ORNL Input to GDSA Repository Systems Analysis FY21

Spent Fuel and Waste Disposition

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To the extent discussions or recommendations in this paper conflict with the provisions of the Standard Contract, the Standard Contract governs the obligations of the parties, and this paper in no manner supersedes, overrides, or amends the Standard Contract.

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REVISION HISTORY

Revision Number	Date Issued	Reason for Revision
0	February 26, 2021	Initial issue

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SUMMARY

This document satisfies the M3 milestone M3SF-21OR010304082 titled "ORNL Input to GDSA Repository Systems." This document describes the current status of Oak Ridge National Laboratory's (ORNL's) efforts related to analyses of dual-purpose canister (DPC) disposal in unsaturated alluvium with a focus on thermal hydrological constraints on criticality timing and power output.

This analysis updates previous analyses of thermal hydrological constraints on timing and power output of a potential criticality event in Dual-Purpose Canisters (DPCs) in a hypothetical repository in unsaturated alluvium using a more realistic representation of heat transport inside dry DPCs. PFLOTRAN was used for the simulations of multiphase thermal hydrology near a single DPC. The scenario considers a DPC failure at 9000 years, allowing water to enter and eventually fill the DPC. Once the DPC is filled to a level that could support a criticality event, different values for criticality power output were added to the decay heat. The main objective is to bound the power output that could be produced by a criticality event without driving water out of the package.

For the conditions analyzed here, following a package breach, the alluvial formation could supply enough water to allow enough accumulation in the DPC to support a criticality event. However, the power output that would be generated is limited to modest values by loss of water moderator due to evaporation and vapor diffusion. In the reference case scenario, the DPC would not start to fill with water until about 16,000 years post closure and would not fill to a level that allows a criticality event until approximately 25,000 years post closure. The long-term average power output that could be sustained without driving off the water and terminating the criticality event is limited to approximately 100 W. Sensitivity to assumed conditions and parameters in the reference case, especially the deep percolation rate, need to be addressed but could not be undertaken because of numerical failures of the PFLOTRAN code running in general mode in the dry conditions of an unsaturated alluvium repository.

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CONTENTS

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LIST OF FIGURES

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ACRONYMS

CADES	Compute and Data Environment for Science
CFR	Code of Federal Regulations
DOE	US Department of Energy
DPC	dual-purpose canister
ORNL	Oak Ridge National Laboratory
PWR	pressurized water reactor
SNF	spent nuclear fuel

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STATUS REPORT SUMMARIZING PFLOTRAN SIMULATIONS OF THERMAL HYDROLOGY OF DUAL-PURPOSE CANISTERS IN UNSATURATED ALLUVIUM

1. INTRODUCTION

The prospect of disposing of spent nuclear fuel (SNF) in existing dual-purpose canisters (DPCs) without cutting the canisters open and repackaging the SNF has potential to reduce costs, the complexity of fuel management, and cumulative worker doses. Although these benefits could be realized, there are several technical challenges to direct disposal of DPCs. Two prominent challenges of the direct disposal of DPCs are thermal management and post-closure criticality control.

Researchers have begun analyzing generic disposal concepts in unsaturated alluvium formations [1,2] in part because alluvium may have thermal and hydrogeologic characteristics that are advantageous for managing the challenges associated with geologic disposal of large DPCs. For example, low water content in unsaturated alluvial deposits could diminish the probability that enough water would be available to fill a breached canister and cause a criticality event.

Previous analyses [3] of DPCs containing 37 pressurized water reactor (PWR) assemblies showed that for dry conditions like those typically associated with unsaturated alluvial deposits in the US Basin and Range Province [4], decay heat alone is sufficient to prevent water from accumulating to sufficient depths to initiate a criticality event for many thousands of years after repository closure. Moreover, even small levels of power produced by a criticality event are sufficient to drive water out of a breached waste package and thus terminate the criticality event. That is, the long-term average power output possible in a criticality event is likely limited by thermal hydrology. However, those previous analyses used the subsurface flow and transport code PFLOTRAN [5], which at the time was not capable of adequately representing heat transport inside dry or partially water-filled DPCs. This summary describes an initial exploration of thermal hydrological constraints on criticality using more realistic models for heat transport recently implemented in PFLOTRAN. As in the previous analyses, the focus is on estimating the power output that can be sustained in a criticality event without driving water out of the package and terminating the criticality event.

