity, U is internal energy, and H is enthalpy, and $\boldsymbol{q}$ stands for Darcy flux/velocity (fluid flow). Saturation (s_l) is the fraction of pore volume occupied by water. Porosity (Φ) is the fraction of the volume which is occupied by gas or liquid.

$$\sum_{\alpha=l,g} \{\frac{\partial}{\partial t}(\Phi s_\alpha \rho_\alpha U_\alpha) + \nabla \cdot (\boldsymbol{q}_\alpha \rho_\alpha H_\alpha)\} + \frac{\partial}{\partial t}((1-\Phi)\rho_{rock} C_{p,rock} T) - \nabla \cdot (\kappa \nabla T) = Q,$$

They assume a radial thermal conductivity, κ_{rad}, which is a temperature-dependent composite depending on the fluid inside of the canister (helium, air, water) surrounding the fuel assemblies stored in the waste package. Conductivity is split into a wet component (κ'_{wet}) and a dry component (κ_{dry}). The wet component depends upon saturation, temperature and porosity. Parameters used are listed in the first column of Table 1. As a starting point, the parameters were taken from Price et al. [7]. The functional form of the assembly-specific radial thermal conductivity model as currently implemented in PFLOTRAN is as follows [8]:

$$\kappa_{rad}(s_l,T,\Phi) = \kappa_{dry}(T) + \left[\kappa'_{wet} - \kappa_{dry}(T)\right]\sqrt{s_l}\,,$$

The dry portion of the thermal conductivity (κ_{dry}) is defined as a constant value plus an exponential fit with regard to temperature with α and β as fit parameters:

$$\kappa_{dry}(T) = \kappa_{dry,0} + \alpha T^{\beta}.$$

The wet thermal conductivity accounts for porosity, Φ, of the medium as well as the conductivities of liquids and solids; it is given by

$$\kappa'_{wet} = \kappa_{liq}\left[1 - \sqrt{1-\Phi} + \frac{\sqrt{1-\Phi}}{1 + \left(\frac{\kappa_{liq}}{\kappa_s} - 1\right)\sqrt{1-\Phi}}\right].$$

For conductivity in the axial direction of the assembly, conductivity of gas is considered negligible due to the longer path length. It is a function of saturation and independent of temperature [8], and it is given by

$$\kappa_{ax}(s_l) = (1-\Phi)\,\kappa_s + \Phi\kappa_{\text{liq}} s_l.$$

The parameters used to calculate the thermal conductivities in the model are given in Table 1.

Table 1. Parameters used in the calculation of the radial and axial thermal conductivities [5].

Parameter	Radial	Axial
Dry $\left(\kappa_{dry,0}\left[\frac{\text{W}}{\text{m}^2\text{K}}\right]\right)$	0.143	
Wet $\left(\kappa_{liq}\left[\frac{\text{W}}{\text{m}^2\text{K}}\right]\right)$	1.72	1.72
Stainless $\left(\kappa_s\left[\frac{\text{W}}{\text{m}^2\text{K}}\right]\right)$	16.7	16.7
ASM Dry coeff $\left(\alpha\left[\frac{\text{W}}{\text{m}^2\text{K}\beta}\right]\right)$	3.83e-5	
ASM Dry exp (β [unitless])	1.67	
Porosity (Φ [unitless])	0.5	0.5

The Van Genuchten function for soil water retention was used in the model with the 'ECPC' unsaturated extension for smoothing a discontinuity at low saturation[8]. The implementation of the smoothing feature was necessary for reliable convergence. The functional forms are shown here, and the parameters used are included in the functional form. A maximum capillary pressure constraint of 0.1 GPa was applied throughout, which can be thought of as the capillary pressure of the smallest pore size, and it is on the order of yield strength of several materials. The saturation function (S_e) used is given as

$$S_e = \frac{1 - 0.1}{[1 + (0.001|\Phi|^2)]^{0.5}} + 0.1.$$

A minimum saturation (S_l) was also applied, which is given by

$$S_l = (1 - 0.1)S_e + 0.1$$

Maulem's model is used for permeability of liquid ($K_{r,l}$) and gas ($K_{r,g}$), which is expressed as

$$K_{r,l} = \sqrt{S_e}\left[1 - \left(1 - S_e^2\right)^{0.5}\right]^2$$

$$K_{r,g} = \sqrt{1 - S_e}\left[1 - S_e^2\right]^1$$

The waste package's outer shell was assigned a very low permeability to prevent water from flowing through it.

