



# Thermal-hydrologic design constraints for the disposal of high-heat waste packages in a deep geologic repository

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## Abstract

The US Department of Energy is considering a variety of waste package configuration options in its generic disposal research program, among them large waste packages that would hold 24 or more pressurized water reactor (PWR) assemblies. 24-PWR assemblies have a high decay heat output. Consequently, they represent unique challenges in tightly-coupled multi-phase thermal/hydrological modelling during the first few hundreds of years after disposal, while the packages generate large amounts of heat that must be dissipated through the engineered and natural barriers. The resulting model is challenging to simulate, as both fluid saturation and temperature change very quickly in the near-field.

In this work, models with different grid resolutions and length scales are used to explore the requirements for accurately simulating 24-PWR disposal. The hypothetical host rock is a partially-saturated alluvium formation 250 m below the surface with small infiltration and a water table 550 m deep. Models are built to study the near-field impacts of disposal of 24-PWRs of 40 GWd/MTU fuel, 100 years out of reactor. Simulations are conducted using PFLOTRAN, a massively parallel reactive flow and transport simulator. The large simulation models are a site-assessment scale array representing disposal of 1350 assemblies and are meshed with four levels of grid resolution. The small-scale model represents a single waste package in the center of an infinite waste-package array and is used as a benchmark.