1.1 SCOPE

The work package SF-21OR01030408, entitled "GDSA–Modeling and Integration–ORNL," describes the scope of work covered by this status report.

The work package states:

> *In collaboration with the Direct Disposal of DPCs team and GDSA modeling teams continue to develop an unsaturated zone (UZ) and Saturated Zone (SZ) repository cases, in order to advance GDSA Framework and PFLOTRAN. Address the technical basis for a UZ repository concept, potential host rocks, environmental considerations. Support development a reference case repository layout and engineered barrier system (EBS) design for the UZ reference case simulation. Identify potentially important features, events, and processes (FEPs) and scenarios.*
>
> *Develop and simulate repository concepts for large (37 PWR/89 BWR) and thermally hot waste packages in (1) unsaturated alluvium or (2) shale. Conceptual repository designs will be developed for DPCs in these host rocks. Specific topics to pursue include:*
>
> *For an alluvium repository concept*
>
> - *Sensitivity analyses on waste package breach area available for inflow (areas smaller than the waste package footprint)*

- *Sensitivity analyses on infiltration rates–lower the recharge flux to 1 mm/yr or even 0.5 mm/yr. This could in part be based on assumptions regarding the creosote plant community and data on penetration of infiltration–the soil chloride profiles from Yucca Flat.*

- *Modeling options for including the potential for flux impinging on the package to be diverted by the overpack, and concentrated at localized corrosion*

- *Prepare a journal article for DOE review documenting findings on modeling large waste packages in alluvium.*

This document provides a summary of the work performed toward meeting these objectives.

2. CONCEPTUAL AND COMPUTATIONAL MODEL

2.1 CONCEPTUAL MODEL

The conceptual model for a geologic repository has been described previously [1,2] and is only summarized here. A sketch of the repository concept is shown in Figure 1.