The simulations were initially initialized without a repository drift to obtain steady state groundwater flow profile. The gas saturation index at the surface was varied to give different percolation rates as a forcing function to examine changes in drying behavior. Repository closure is assumed at t=0, using results from the steady state as initial conditions, but with waste package internals, shell, and drift backfill in place. At 9,000 years, the top of the waste package shell is assumed to be breached, which is modeled by replacing the mesh cells associated with the waste package shell with those associated with drift backfill. The low permeability cells of the waste package shell sides and bottom remain intact, allowing the waste package to fill with water with no way to drain out.

A variety of critical powers and percolation rates were considered as follows:

Percolation rate (mm/year)	Extra power from criticality (W)	Fraction of upper side breached (%)
2	100	100
2	138	100
2	139	100
2	100	50
5	0	100
5	108	100
5	0	50

3. RESULTS

The observation point for all the line plots discussed hereinafter is at the center of the DPC. The variation of the temperature at the center of the DPC for the reference case of 2 mm/year percolation rate is shown before DPC package breach in Figure 3, similar to that in Painter [5]. The temperature peaks at ~319°C but decays to ~ 75°C around the time of the waste package breach which, as mentioned previously, is assumed to occur at 9,000 years.

The liquid saturation index cross sectional contour plots at different times post the DPC waste package breach are shown for 2 mm/year in Figure 4, similar to Painter [5]. With this reference percolation rate, water begins to fill the DPC only around 16,200 years and initiates a criticality event at ~25,000 years. A 100 W criticality event was assumed, which is in addition to the decay heat is sufficient to drive off most of the water, as discussed in the following figures.

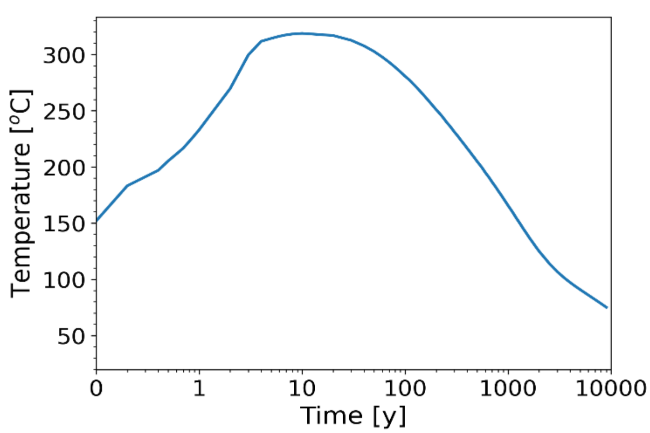

Figure 3. DPC internal temperature vs. time prior to waste package breach, similar to Painter [5].