## I. Conceptual model

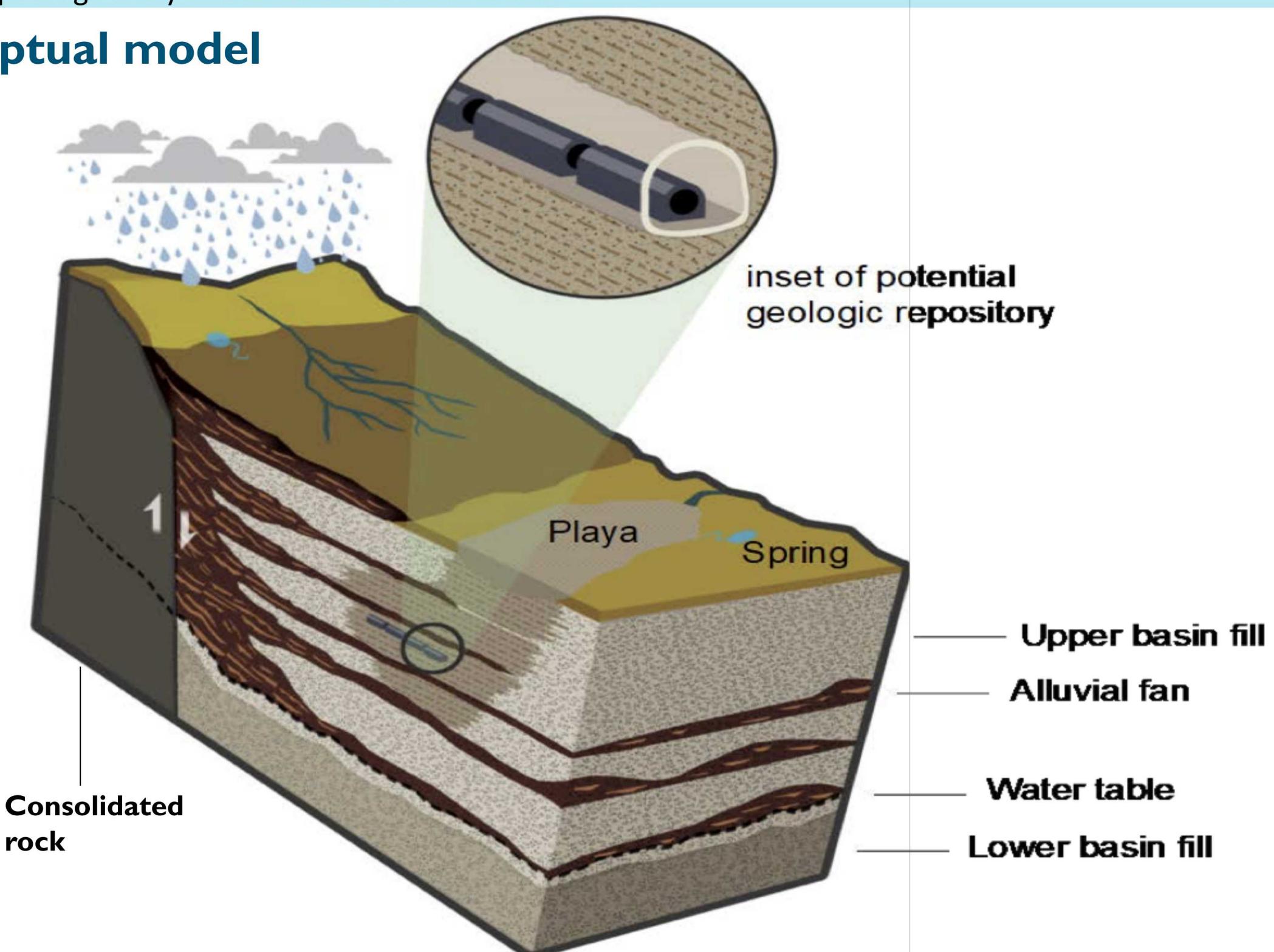


Figure 1: Arid environment with little infiltration. The repository is above the water table and could be used for disposal of 24-PWRs. Drifts are backfilled with crushed alluvium modified to increase thermal conductivity.