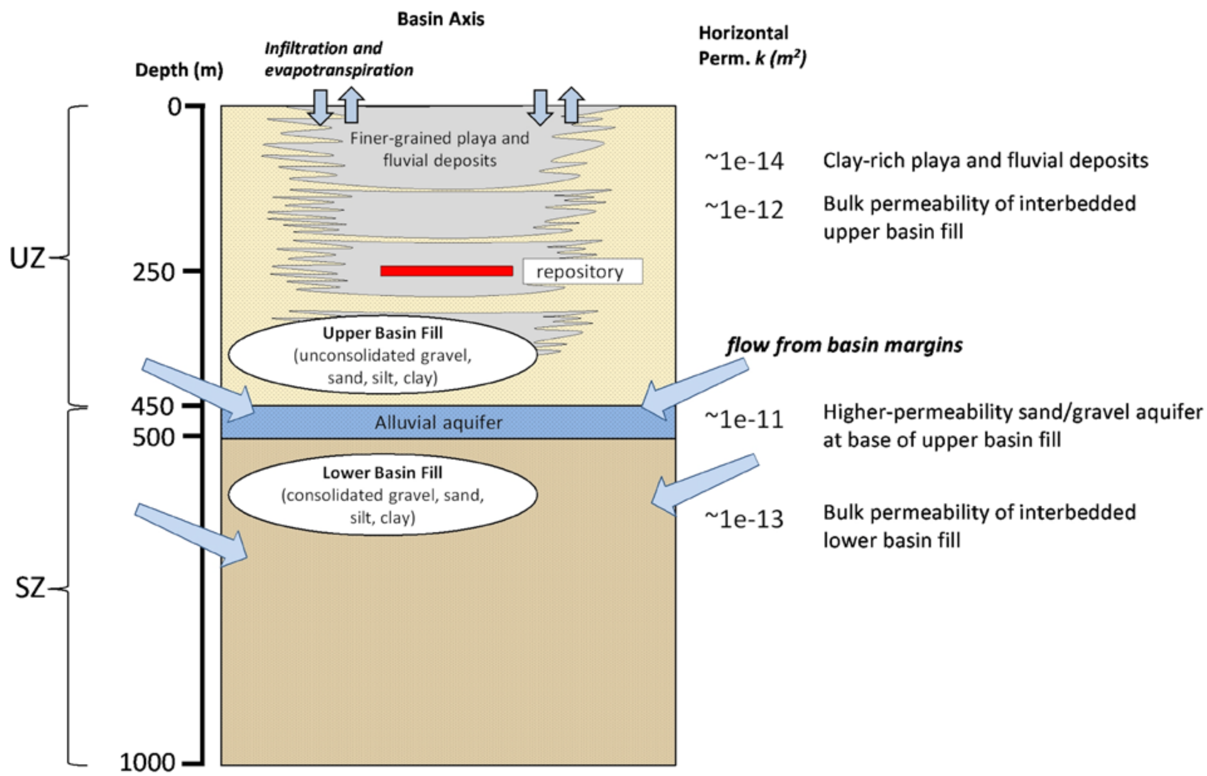

Figure 1. Schematic cross section of the unsaturated zone model [1,2] considered in these analyses. UZ = unsaturated zone; SZ = saturated zone

As shown in Figure 1, the alluvial fill of a generic unsaturated zone natural barrier system may be subdivided into two hydrogeologic units: an upper basin-fill aquifer unit representing the upper two-thirds of alluvial fill; and a lower basin fill aquifer unit representing the lower one-third of alluvial fill. Since the focus of the current analyses is related to the behavior of the near-field repository system (the area near the waste package and surrounding geologic formation), the lower basin fill unit is not represented in the numerical representation.

2.2 Representation of DPCs in Alluvial UZ Using PFLOTRAN

The parallel subsurface multiphase thermal hydrology simulator PFLOTRAN [5] was used for these analyses. PFLOTRAN solves the highly nonlinear conservation equations for mass and energy in variably saturated porous media. This work used PFLOTRAN's so-called general mode, which includes conservation equations for energy, water as liquid and vapor, and air as gas and dissolved in liquid.

The model domain includes a single waste package positioned in a backfilled emplacement drift (tunnel) in a repository situated in unsaturated alluvium at a depth of 250 m. The waste package and drift are both approximated as having a square cross section, which is 1.67×1.67 m for the waste package and 4×4 m for the emplacement drift. The centerline-to-centerline drift spacing is 40 m. The waste packages are 5 m long with centers spaced at 40 m along the drift. The drift and waste package volumes are consistent with the GDSA UZ reference case design (Table 4.1 in Sevougian et al. 2019 [7]; see also Hardin and Kalinina [8]). 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 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 2 shows a detail from the computational mesh in the vicinity of the waste package and drift.

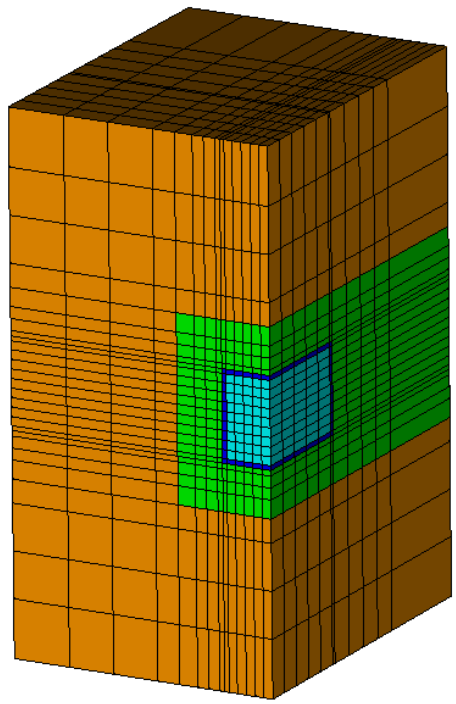

Figure 2. Cut through the computational domain showing a 6×6×12 m detail of the mesh with backfilled drift (green), host formation (brown), waste package internals (light blue), and waste package shell (dark blue). This 3-D perspective is cut through the drift centerline and waste package midpoint and thus shows only one-quarter of the waste package.

The alluvium host medium for the repository is assumed to have a dry thermal conductivity of 1.0 W/m^2-K and a wet thermal conductivity of 2.0 W/m^2-K [1]. Backfill material is assumed to have the same thermal properties as the alluvium but with higher permeability (10^{-14} m^2 for the host medium versus 10^{-13} m^2 for the backfill). The internals of the waste package are assumed to have the same moisture retention properties as the backfill material. That assumption is conservative because it prevents the formation of a capillary barrier once the waste package fails. The waste package outer shell is assigned a very low permeability to prevent water from flowing through it.

