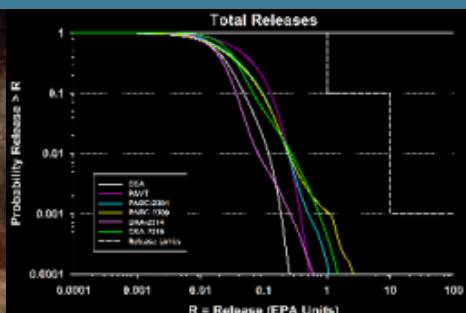
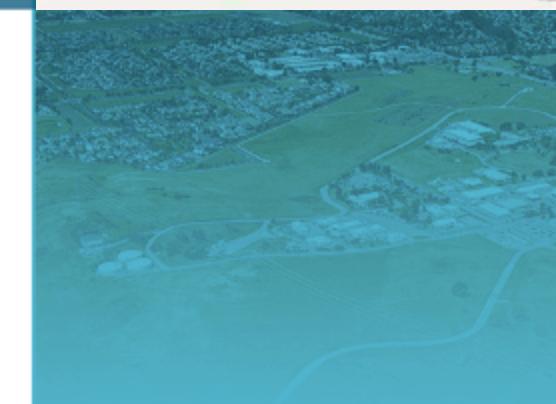


# APPA Peer Review Questions and Concerns Response



Seth King, Tara LaForce, and Clifford Hansen

July 2021



Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This research is funded by WIPP programs administered by the Office of Environmental Management (EM) of the U.S. Department of Energy

# Table of Contents



This presentation will address some follow up questions asked by the Peer Review Panel:

1. DBR Model: B. Brine flow rate versus time over the 4 1/2-day release duration – **Slides 3 and 4.**
2. Repository Fluid Flow: Gas saturation plots and Brine pressure over time – **Slides 6 through 19.**
3. Plots of the PFLOTRAN spiderweb mesh – **Slides 20 through 28.**
4. Please provide the Sandia definitions for Eulerian and Lagrangian grid deformation and specify which is being used in the above – **Slide 29.**
6. Please provide a technical description and/or references for the details of the numerical methods used in BRAGFLO - **Slides 30 through 32.**

Note that question 1A asking for a DBR grid refinement study will be responded to at a later time.  
Question 5 on actinide concentration was answered verbally during the peer review meeting.

# Peer Review Panel follow up question



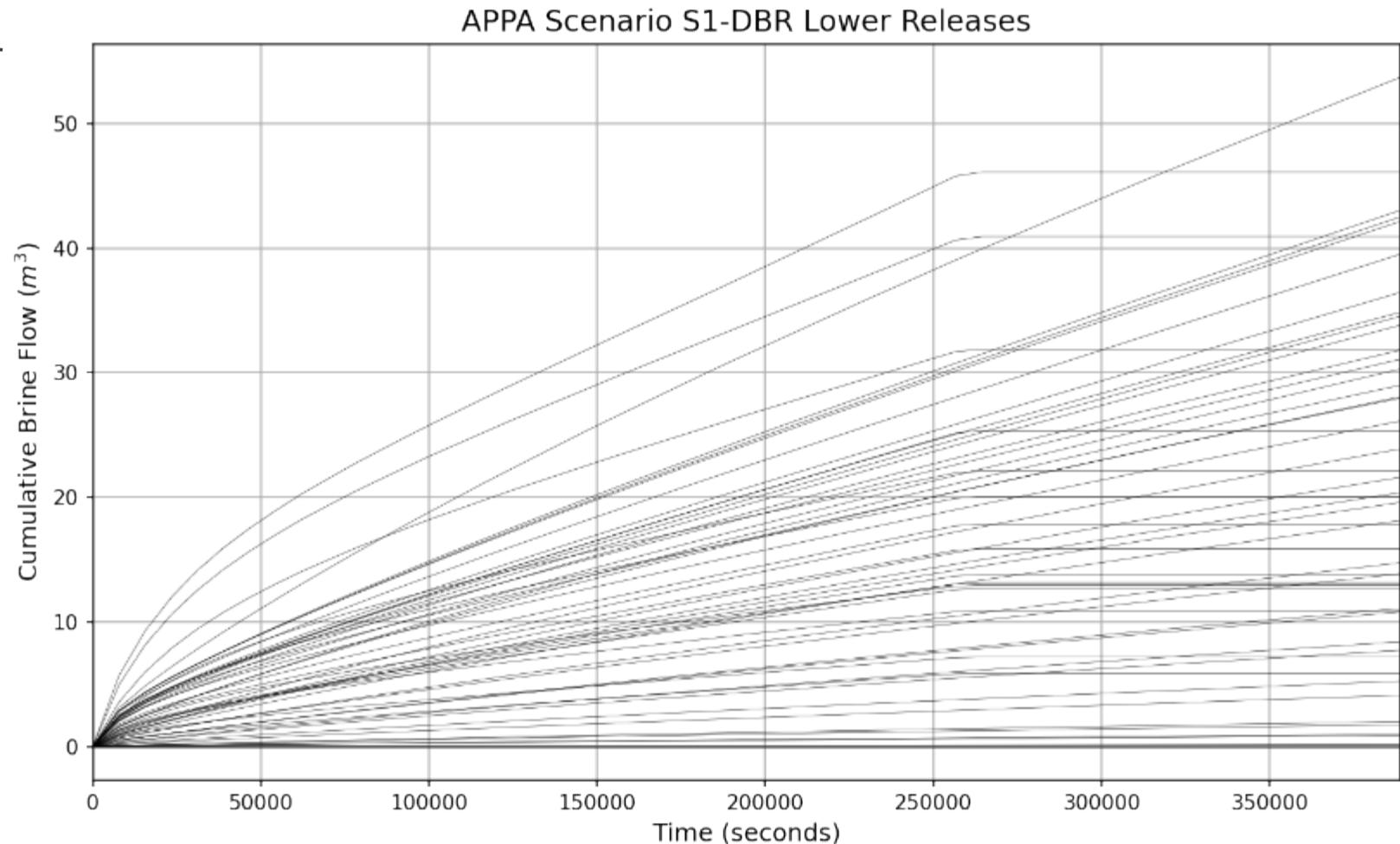
## 1. DBR Model

### B. Brine flow rate versus time over the 4 1/2-day release duration

Cumulative brine flow ( $m^3$ ) over time are plotted for Lower intrusions in the S1-DBR scenario. Note some flow rates cut off at 259,200 seconds (3 days), as the gas flow rate is below the cutoff for a blowout and the DBR event ends at 3 days.

S1-DBR models a DBR event from a previously unintruded repository.

(continued)



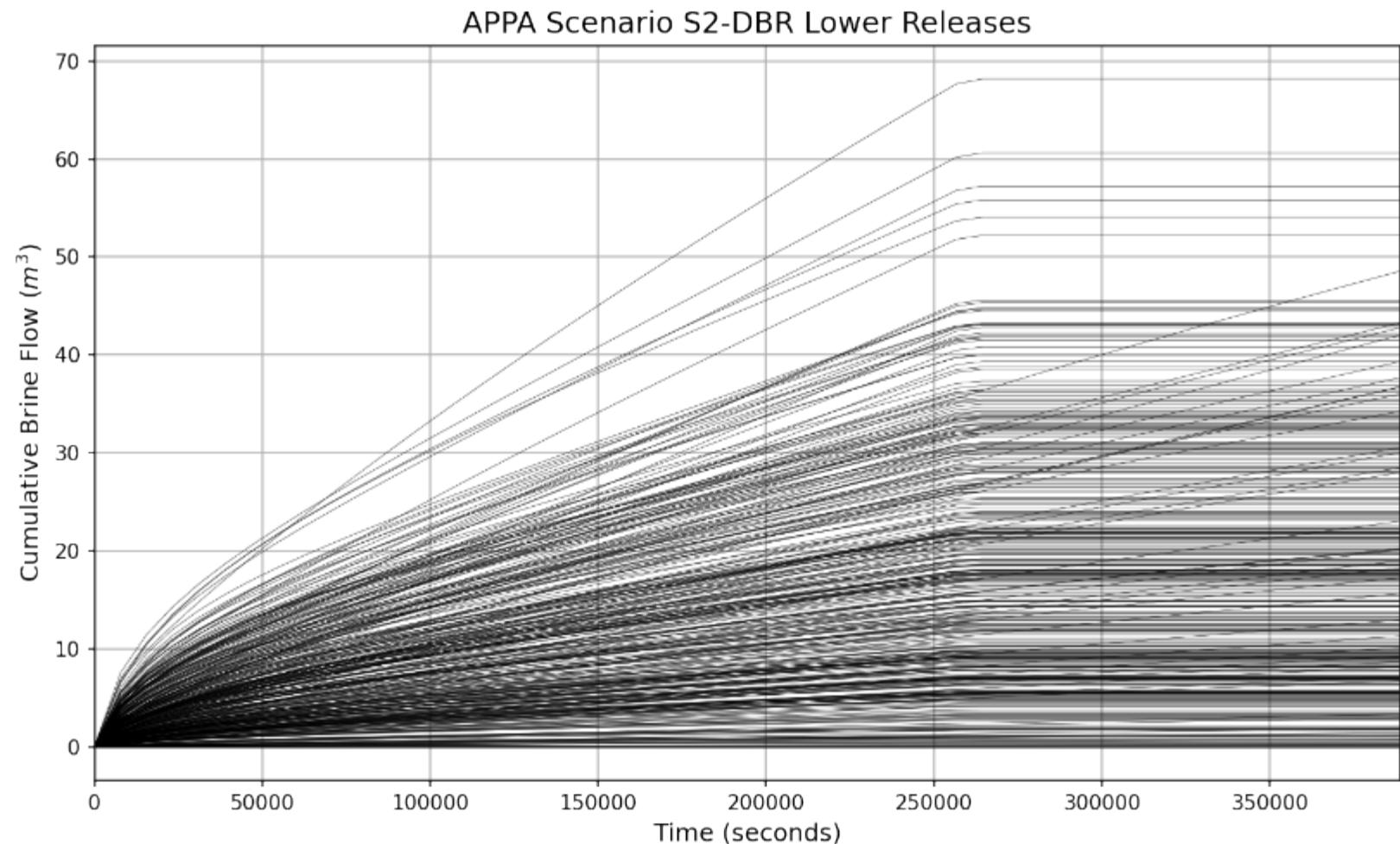
# Peer Review Panel follow up question



## 1. DBR Model

### B. Brine flow rate versus time over the 4 1/2-day release duration

Cumulative brine flow rates over time are plotted for Lower intrusions in the S2-DBR scenario. The S2-DBR scenarios generally have higher brine saturation initial conditions from the Salado Flow model, leading to lower gas flow rates, cutting off more vectors at 3 days into the DBR event.