## 2.1 Site-scale simulation models

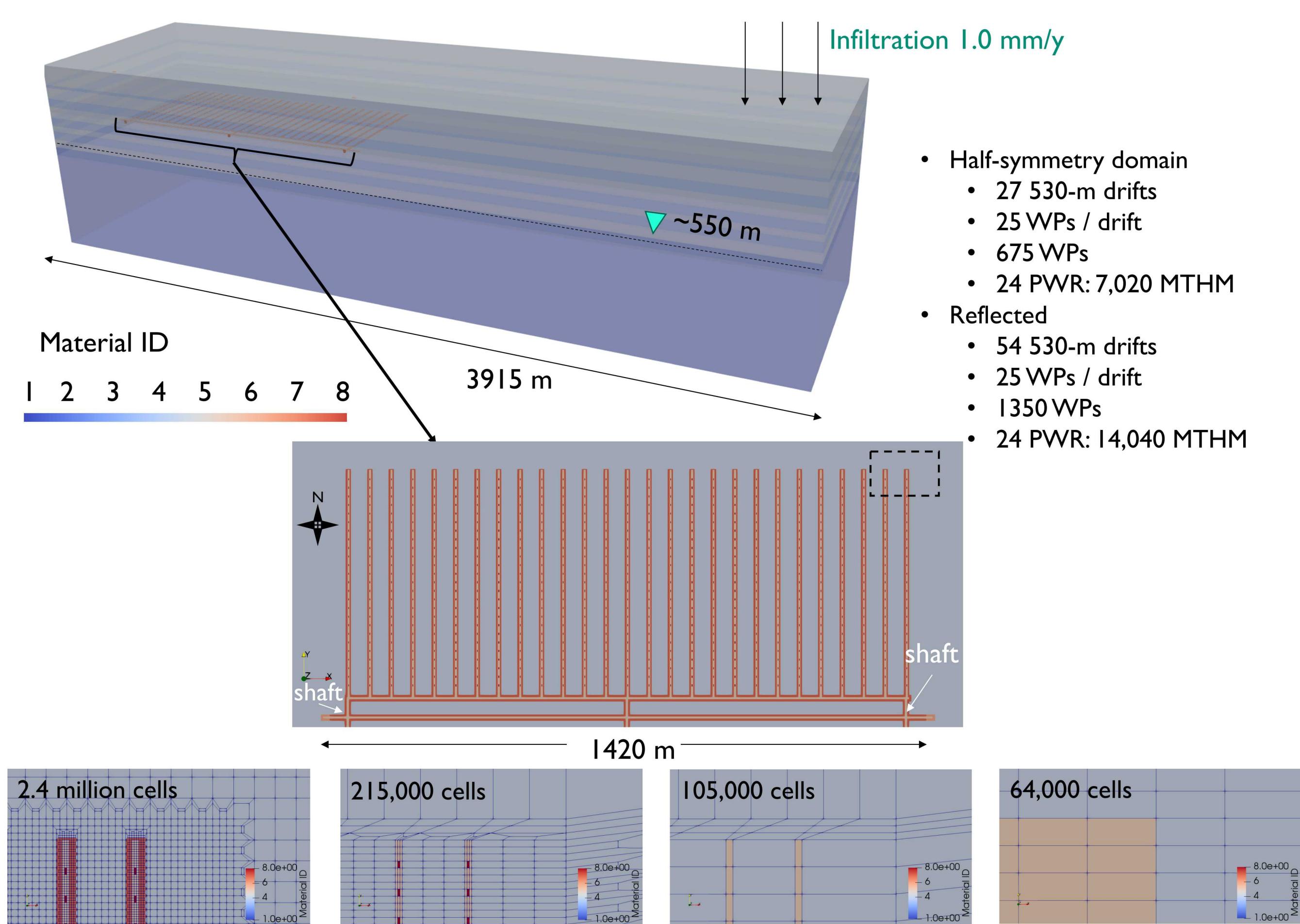


Figure 2: Top: model of the full domain with 50m center-to-center drift spacing and 20m center-to-center waste package spacing. Middle: XY plane view of drifts (ID=5) and waste packages (ID=8). Bottom: detail of the four simulation meshes in the northeast corner of the repository. Only the 2.4 million and 215,000 cell models resolve the waste packages. The 105,000 cell model resolves the drifts only, and the 64,000 cell model does not resolve waste packages or drifts.

## 2.2 Site-scale simulation results

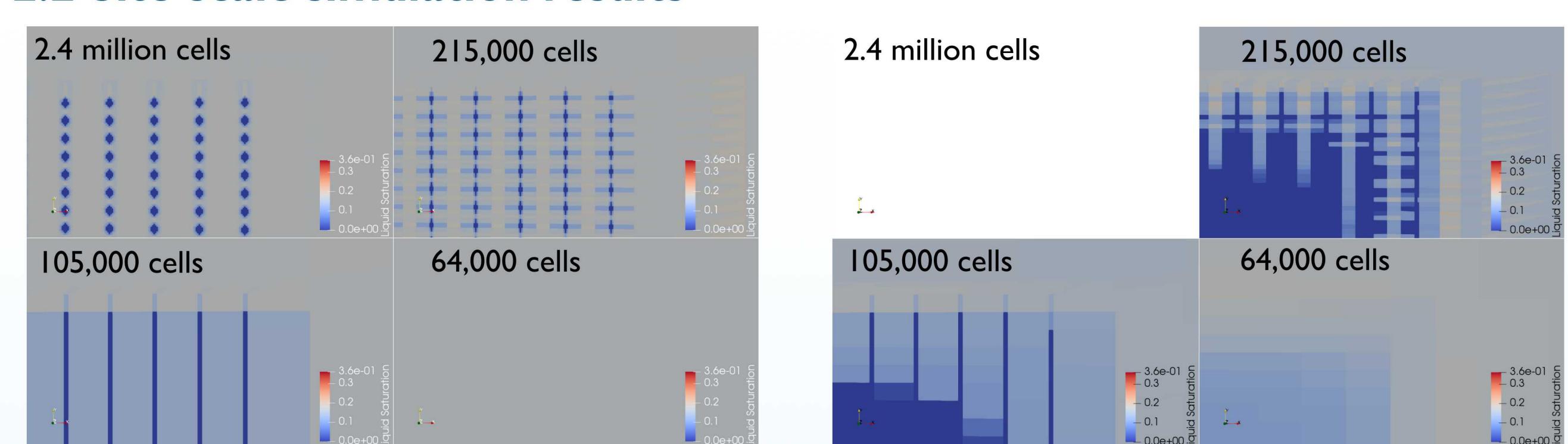


Figure 3: Liquid saturation in the XY plane view of the northeast corner of the repository 20 years (left) and 500 years (right) post-closure on the four simulation meshes. Maximum temperature in the waste packages occurs at 20 years, and maximum dry out of the repository occurs at 500 years. The finest model was run for 48 hours of computation time on 64 cores of a parallel super-computer, but did not finish the simulation due to small time steps. The coarsest mesh does not capture the dry-out of the drifts.