A series of PFLOTRAN simulations were undertaken using ORNL's high-performance computing resource CADES (Compute and Data Environment for Science) The simulations were initially spun up without the repository. Repository closure is assumed at t=0, using results from the spinup phase as initial conditions, but with waste package internals, shell, and drift backfill in place. The DPCs are assumed to contain 37 PWR assemblies from a reactor that was shut down before calendar year 2000. Decay heat in the DPC produces about 4 kW at the time of repository closure (assumed to be in calendar year 2100) and produces only 249 W at 9,000 years post-closure, the assumed time of the waste package breach in this work.

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 cells 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. The criticality event is assumed to start when the waste package is filled to a level of ~1 m. The reference case has an assumed deep percolation rate of approximately 2 mm/year. Aquifer recharge estimates (equivalent to areal averaged deep percolation) in the Basin and Range Province typically range from about 2 mm/year in hyper-arid basins to an average of 17 mm/year in the Great Basin [9].

The objectives are to identify the time at which the DPC fills with water to 1 m potentially initiating a criticality event and to bound the power output that could be produced by a criticality event without driving water out of the package.

2.3 Representation of Thermal Conductivity in Dry and Partially Filled DPCS

PFLOTRAN is a porous-medium code designed to represent thermal hydrology and reactive transport processes in geologic formations. Therefore, it is necessary to homogenize the DPC internals and represent them as an effective porous medium containing a spatially distributed heat source. Previous analyses [9] have shown that heat transport resulting from a combination of thermal radiative transfer, conduction, and convection in dry DPCs can be accurately represented as thermal conduction with an appropriately chosen effective thermal conductivity, consistent with PFLOTRAN's porous-medium conceptualization. However, the effective thermal conductivity is a strong function of temperature in this approach. In addition, anisotropic thermal conductivity is needed because the thermal conductivity is significantly different along the DPC axis and perpendicular to it. Models for radial and axial thermal conductivity appropriate for dry, water filled, and partially water filled DPCs are developed here. Those models were recently added to PFLOTRAN [A. Salazar, personal communication, Dec. 22, 2020].

The thermal conductivities depend on the PFLOTRAN variables s_l and T, the liquid saturation index and temperature in °C, respectively. Thermal conductivity in partially saturated porous media is typically assumed to vary as the square root of liquid saturation index s_l. Adopting the same dependence on the liquid saturation index and adding a temperature dependence for thermal conductivity in dry conditions results in the following model for thermal conductivity in the plane perpendicular to the DPC axis κ_{xz}

$$\kappa_{xz}(s_l,T) = \kappa_d(T) + \left(\kappa_w - \kappa_d(T)\right)\sqrt{s_l}\ , \qquad \textit{Equation 1}$$

where $\kappa_d(T)$ and κ_w are thermal conductivity in dry and water filled conditions, respectively.

In dry conditions, the effective thermal conductivity of SNF assemblies has been studied previously in the Yucca Mountain Project [10]. Owing to the role of thermal radiation in controlling heat transfer in dry SNF assemblies, the effective thermal conductivity depends on temperature. In nitrogen, the $\kappa_d(T)$ ranges from 0.14 W/m-K at 25°C to 0.98 W/m-K at 400°C [10]. A power-law relationship

$$\kappa_d(T) = \kappa_{d0} + a_{tc}T^{\alpha_{tc}}, \qquad \textit{Equation 2}$$

represents the dry radial thermal conductivity well over the relevant range of temperatures (Figure 3). The empirical parameters were determined by fitting data from [10] to obtain $k_{d0} = 0.143$ W/m-K, $\alpha_{tc} = 1.67$, and $a_{tc} = 3.83 \times 10^{-5}$.

To calculate the effective thermal conductivity of a water-filled fuel assembly κ_w, we use results from Cheng and Hsu (1999) [11] who evaluated several approaches for calculating the thermal conductivity of a regular array of cylinders embedded in a stagnant fluid. They found a lumped parameter model proposed by Hsu et al. (1995) [12] to be accurate over a wide range of geometries. Adopting that model and approximating the cylinders as having square cross-sections, κ_w can be estimated from Eq. 15 of Cheng and Hsu (1999) [11]

$$\frac{\kappa_w}{\kappa_l} = 1 - \sqrt{1-\phi} + \frac{\sqrt{1-\phi}}{1+(\lambda-1)\sqrt{1-\phi}} \qquad \textit{Equation 3}$$

where κ_l is thermal conductivity of liquid water, ϕ is porosity of the assembly, $\lambda = \frac{\kappa_l}{\kappa_s}$ and κ_s is thermal conductivity of the solids (SNF rods and basket assemblies).