## Peer Review Panel follow up question

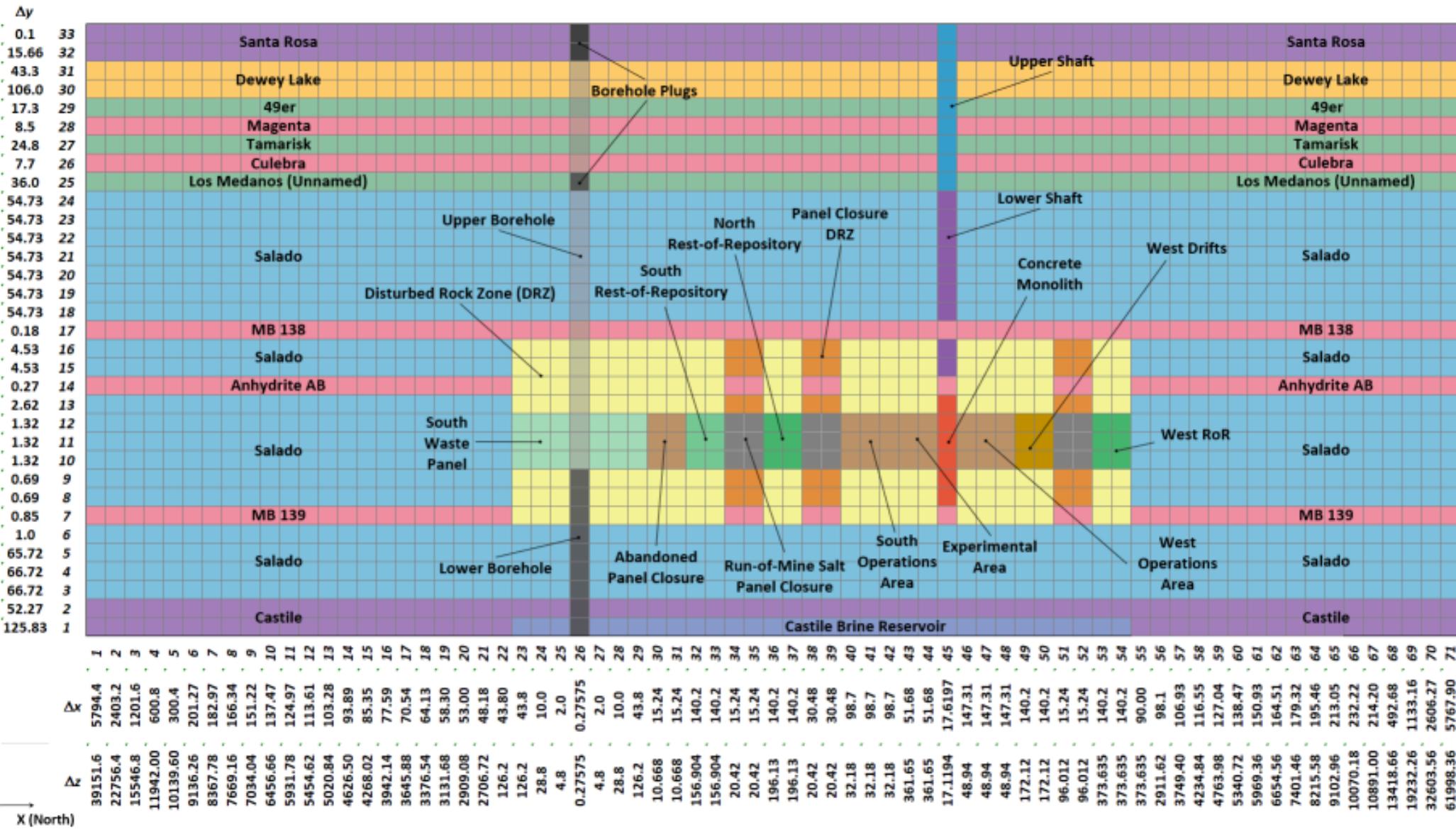


2. Repository Fluid Flow (everyone liked the movie)

- A. Gas saturation plots over 5-time steps
- B. Brine pressure over 5-time steps

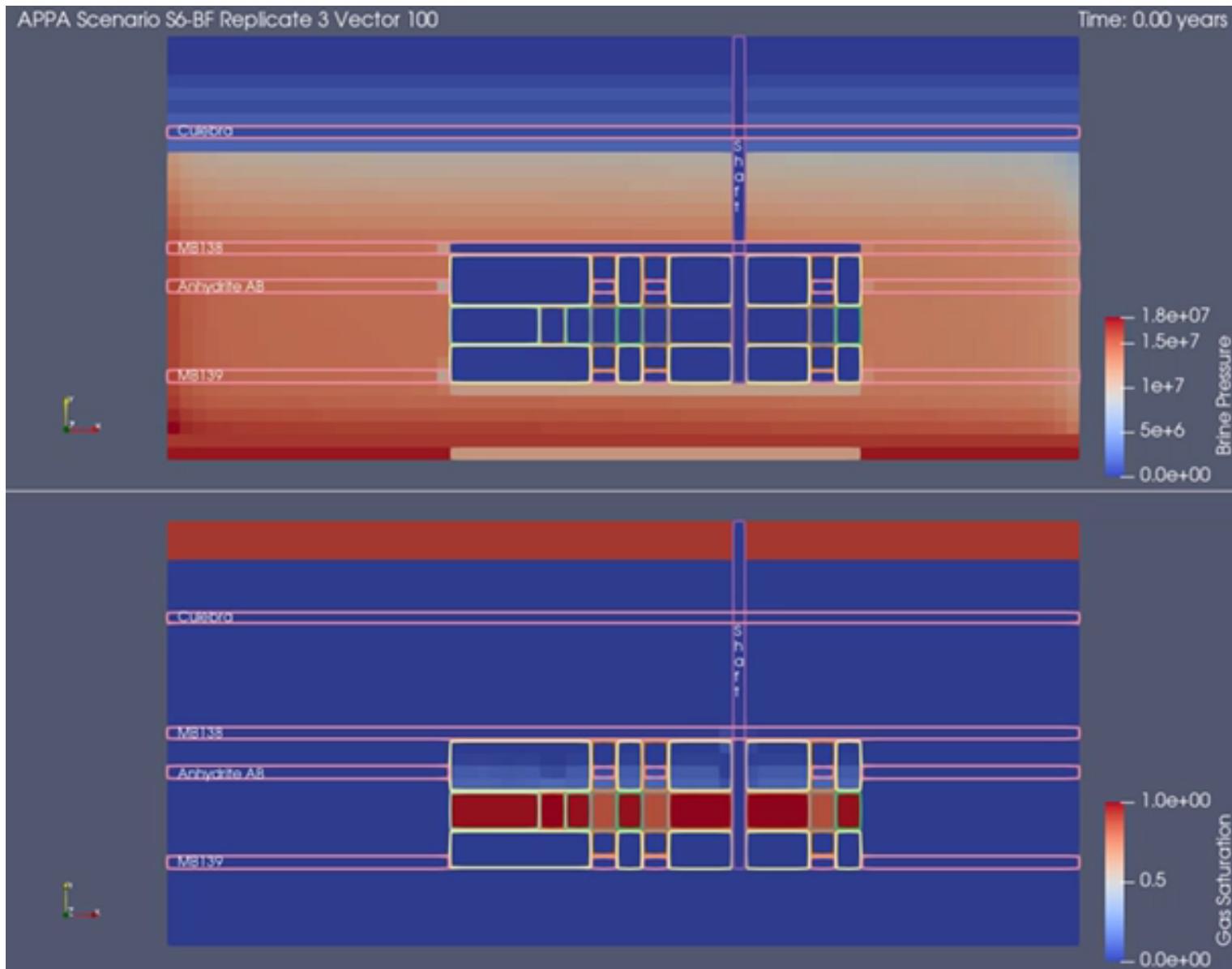
An animation of the Salado Flow results for an example vector in Scenario S6-BF will be shown.

Following slides will pull out screenshots at important times in the simulation and provide some description of the system behavior.