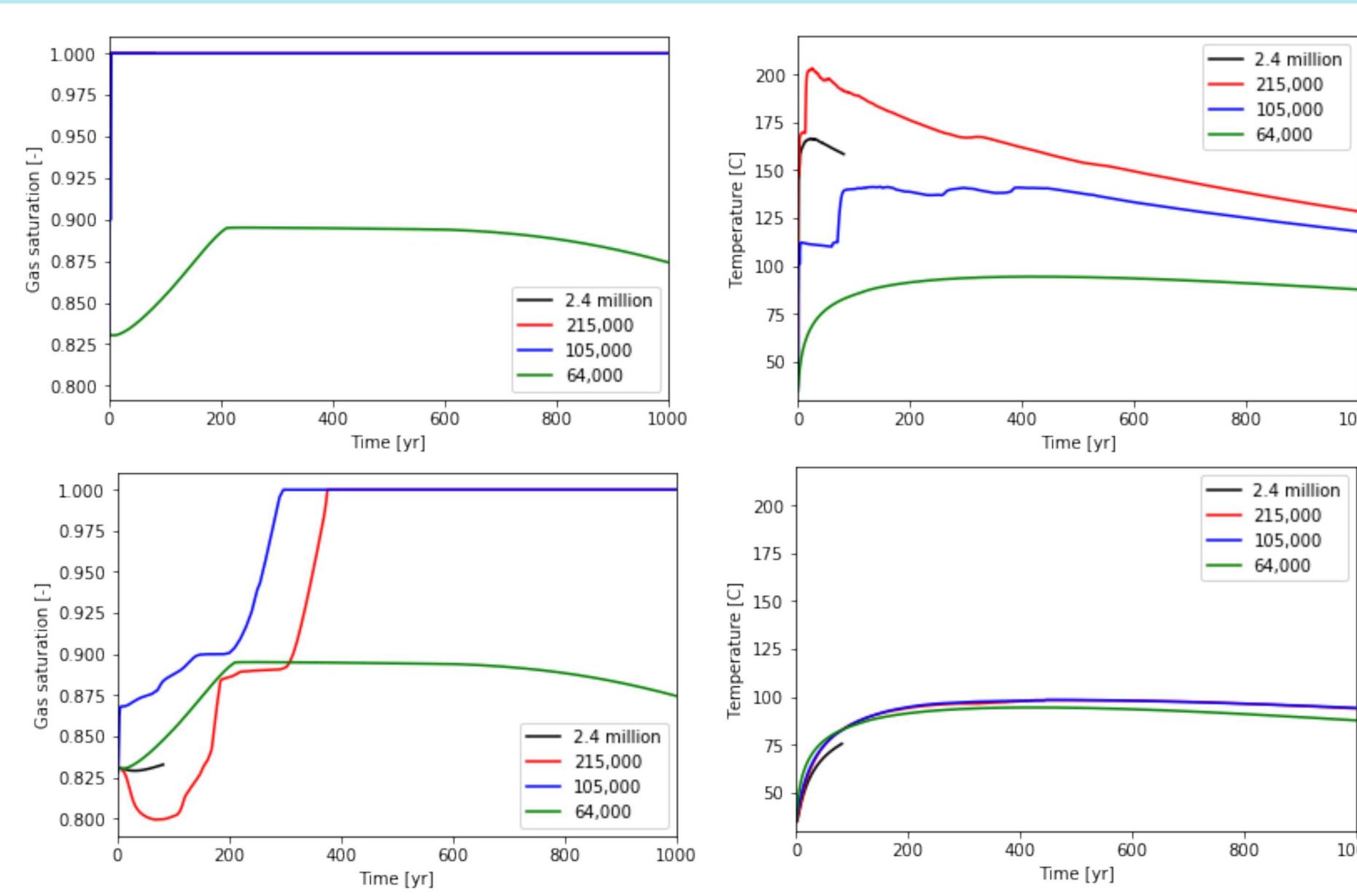


Figure 4: Gas saturation (left) and temperature (right) in the cell containing the waste package for the 4 site-scale simulation models. The coarsest model does not resolve dry out or the high temperatures in the waste package.