The thermal conductivity along the axis κ_y can be approximated by considering the solids (SNF rods and basket assemblies) and liquid water are providing parallel paths for heat conduction

$$\kappa_y = (1-\phi)\kappa_s + \phi s_l \kappa_l \qquad \textit{Equation 4}$$

where κ_l is thermal conductivity of liquid water, s_l is the liquid saturation index, ϕ is porosity of the assembly, $\lambda = \frac{\kappa_l}{\kappa_s}$ and κ_s is thermal conductivity of the solids.

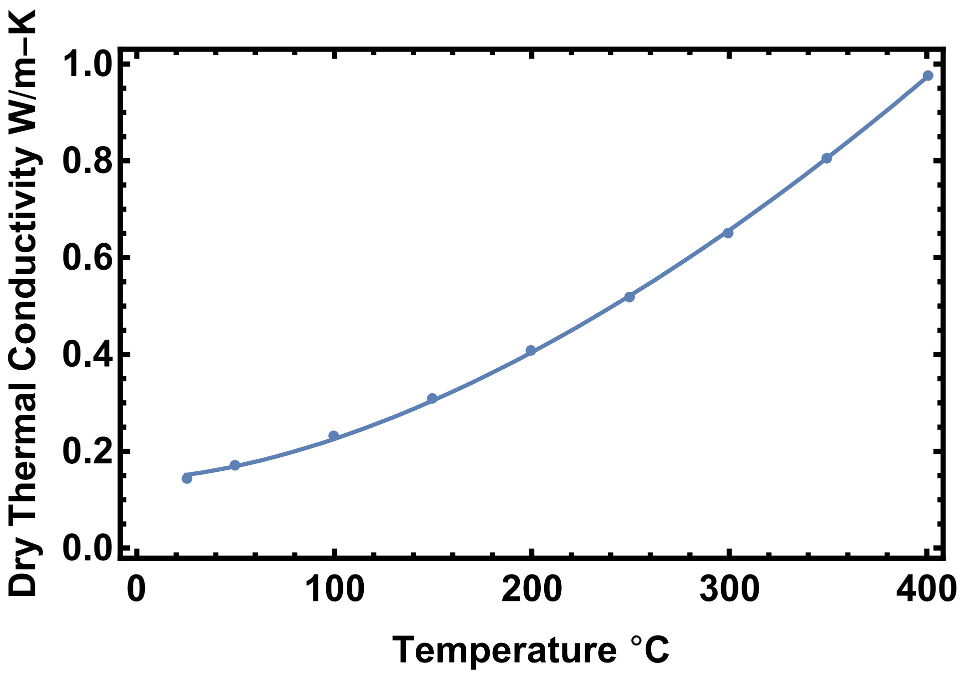

Figure 3. Power-Law Curve Fit (solid curve) to Thermal Conductivity for PWR SNF Assemblies in Dry Conditions. Individual data points were extracted from [9].

3. PRELIMINARY RESULTS

3.1 EXPERIENCE with PFLOTRAN'S GENERAL MODE

PFLOTRAN's general mode solves conservation equations for water mass, air mass, and energy in the gas and liquid phases. General two-phase capability allowing for phase disappearance/reappearance is necessary to address thermal hydrology in unsaturated repositories with waste packages that generate significant decay heat. Numerical challenges associated with this class of subsurface simulation are well known. The model configuration of interest here with high-resolution explicit representation of the DPC is particularly challenging based on our previous experience [3]. Unfortunately, the addition of the temperature-dependent thermal conductivity appears to make it even more difficult for PFLOTRAN to converge for this model configuration. As a result, we were able to obtain solutions only for a single reference case, despite repeated efforts to tune numerical solution parameters. We will continue working with the PFLOTRAN developers to find a more robust solution method.