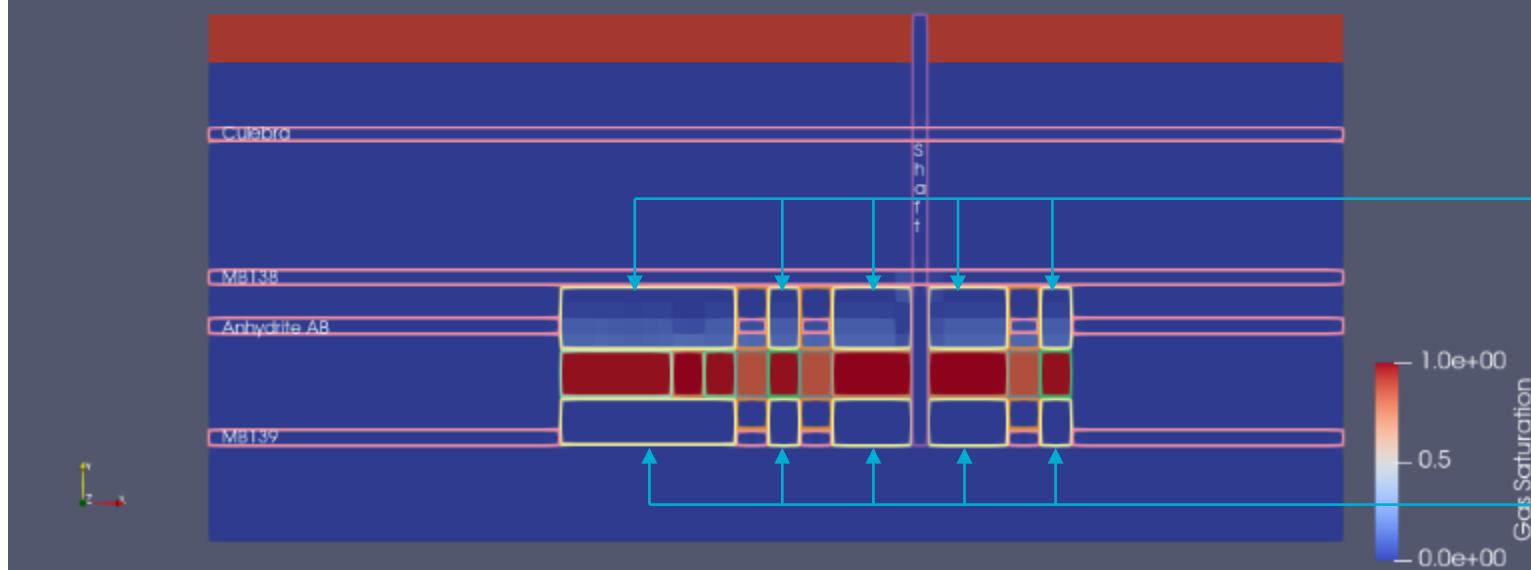
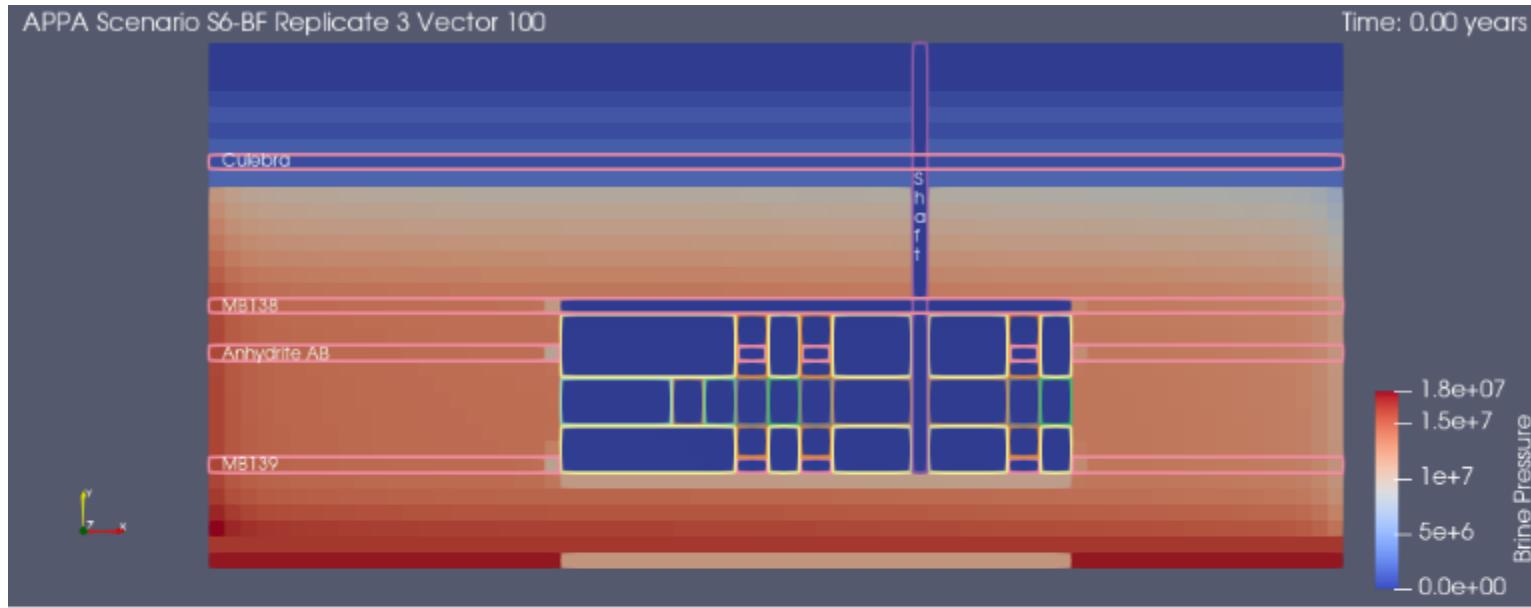
An animation of the Salado Flow results for an example vector in Scenario S6-BF will be shown. Please refer back to this image for grid area materials and grid block dimensions.

# Animation of flow results



An animation of the Salado Flow results from an example vector is provided to address concerns expressed by the peer review panel over the lack of spatial plots of results. The animation shows the S6-BF scenario with an E2 intrusion at 1000 years and an E1 intrusion at 2000 years. The following slides will pull out screenshots at important times in the simulation and provide some description of the system behavior. The remaining slides will discuss important points to keep in mind when visualizing results in this manner.

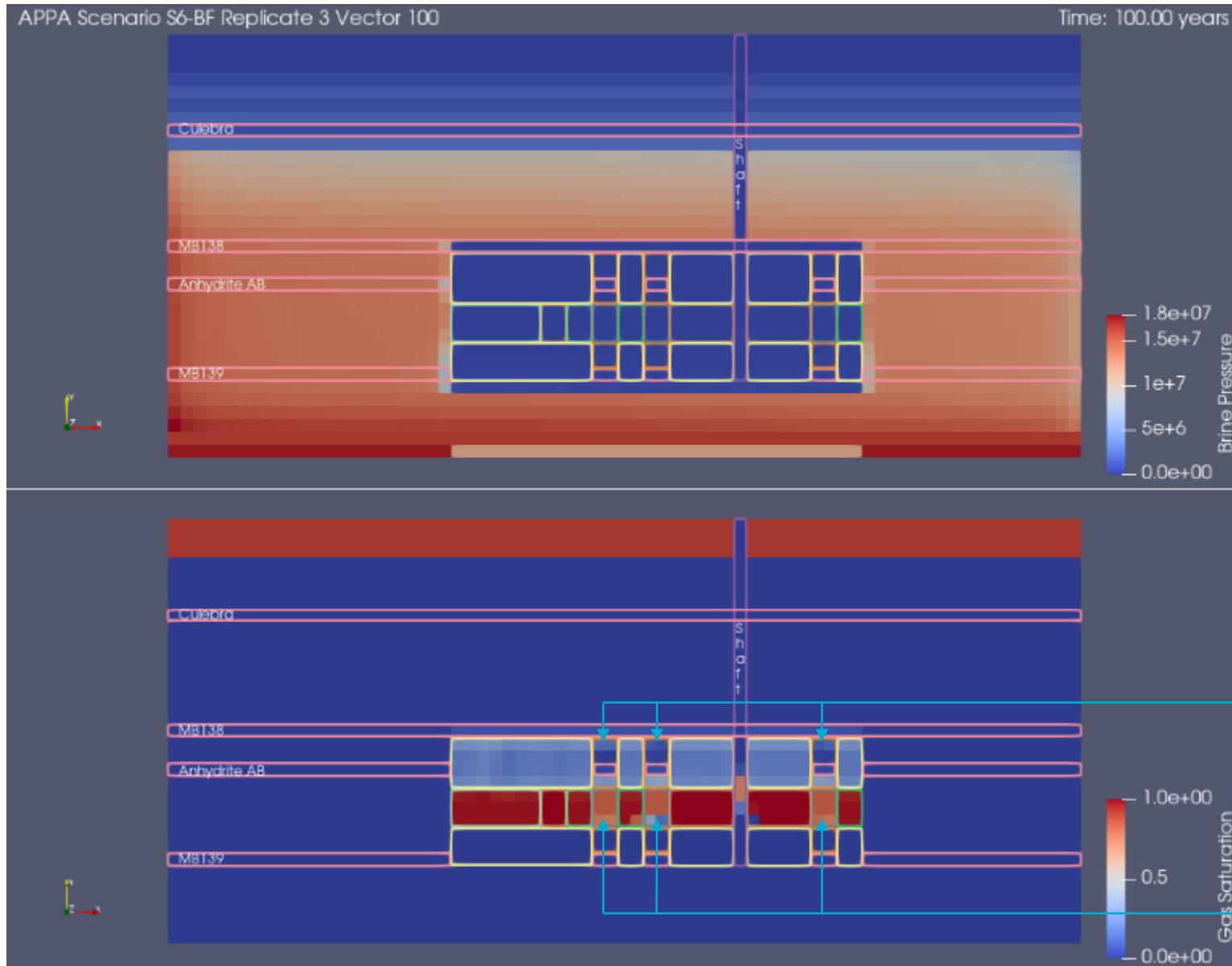
# Scenario S6-BF Replicate 3 Vector 100 – 0 years



Note the reduced brine saturation (increased gas saturation) in the DRZ from the -5 year pre-closure time.

At closure ( $t=0$  years) waste is introduced, pressures and saturations in the excavated areas are reset.

# Scenario S6-BF Replicate 3 Vector 100 – 100 years

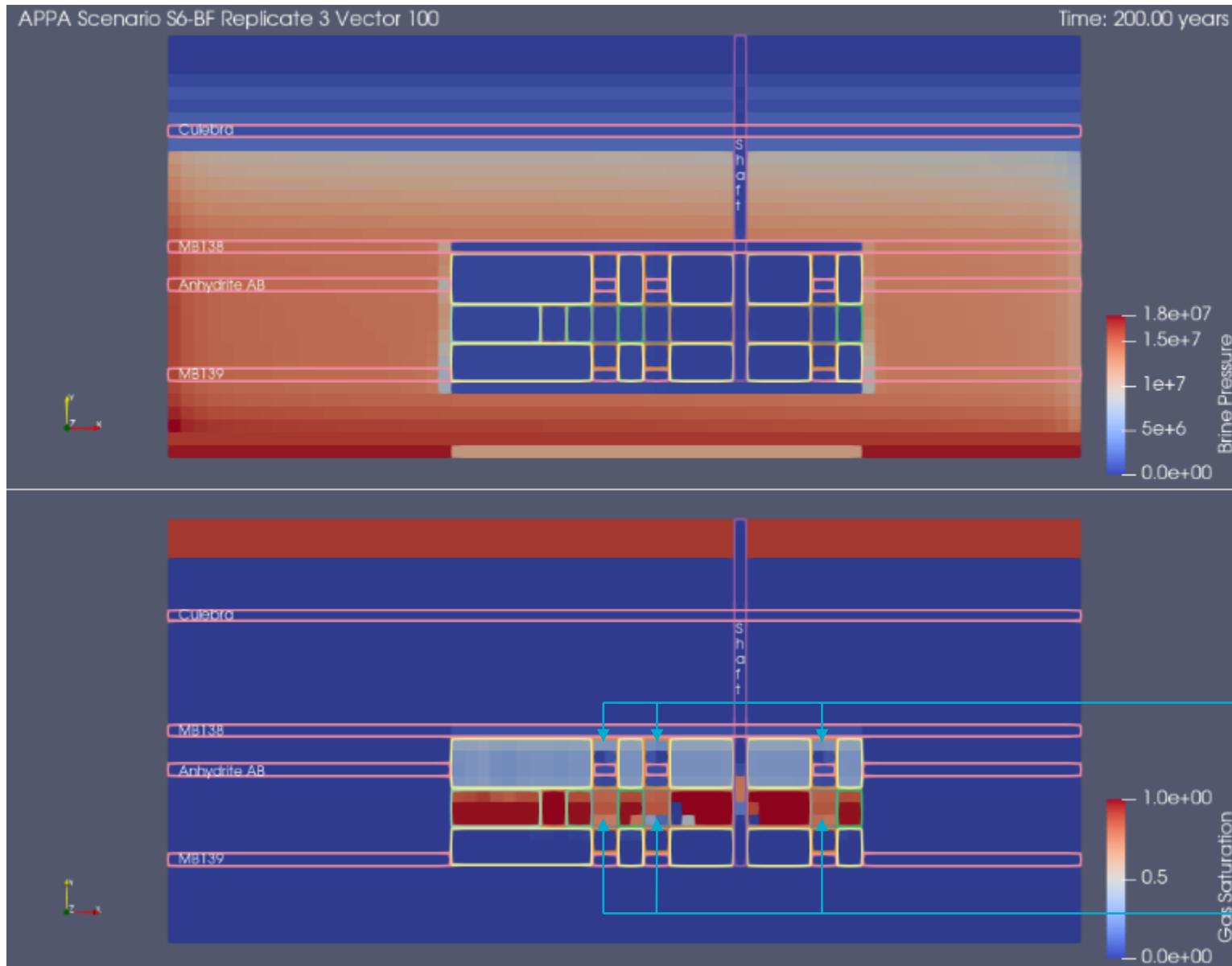


Further reduction of brine saturation (increased gas saturation) in the overlying DRZ and some drainage of the markerbeds.