## 3.1 Single waste-package simulation model

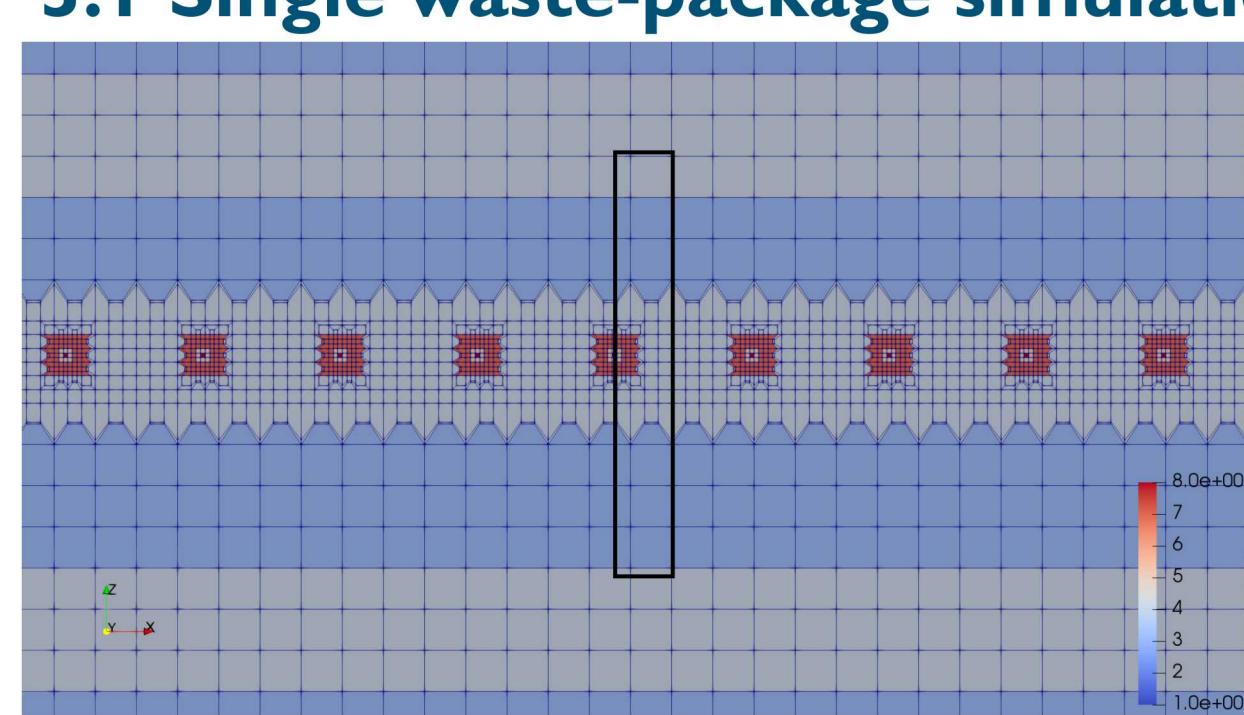


Figure 5: Gas saturation (left) and temperature (right) between two central drifts for the 4 site-scale simulation models. The coarsest model does not resolve dry out but does capture the temperature increase between the waste packages.