3.2 REFERENCE CASE RESULTS

Temperature versus time in the center of the DPC is shown in Figure 4 for our reference case, which has a deep percolation rate of 2 mm/year. These plots stop before the criticality event. The temperature peaks at 322°C at approximately 10 years post-closure, which is significantly higher than the ~240°C found previously without the new and more realistic thermal conductivity model. By the time of the assumed DPC breach, the DPC temperature has decayed to about 75°C.

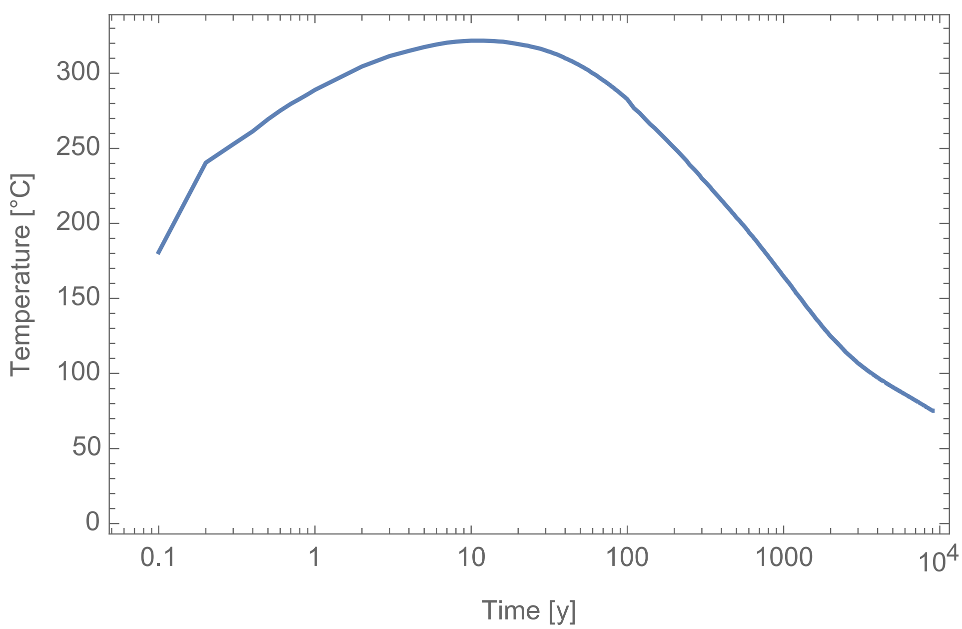

Figure 4. DPC internal temperature vs. time prior to waste package breach.

The liquid saturation index field is shown in Figure 5 at 500 years post-closure, which is near the time of the maximum extent of the dry zone. The black box in the center is the waste package shell. The region of zero liquid saturation extends several meters into the host formation in all directions. It is vertically asymmetric, extending further in the downward direction. Significantly, the dry-out zone does not extend to the pillar centerline between drifts. As a result, water is able to drain between drifts without forming a perched zone of higher water content above the repository.