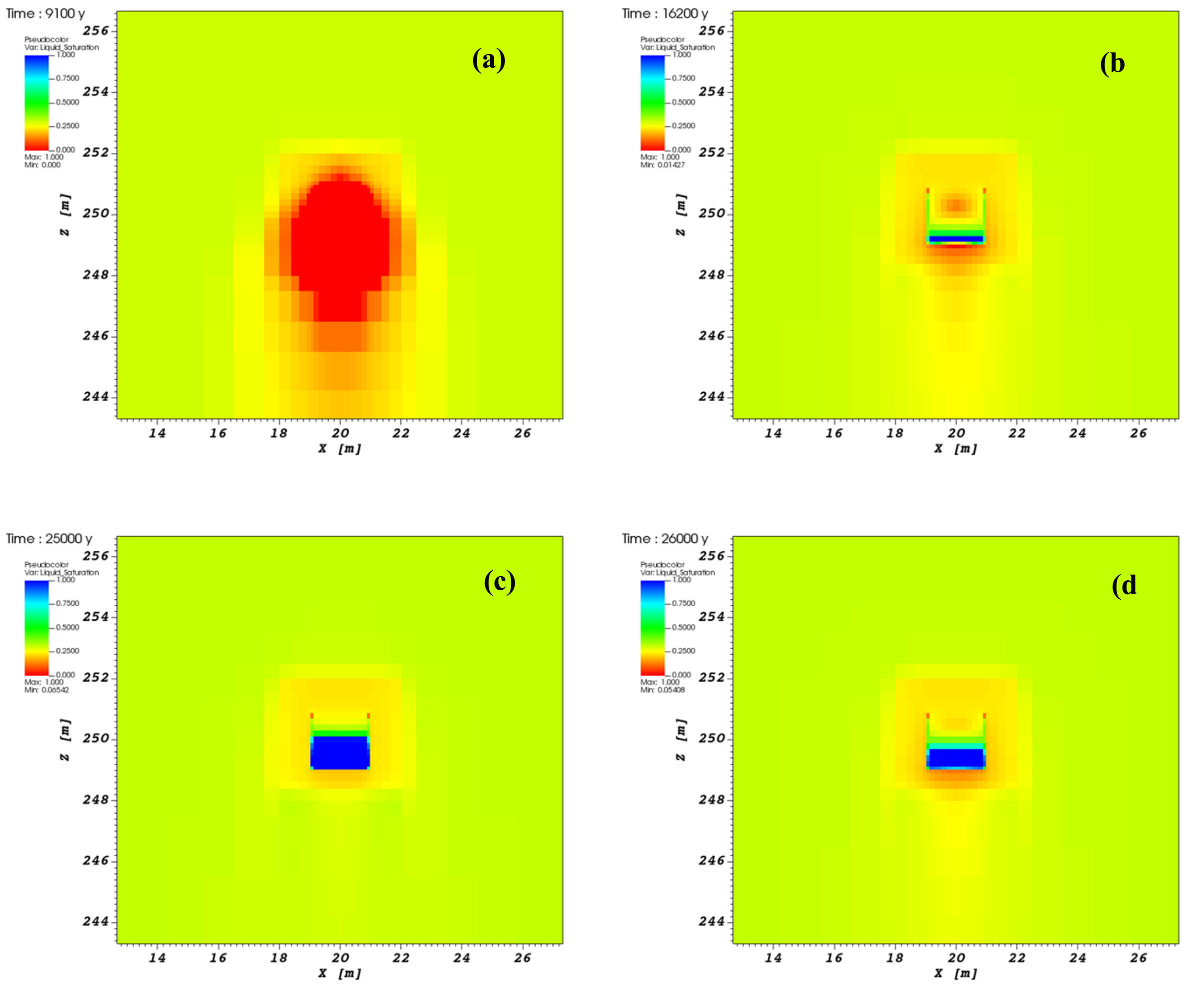

Figure 4. X-Z cross-sectional contour plots of the liquid saturation index for the following conditions for a percolation rate of 2 mm/year (a) just after DPC failure, (b) the DPC starts to be filled with water, (c) the DPC is filled with water to 1 m triggering criticality, and (d) 1,000 years. after the start of a 100 W criticality event, similar to [5].

Assuming only a certain percentage of the cap region of the DPC is breached (say 50%) would delay the criticality event as shown in Figure 5(a). With a higher percolation rate of 5 mm/year. (2.5 × 2 mm/year.), the package is filled to ~1 mm just 500 years post breach, which is more than 32 times faster (~16,000 years) than the 2 mm/year. percolation rate post breach.