## 3.2 Single waste-package simulation results

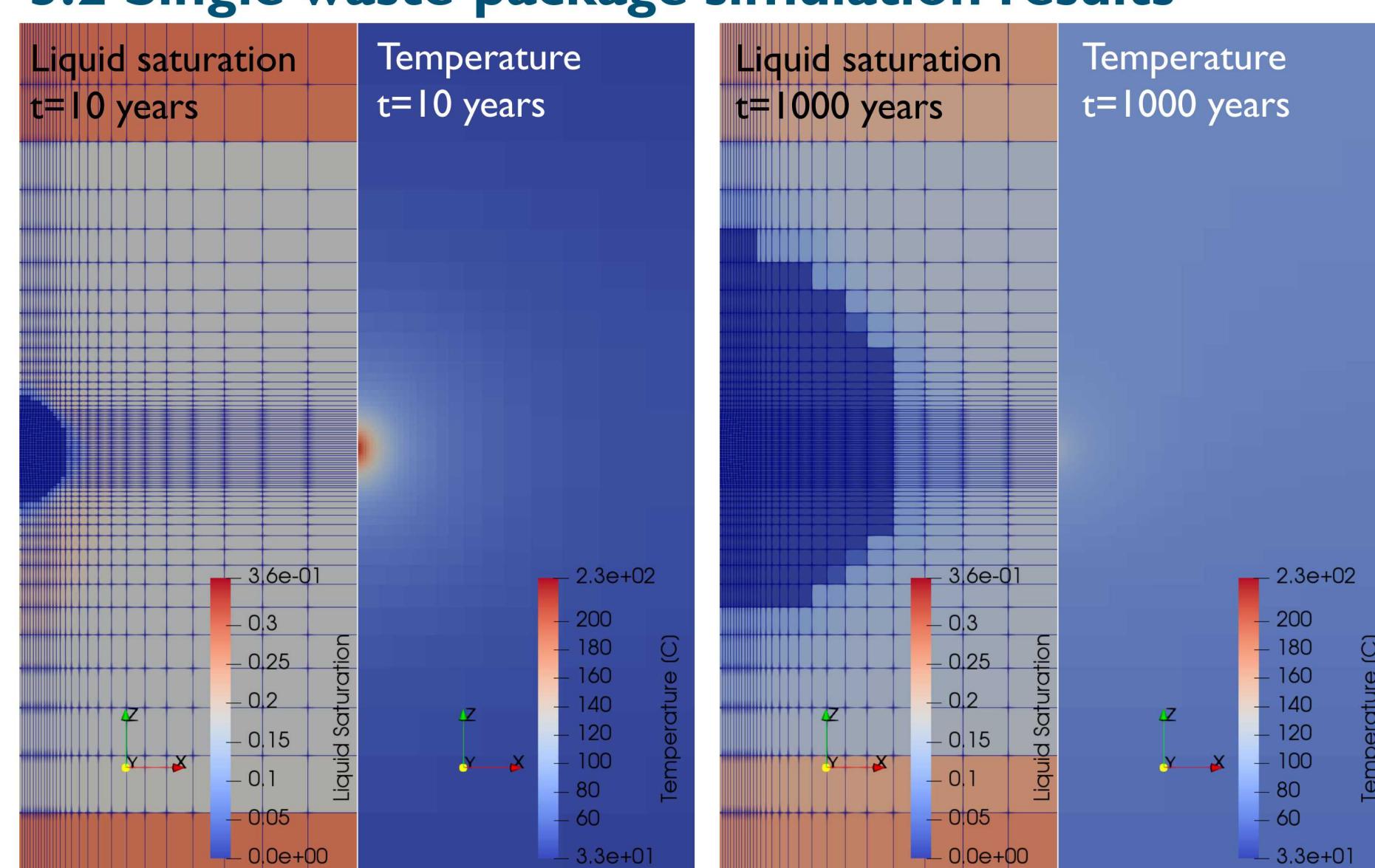


Figure 6: The black rectangle indicates the area of the array included in the single waste package model. Only 1/4 of the waste package is simulated and the rest is captured by reflective boundaries.