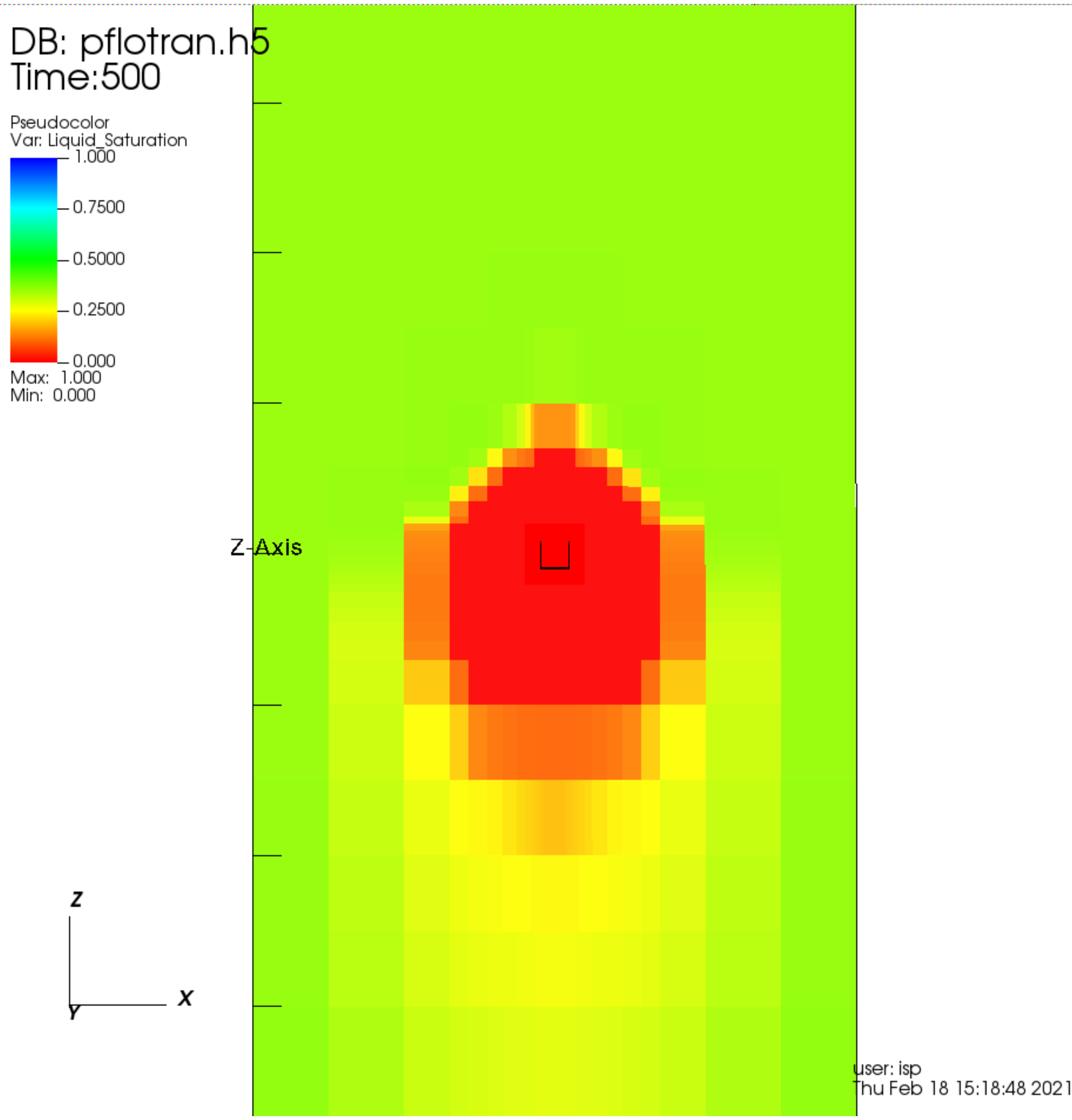

Figure 5. Liquid saturation index for the reference case at 500 years postclosure, the time of maximum dry-out. The black box is the waste package outer shell. The subdomain shown is 40 m wide.

At the time of the assumed breach of the DPC, the environment around the DPC is still dry (Figure 6a). Because of the low background percolation rate water does not begin to pool in the bottom of the DPC until approximately 16,200 years (Figure 6b) and does not reach the level required to initiate a criticality event until approximately 25,000 years post-closure (Figure 6c).