At t=100 years, Run Of Mine Panel Closure System (ROMPCS) material change to represent creep closure.

DRZ PCS  
Panel Closures

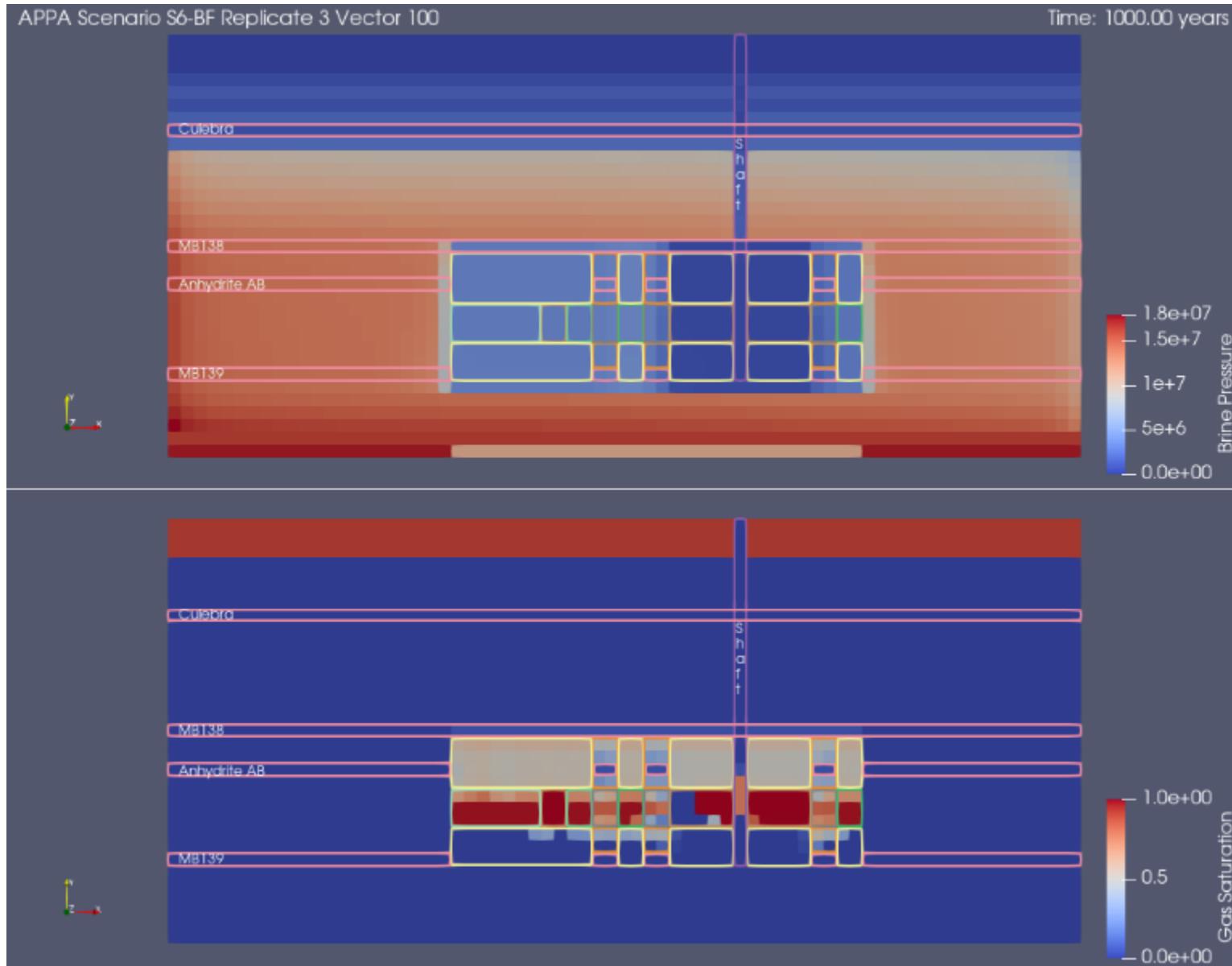
# Scenario S6-BF Replicate 3 Vector 100 – 200 years



Still more drainage of the overlying DRZ and markerbeds. Brine build up in the repository floor around panel closures.

At time 200 years, ROMPCS material transition to represent further creep closure, healed regions of the DRZ above and below the panel closures, lower shaft material transitions to represent creep closure.

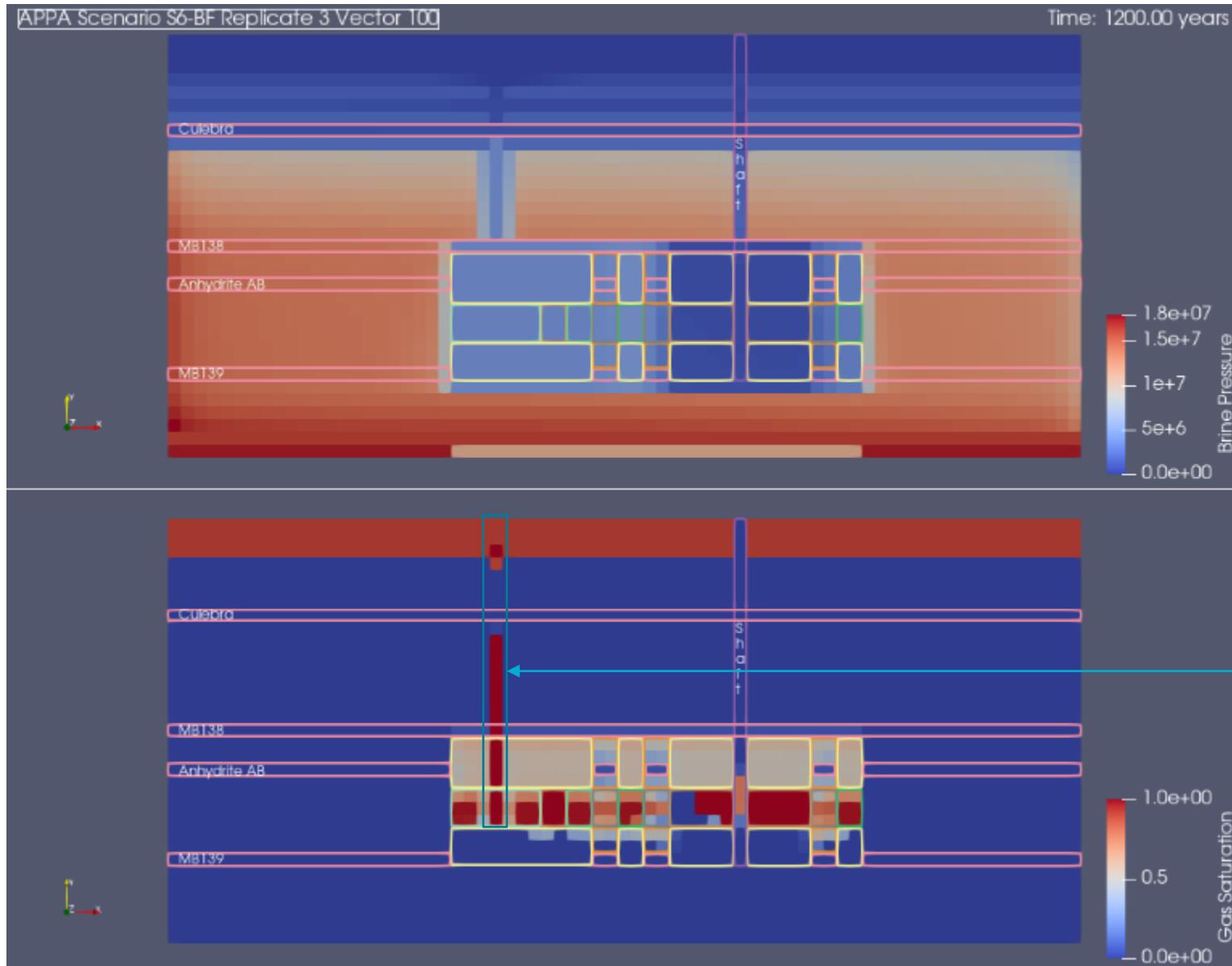
# Scenario S6-BF Replicate 3 Vector 100 – 1000 years



Still more drainage of the overlying DRZ and markerbeds. Brine pooling in the repository floor and against panel closures.

At time 1000 years E2 intrusion into the repository. An E2 intrusion does not intersect the pressurized brine pocket in the Castile formation, therefore the borehole is modeled as ending at the repository floor.