## 3.3 Comparison of results across scales

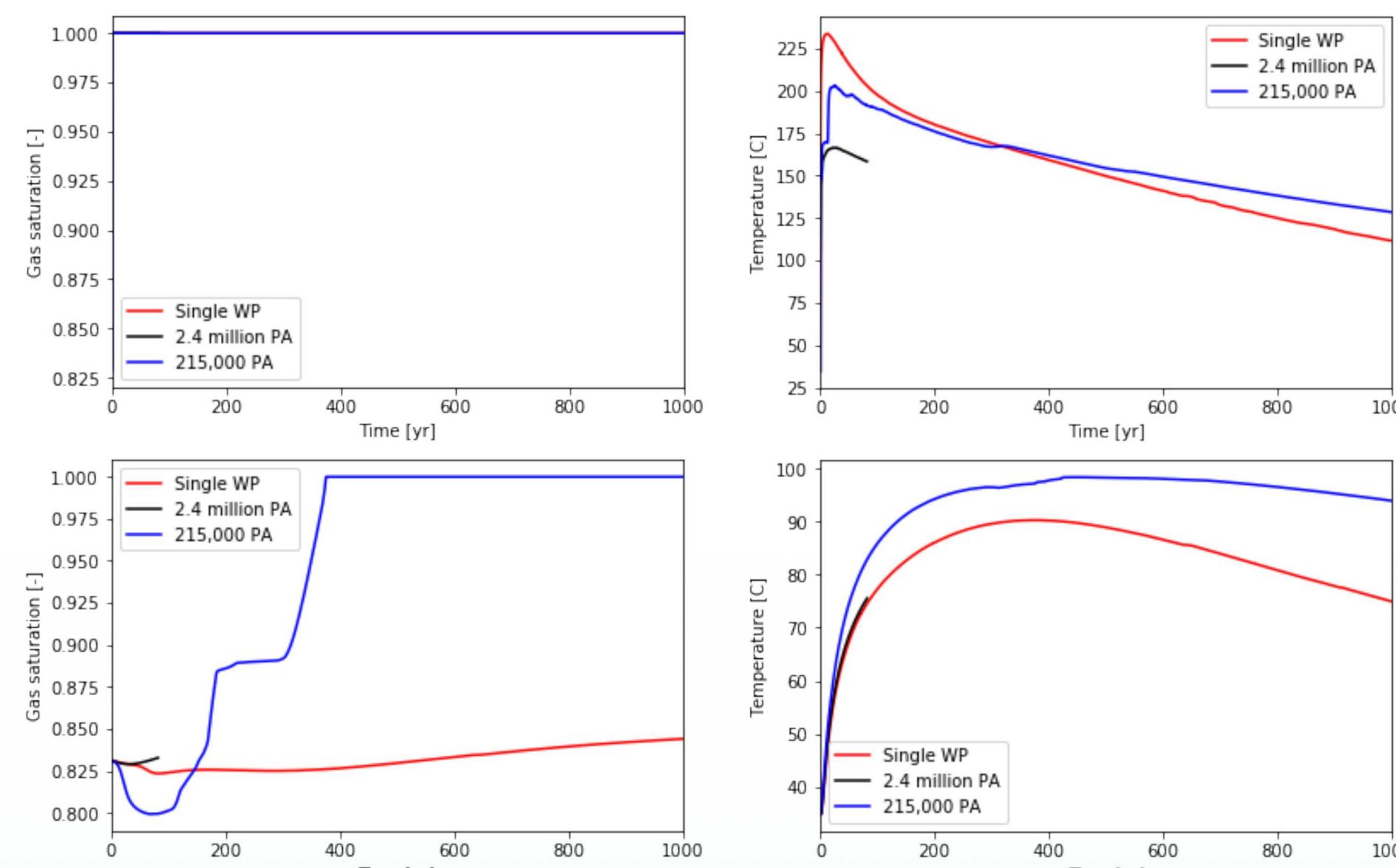


Figure 7: Simulation results on the highly-refined single waste package model. Left: liquid saturation and temperature after 10 years, the time of peak temperature in the waste package. The dry out region propagates away from the drift more quickly than the thermal front. Right: liquid saturation and temperature after 1000 years, the time of maximum dry out. The waste package has cooled and the dry out region has a teardrop shape due to upward migration of gas.

## 4 Conclusions and future work

- The two coarse meshes of the site-scale model are clearly too coarse to model the near-field fluid flow, while the finest takes too much simulation time.
- The remaining 215,000 cell model predicts dry out of the entire area between many of the drifts, which was not observed in the single waste-package benchmark or an intermediate scale model (not shown). It remains unclear whether the level of resolution in this model would be sufficient for site-scale simulations in the unsaturated alluvium conceptual model including radionuclide transport.
- This work highlights the need to explore upscaling properties and/or using nested models to capture near-field temperature and saturations along with far-field radionuclide transport in the site-scale alluvium conceptual model.