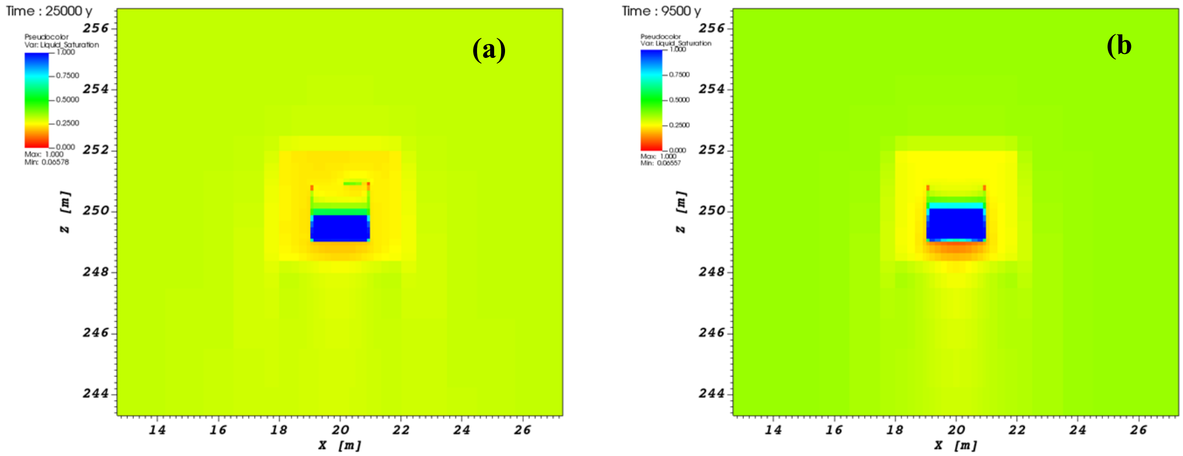

Figure 5. X-Z cross-sectional contour plots of the liquid saturation index for the following conditions (a) 2 mm/year percolation rate with 50% breached at 25,000 years with a slower fill rate, (b) 5 mm/year percolation rate with a criticality event triggered at just 9,500 years.

The figures below show an example of dry-out following a breach at 9,000 years with a 2 mm/year percolation rate. At the time of breach, no filling occurs due to the thermal gradient, but as the decay heat declines, water infiltrates, and a constant power, un-terminating criticality is assumed to occur with 100% saturation at a constant power. The goal here is to probe only the dry-out behavior, and this unrealistic assumption is a means to that end. It can be seen on Figure 6(a) that a 138 W power increase almost causes dry-out, but a 139 W increase causes dry-out briefly (Figure 6(b)). Some numerical noise is notable at the low liquid saturation points, and this requires further examination. Further study could aim to produce dry-out curves showing steady-state saturation indexes corresponding to various power levels at various infiltration rates. They could be used to understand consequences of slow-burn type events. To see some effect of the size of the DPC breach upon wetting behavior, the opening on the top of the DPC as part of the problem definition was assumed to be half of its regular size. Again, no drainage path is assumed. The reduced breach area reduced the wetting behavior. In this case, no criticality is assumed, and only the decay heat is driving moisture away. Initial ingress occurs at a similar rate, but full saturation is substantially delayed, as shown in Figure 7 at the center of the DPC.

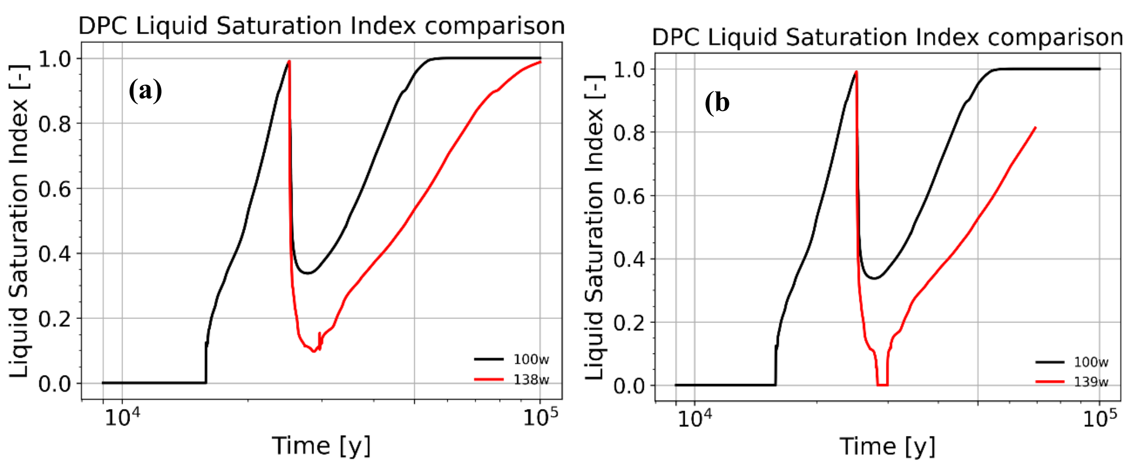

Figure 6. Liquid saturation index plots showing dry out behavior post breach for 2 mm/year percolation rate assuming a criticality event (a) producing 138 W, just before complete dryout and (b) producing 139 W, which is the bounding power.