# Scenario S6-BF Replicate 3 Vector 100 – 1200 years

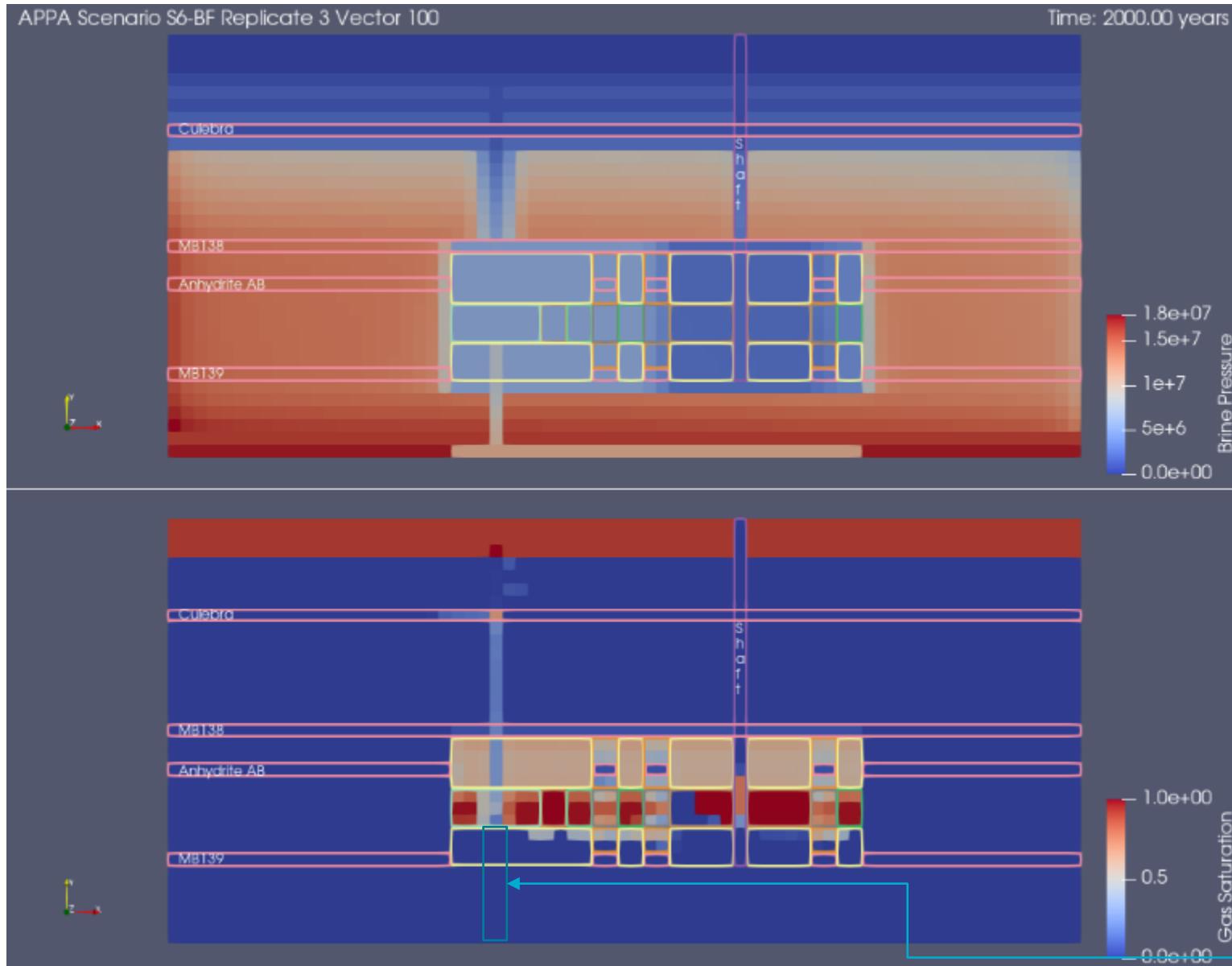


Borehole has filled with gas, and reduced some of the pressure in the repository.

At 1200 years, borehole plugs fail, entire borehole is modeled as sand.

Upper Borehole

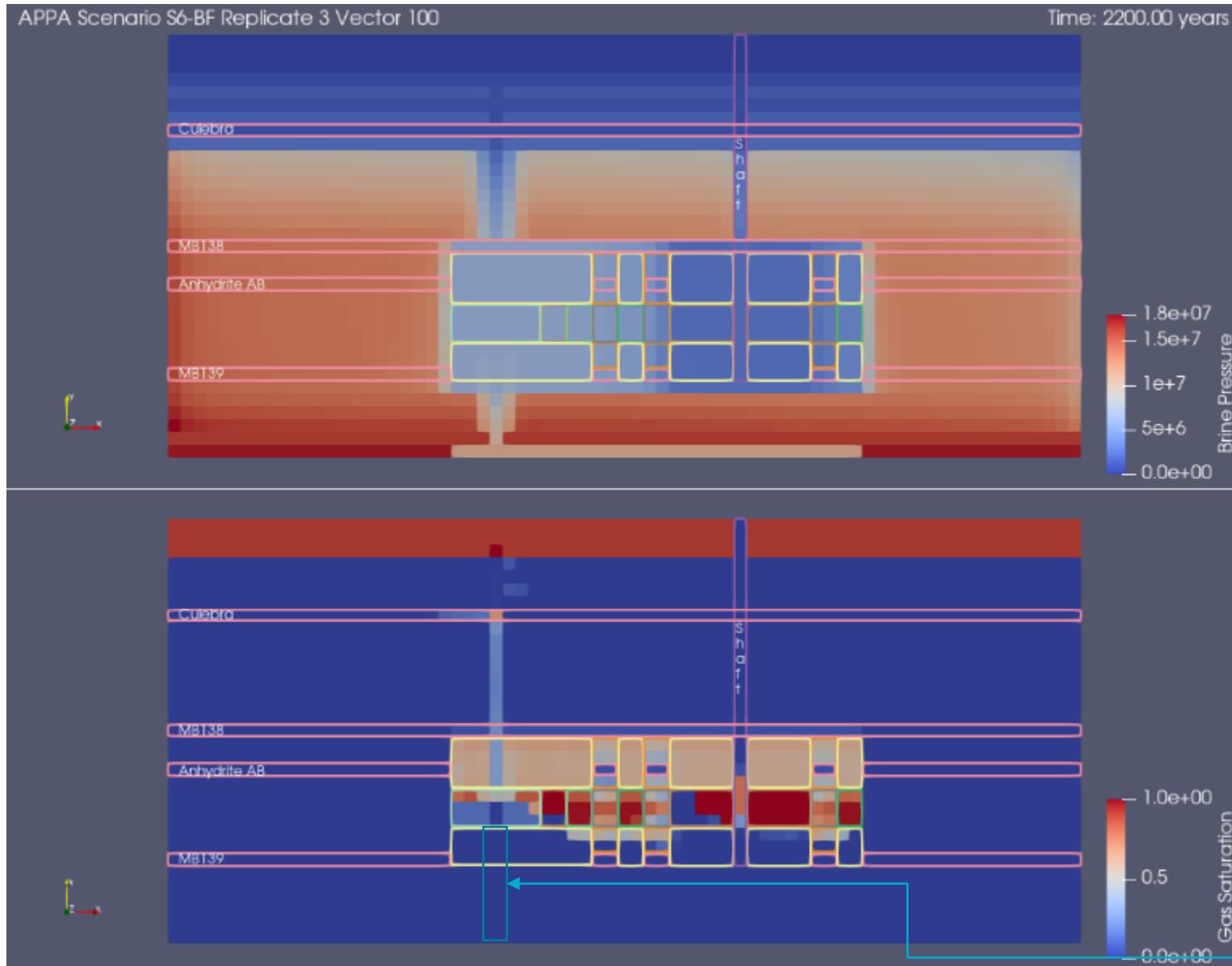
# Scenario S6-BF Replicate 3 Vector 100 – 2000 years



The degraded borehole has allowed communication with the Culebra, primarily allowing gas to flow into the Culebra and brine to flow from the Culebra to the repository.

At 2000 years, E1 intrusion occurs, the lower wellbore with open borehole material is placed down to the Castile reservoir, upper portion of borehole models original intrusion and stay as sand.

# Scenario S6-BF Replicate 3 Vector 100 – 2200 years

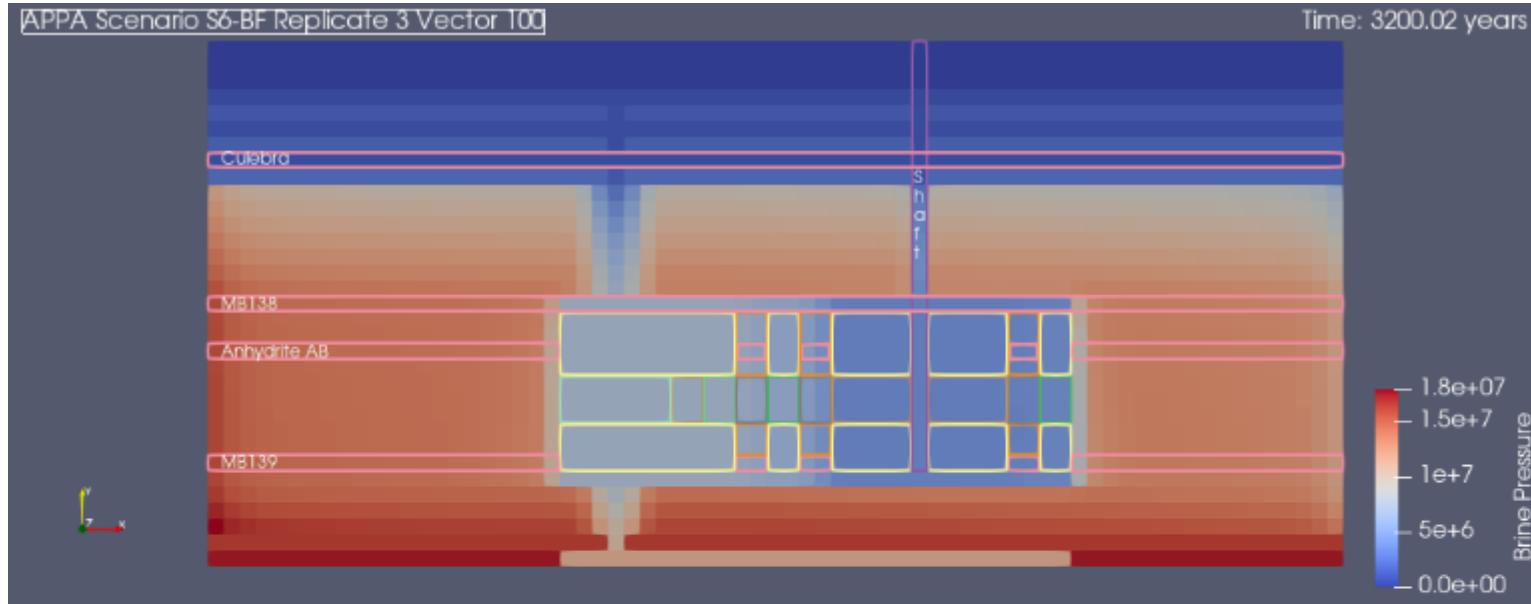


Brine from the Castile has started to flood the repository driving the brine saturation in the intruded waste panel (and South Rest-of-Repository) up.

At 2200 years, Lower borehole (E1 intrusion) plugs fail, degrades to sand.