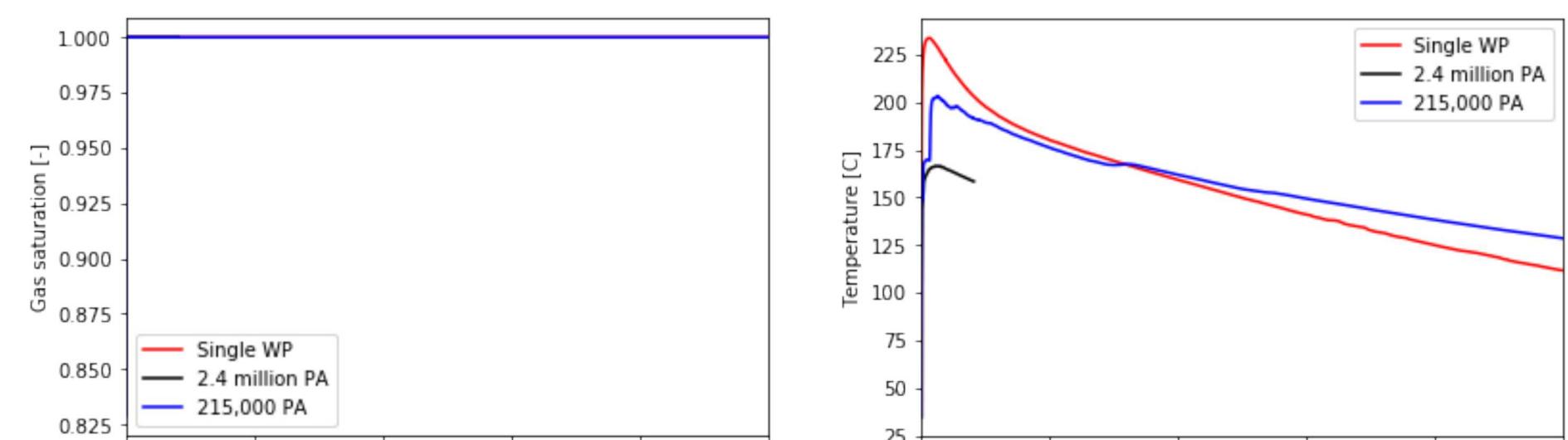


Figure 8: Gas saturation (left) and temperature (right) in the waste package for the single waste package model and the two finest mesh site-scale models. The results across the three models are broadly consistent.

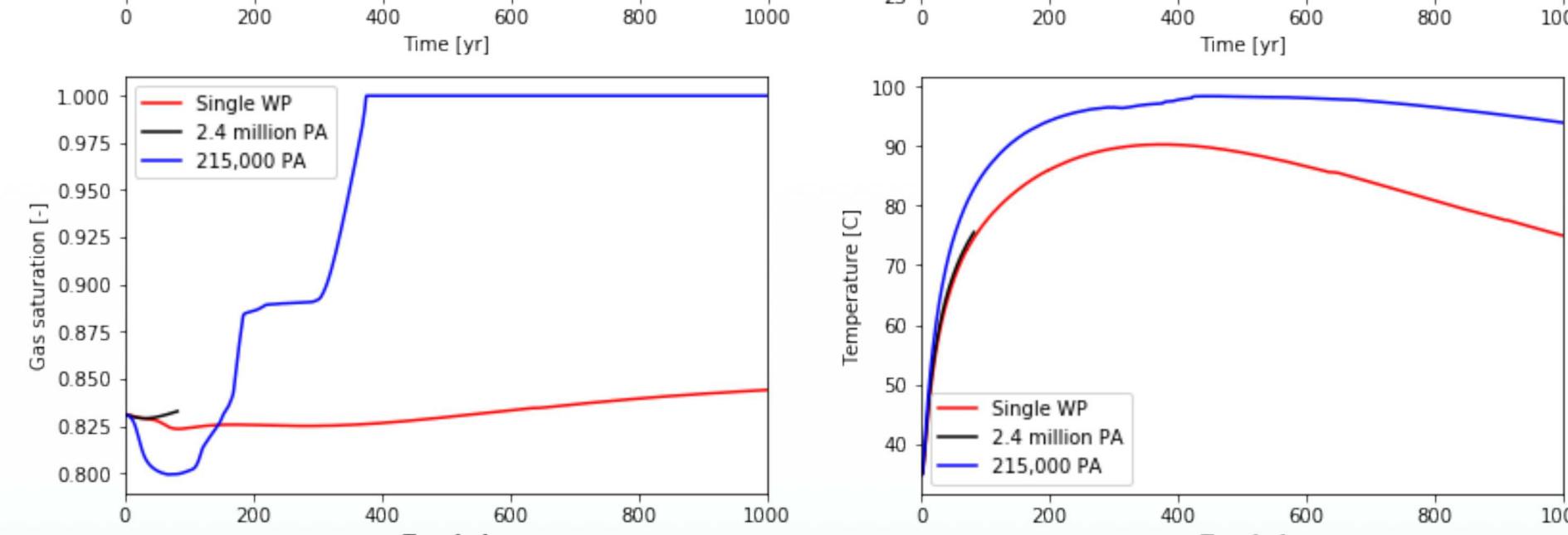


Figure 9: Gas saturation (left) and temperature (right) at the midpoint between drifts for the single waste package model and the two finest mesh site-scale models. The saturation profiles are inconsistent between the models.