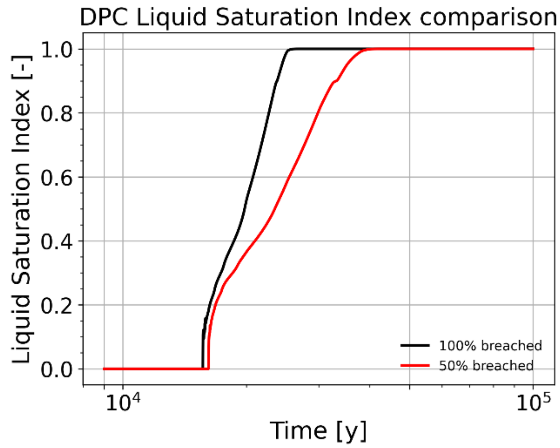

Figure 7. Liquid saturation index plot for 2 mm/year percolation rate assuming 100% of the DPC cap is breached vs. 50% of the DPC cap is breached.

The final set of liquid saturation index lines plots the center of the DPC, showing the maximum bounding sustained criticality event power (Figure 8(a)) and variation in breach rates (Figure 8(b)) for 5 mm/year percolation rate. The 5 mm/year. percoaltion has a lower bounding power than the 2 mm/year percolation rate because the decay heat rate is higher at 9,500 years in comparison to 25,000 years. The 5 mm/year percoaltion rate is also less sensitive to the breach size in comparison to 2 mm/year. percolation rate. This suggests that for a constant heating rate, there exists a kind of threshold percolation rate.

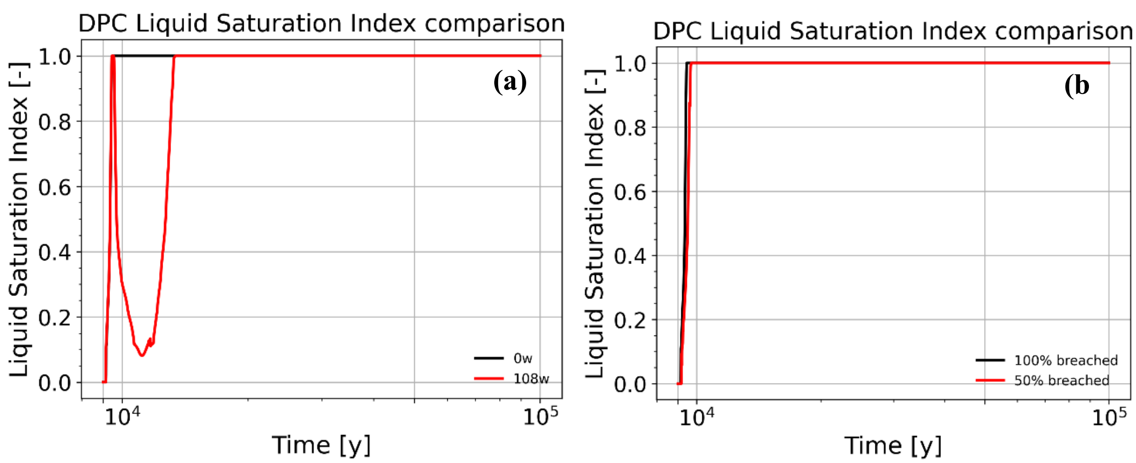

Figure 8. Liquid saturation index plots for 5 mm/year percolation rate for (a) 108 W criticality event (close to the bounding power), and (b) comparison between 100% and 50% breach.

4. CONCLUSION

This year's work demonstrates that the improvements in the production version of PFLOTRAN enable the simulation of thermally induced water flow following a DPC breach. Though no pressing needs for code improvement were identified, numerous further avenues of study exist for thermally driven DPC dry-out following a breach. Overall, it was shown that the size of the breach may affect dry-out/wetting behavior when heat production is sufficient to drive water from the DPC. There also may exist some threshold percolation rate for a given DPC heating rate after which water ingress becomes rapid. This is of course further complicated if potential for criticality exists. Future items to examine are as follows:

- Fill behavior of voids in the DPC.

- A fuller matrix of fill materials.
- Draining of the DPC.
- Further examinations of numerical behavior, especially for limiting conditions.
- The range of power profiles.
- The role of feedback mechanisms.
- The effect of boiling.
- Identification of bounding mechanisms and assumptions.
- Further study could aim to produce dry-out curves showing steady-state saturation indexes corresponding to various power levels at various infiltration rates. They could be used to understand consequences of slow-burn type events.
- Eventually, partial coupling to criticality modeling of specific DPC configurations.

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