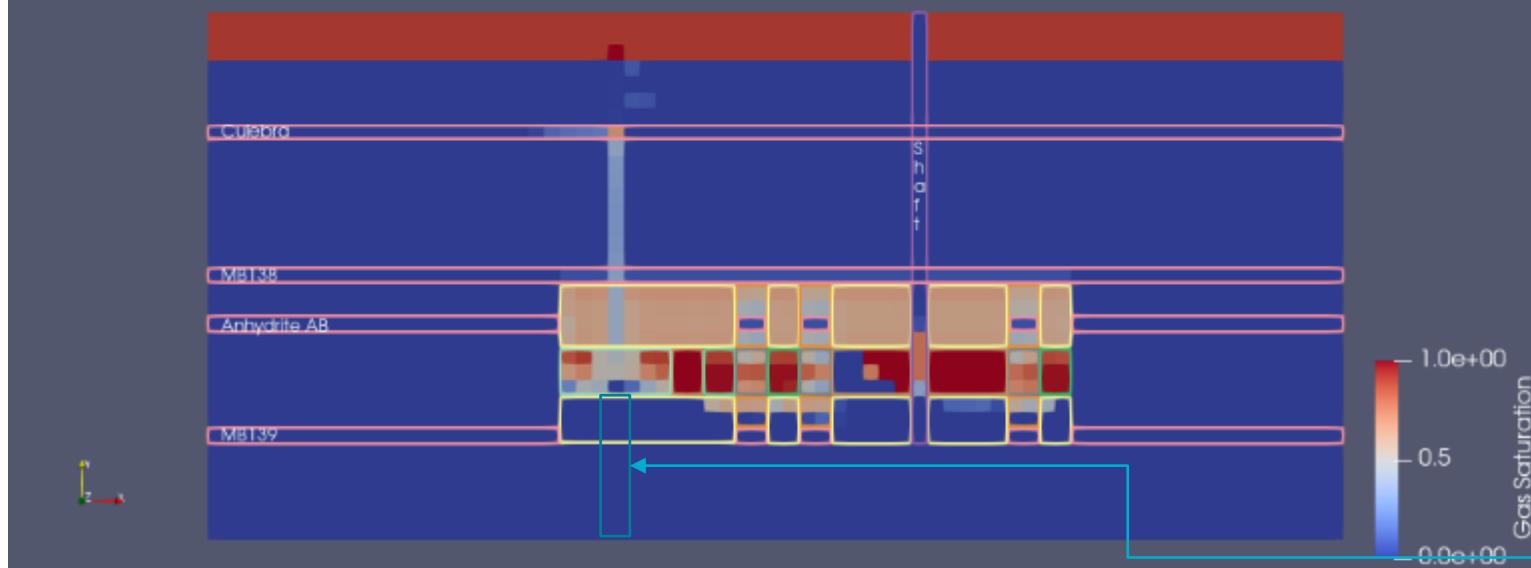
Lower Borehole

# Scenario S6-BF Replicate 3 Vector 100 – 3200 years



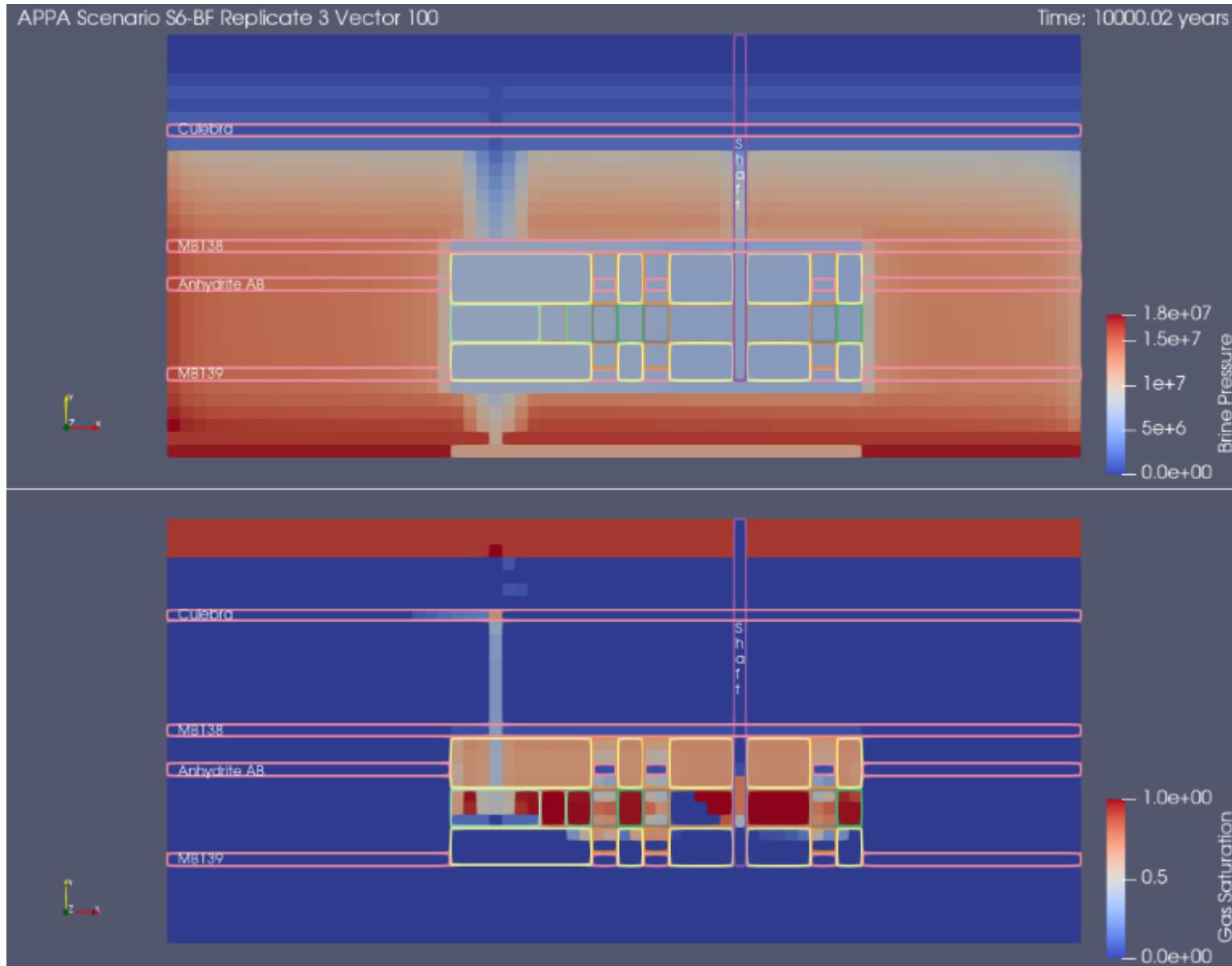
Brine and Gas flow up the borehole and into the rest of the repository have began reducing the brine pressure and saturation in the intruded Waste Panel and South Rest-of-Repository.

At 3200 years, Lower borehole (E1 intrusion) undergoes creep closure.



Lower Borehole

# Scenario S6-BF Replicate 3 Vector 100 – 10,000 years



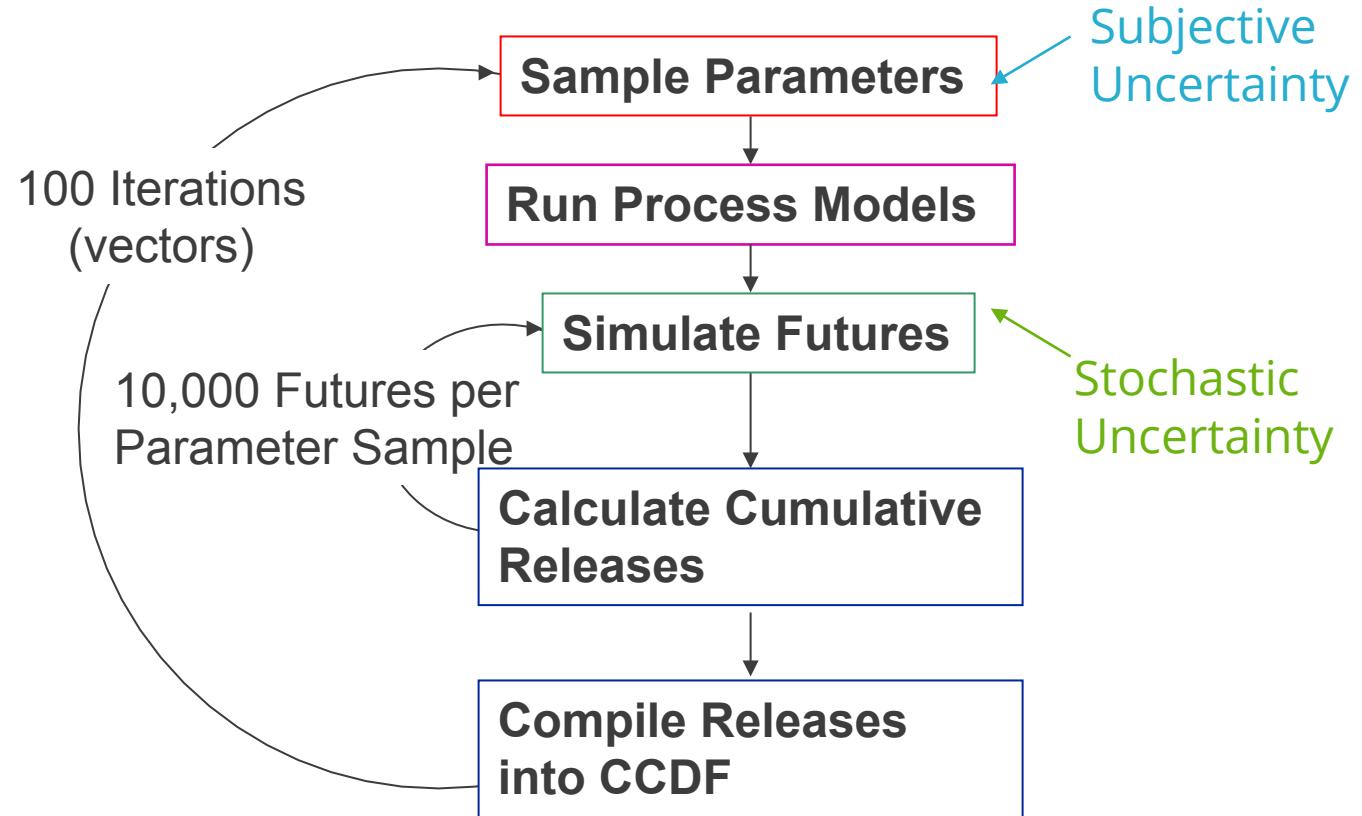
Brine pressures and saturations have reached a reasonably steady state.

End of simulation at 10,000 years.