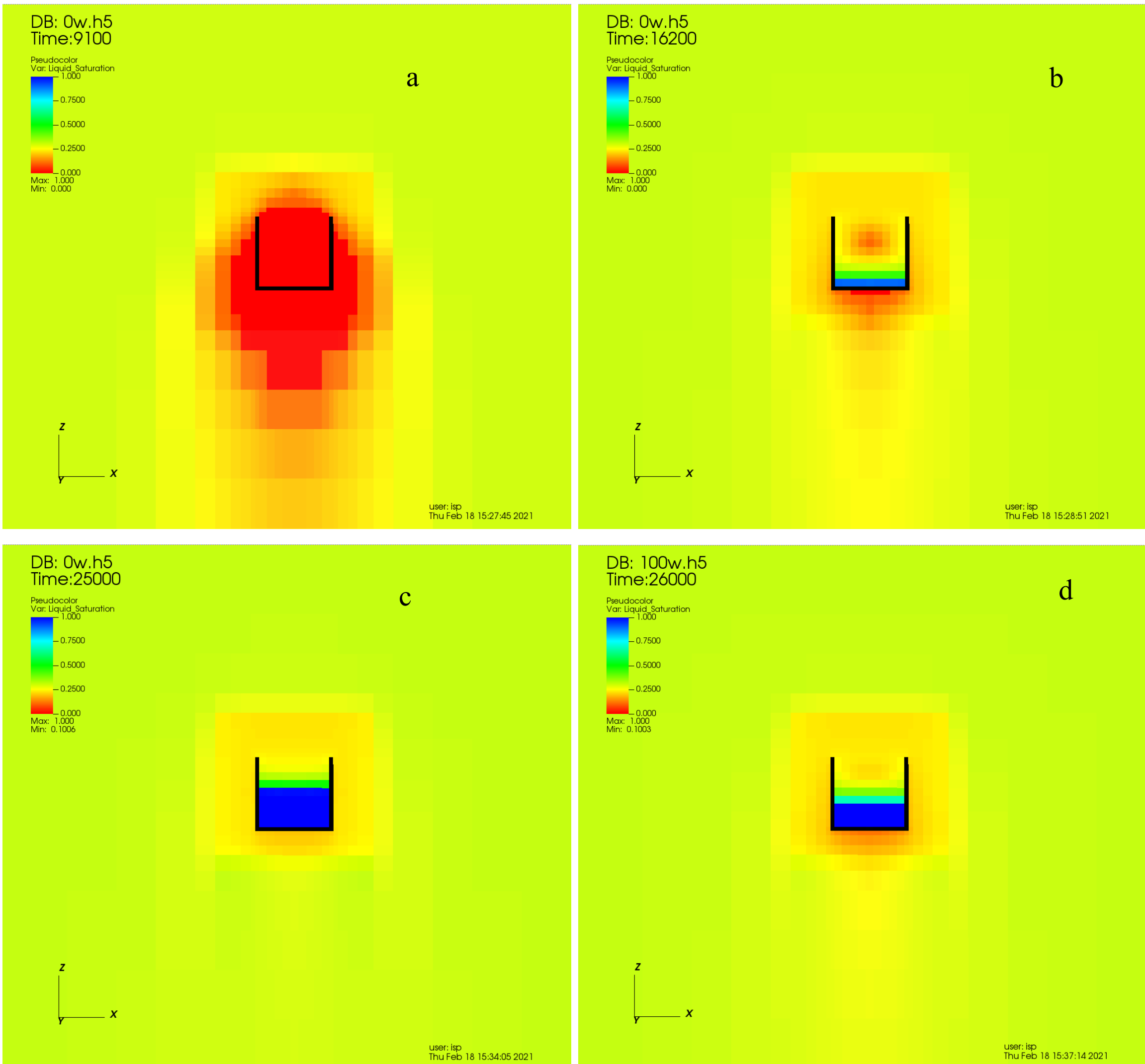

Figure 6. Details from the PFLOTRAN simulation of the reference case showing liquid saturation index in cross section at different times: (a) just after DPC failure, (b) when water starts to fill the DPC, (c) when the DPC is filled with water to 1 m triggering a criticality event, and (d) 1000 years after the start of a 100 W criticality event.

At 25,000 years post-closure, a criticality event producing 100 W is initiated. That small power output is sufficient to drive off the water (Figure 6d). However, the process is slow because evaporation losses are almost balanced by incoming water from deep percolation. Because loss of moderator would shut down the criticality event, we can conclude that the maximum power output is limited by thermal hydrological processes to about 100 W for this reference case.

4. CONCLUSIONS

These results update previous analyses of thermal hydrological constraints on timing and power output of a criticality event in DPCs in a hypothetical repository in unsaturated alluvium using a more realistic representation of heat transport inside dry DPCs. For the conditions analyzed here, following a package breach, the alluvial formation could supply enough water to allow enough accumulation in the DPC to trigger a criticality event. However, the power output that would be generated is limited to modest values by loss of the water moderator due to evaporation and vapor diffusion. In the reference case scenario, the DPC would not start to fill with water until about 16,000 years post closure and would not fill to a level that allows a criticality event until approximately 25,000 years post-closure. The long-term average power output that could be sustained is limited to approximately 100 W. Sensitivity to assumed conditions and parameters in the reference case, especially the deep percolation rate, need to be addressed but could not be undertaken because of numerical failures of the PFLOTRAN code running in general mode in the dry conditions of an unsaturated alluvium repository.

5. REFERENCES

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