# Terminology



- The APPA includes 64 uncertain parameters
  - A *vector* is a set of one value for every parameter
  - PA uses Latin hypercube sampling (LHS) to create a sample of size 100 (100 vectors)
  - LHS ensures that extremes of each parameter's range are included in the sample
  - The LHS technique used enforces any correlation between parameters (or lack thereof)
  - Three replicates (three independent LHS) are performed in order to generate a confidence interval on the mean CCDF
- A *future* is a sequence of borehole intrusions (and mining) events
  - PA uses random sampling to generate *futures* to estimate the CCDF of releases for each *vector*
- A *scenario* is a specific event (e.g., E1 intrusion at 1000 yr) for which results are calculated (e.g., pressure, saturation, brine flow, radionuclide transport) within the process models
  - Releases for each intrusion in a *future* are computed from *scenarios* using interpolation and time-shifting
  - Scenario results are calculated for each *vector*





## Issues in looking at single vector results

The LHS sample size of 100, generates 100 vectors that represent the system uncertainty as an ensemble. Vectors are not independent samples as you would get in a simple random sampling method. PA generally looks at results as an ensemble.

The grid blocks are not shown to scale due to the highly variable grid block sizes. If the grid blocks were scaled to size, features like the borehole would be too small to see.

The 1° dip will result in more elevation change across large grid blocks than small grid blocks. The pooling of brine in the Operations/Experimental areas might seem exaggerated compared to other areas, due to the logical unit display of these grid blocks.

Time is not normalized, it follows the simulation time steps. This means in the animation time will slow down around events with more changes (like intrusion) and speed up during times of little change (late time).

The replicate 3 vector 100 example shown was chosen as being close to the mean output for some simulation results. As shown in the horsetail plots, there is a lot of uncertainty in the ensemble simulation results, other vectors can show much different behavior.

# Peer Review Panel follow up question



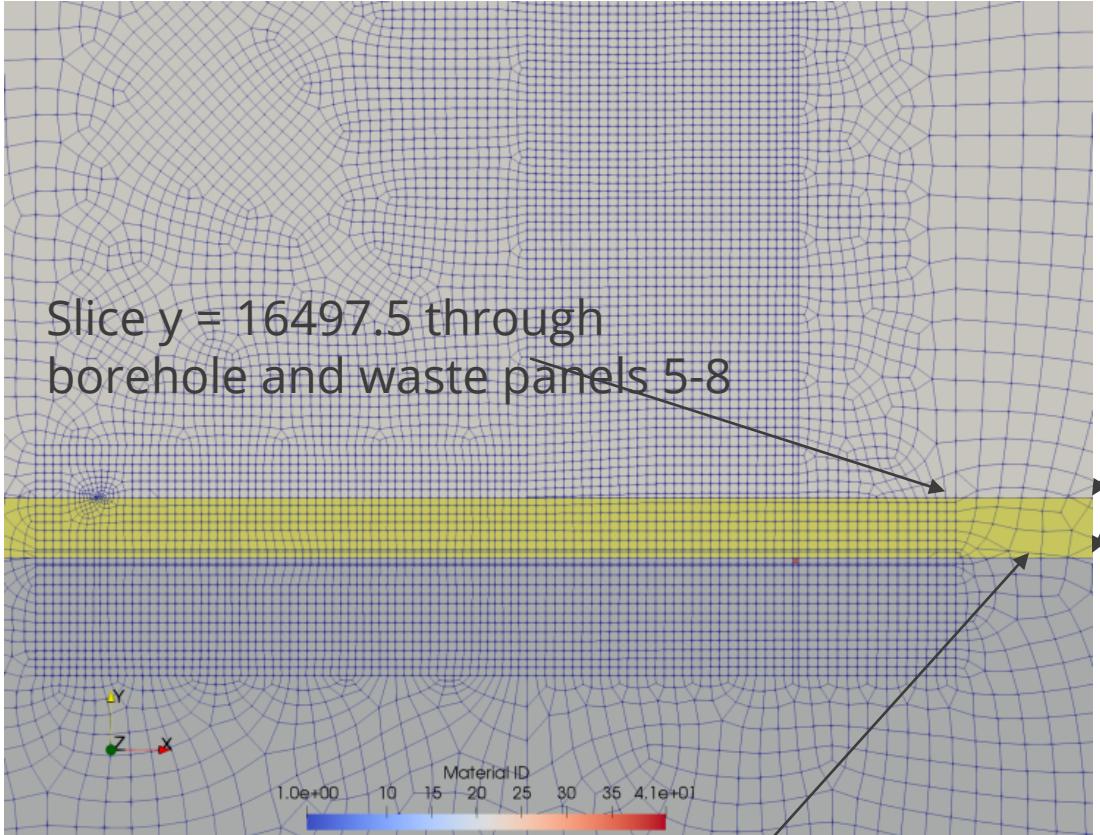
3. Plots of the numerical meshes that are used in the Repository Fluid Flow model and the two DBR models.
  - A. Provide high-resolution images so that meshes near the repository can be seen and label the numerical mesh with geomaterial types.

This comment has been clarified as a desire for high-resolution images of the PFLOTRAN 3D mesh near the repository. The following slides will provide these images.

Minor grid orientation effects around the repository features are seen. The effects are not seen around the borehole. These effects are discussed in LaForce et al. (2020).

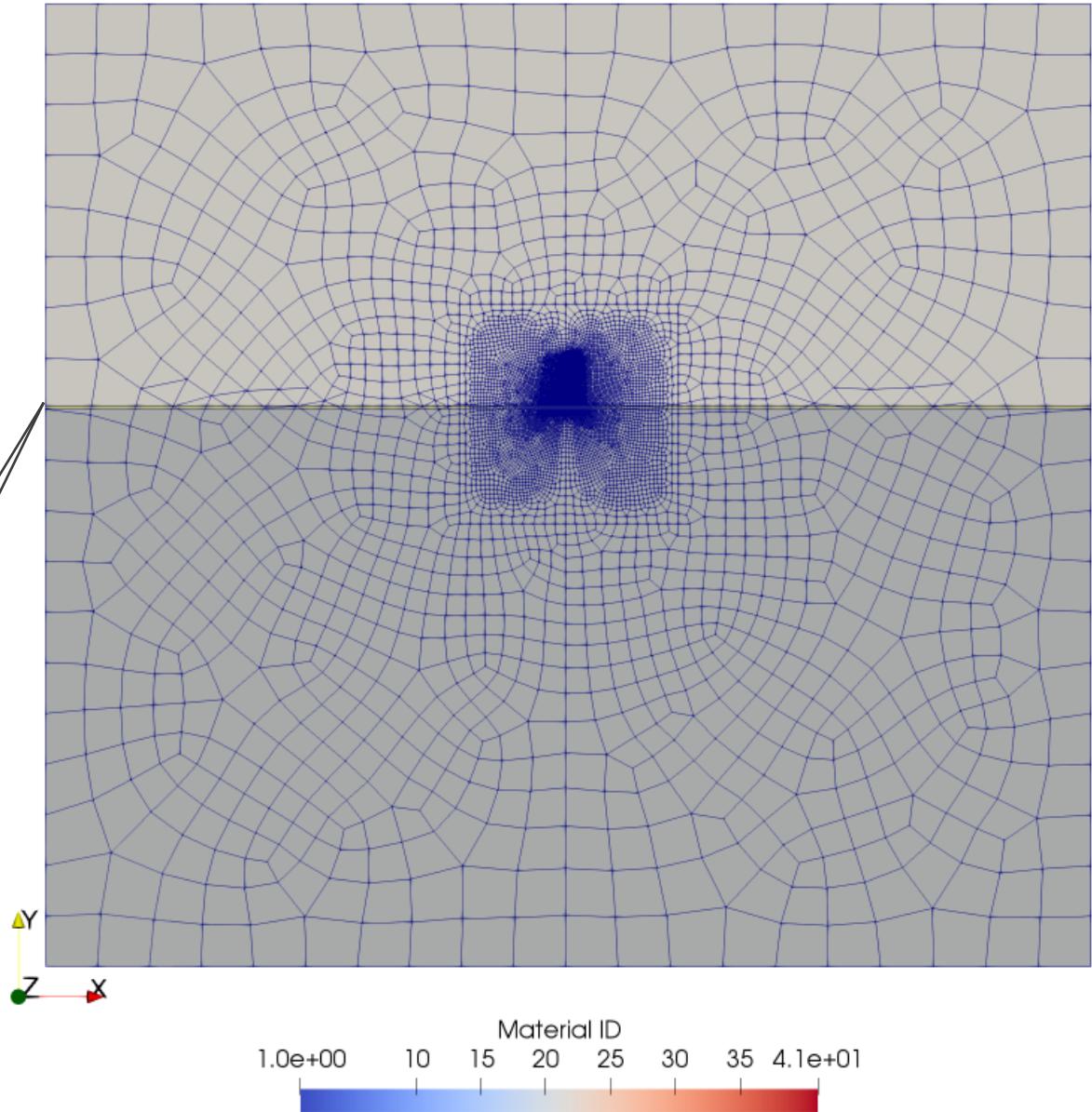
LaForce, T., C. Hansen, E. Stein, 2020. Development of 3D model of the WIPP with proposed additional panels. Albuquerque, NM: Sandia National Laboratories. ERMS 573646

# Top Surface



Slice  $y = 16497.5$  through  
borehole and waste panels 5-8

Slice  $y = 16402.5$  through  
midline of waste panels 9 and  
10



# Slice $y = 16402.5$ through midline of WP 9 and 10



Full model



Repository area only

Dark blue = Salado

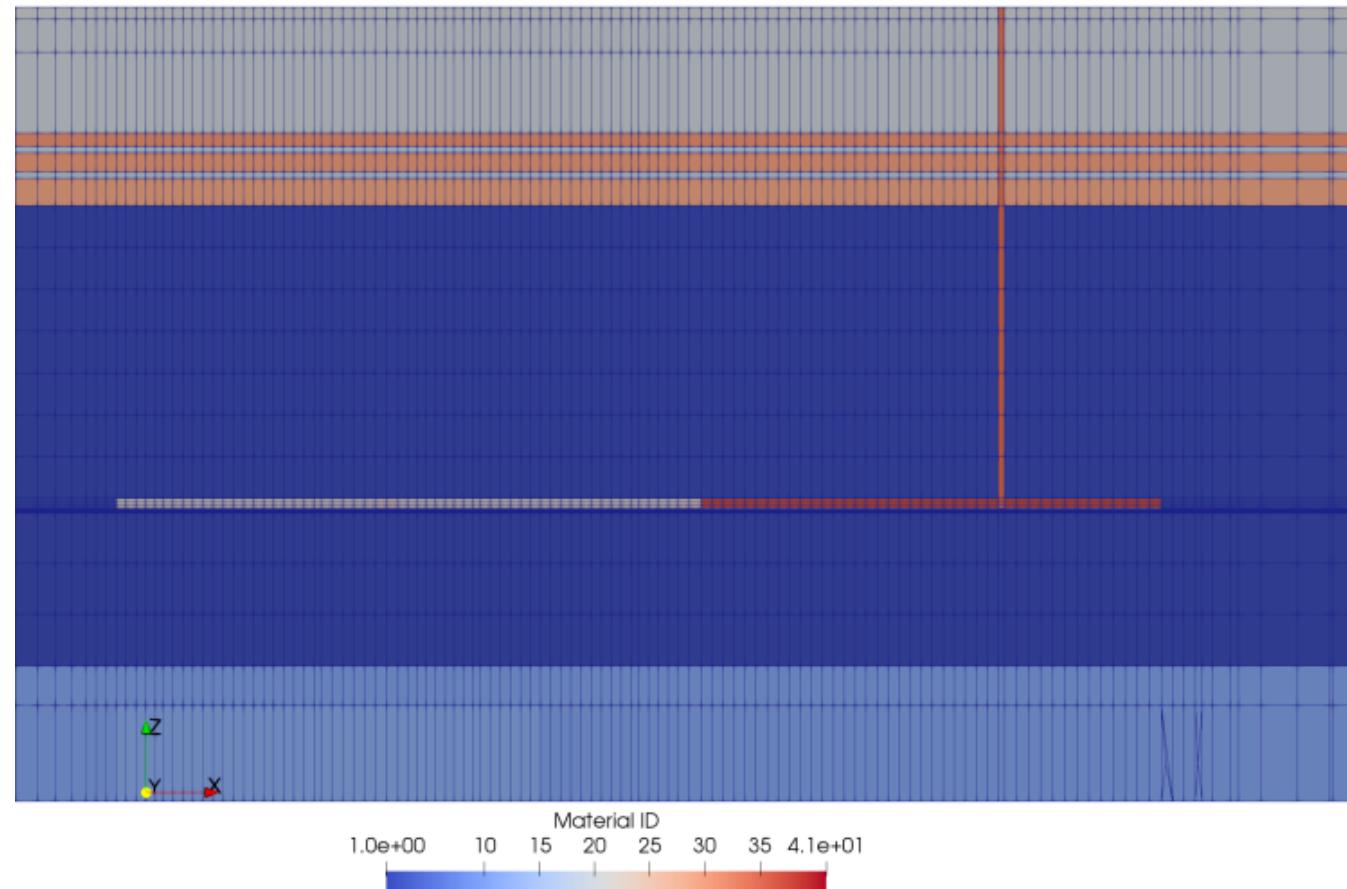
Light orange and gray = overlying sediments

Light blue = Castille reservoir

Dark orange = Shaft

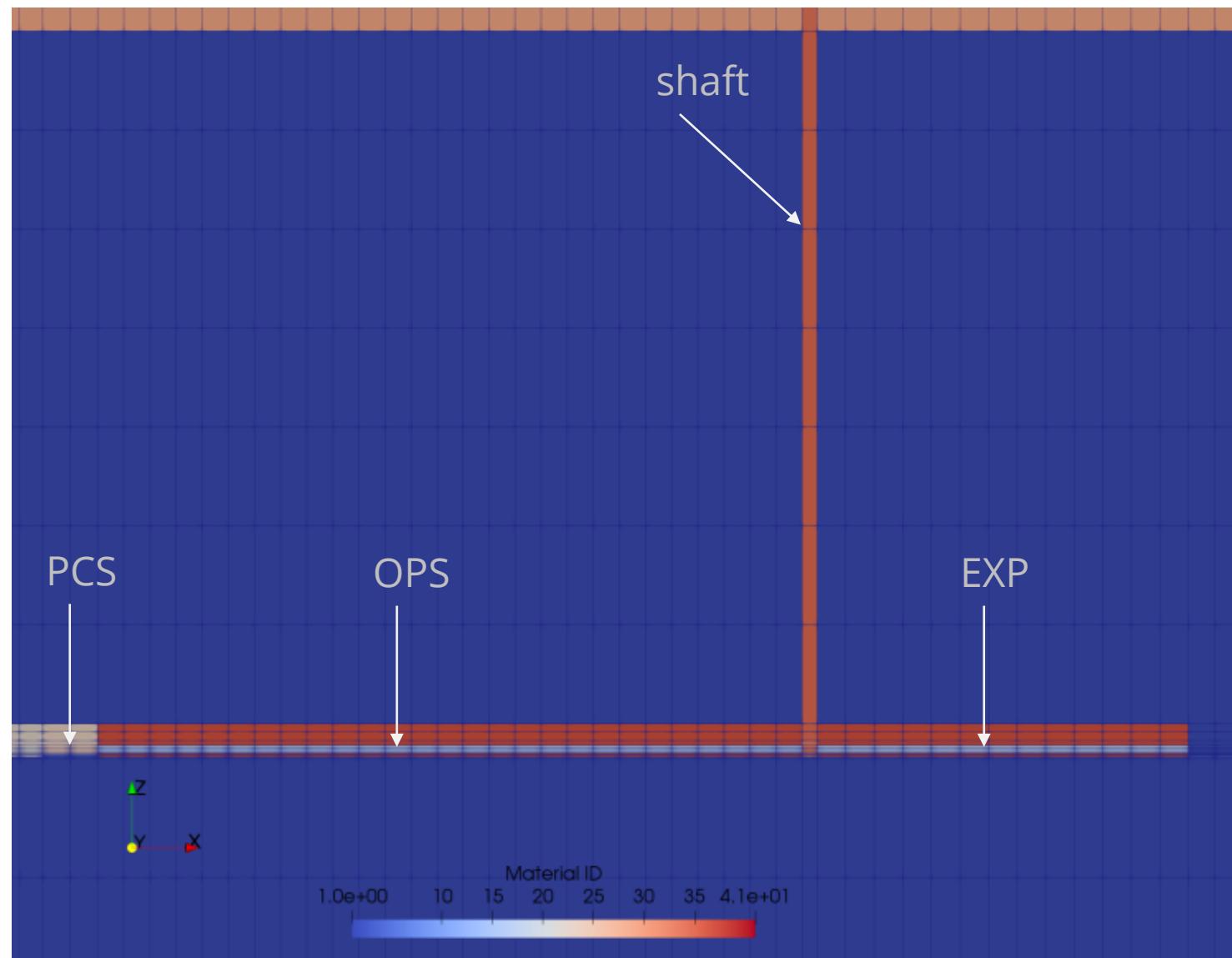
Red = Damage zone over Operations (OPS) and Experimental (EXP) areas

Pink/gray = Damage zone over waste panel (WP) 9-10 and Panel Closures (PCS)



# Slice $y = 16402.5$ through midline of WP 9 and 10

Area near OPS and EXP only  
Dark blue = Salado  
Dark orange = shaft  
Red = damage zone over OPS and EXP  
Light blue = OPS and EXP



# Slice $y = 16497.5$ through borehole and WP 5-8



Area near WP only

Dark blue = Salado

Dark orange and gray = overlying sediments

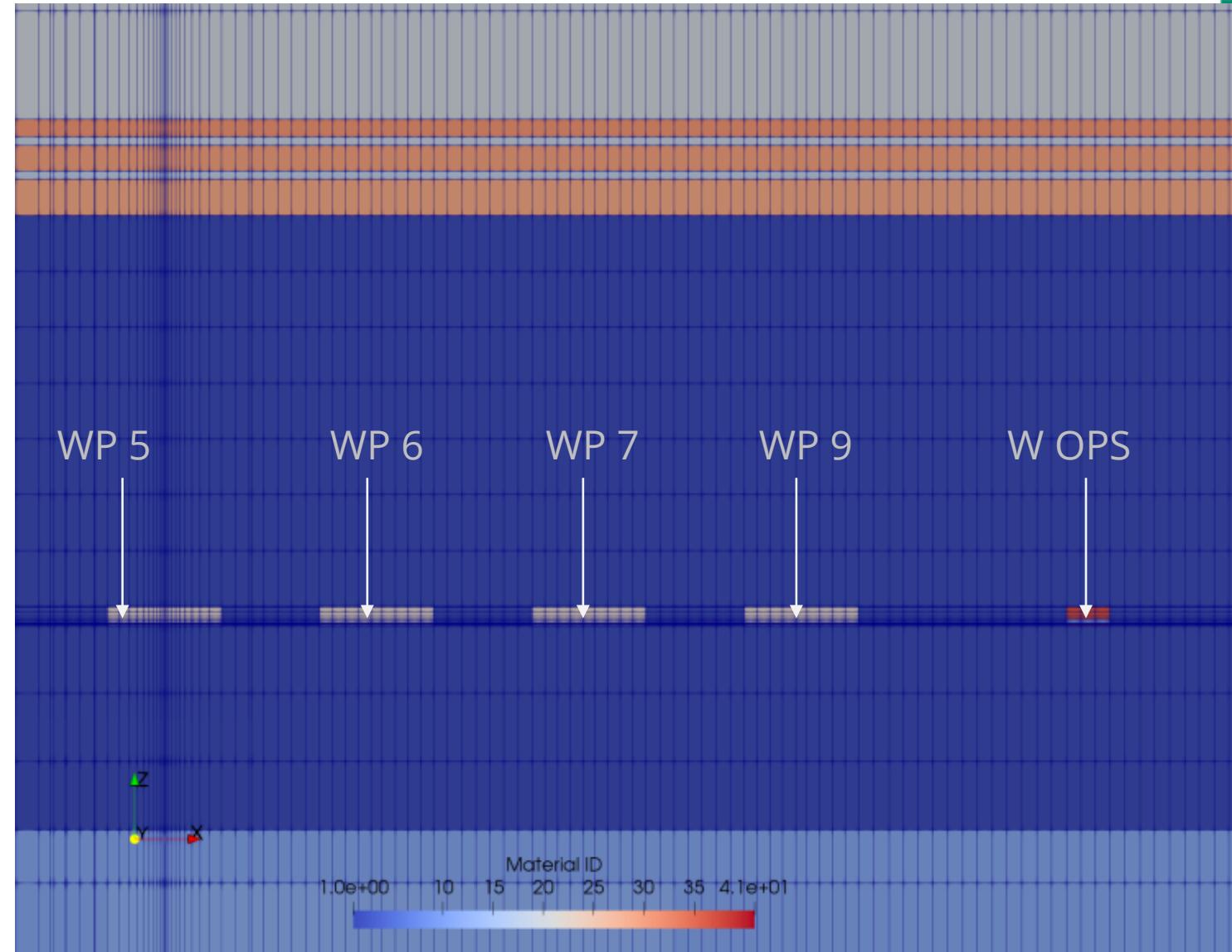
Light blue = Castille reservoir

Pink/gray = damage zone over WP

Light gray = WP

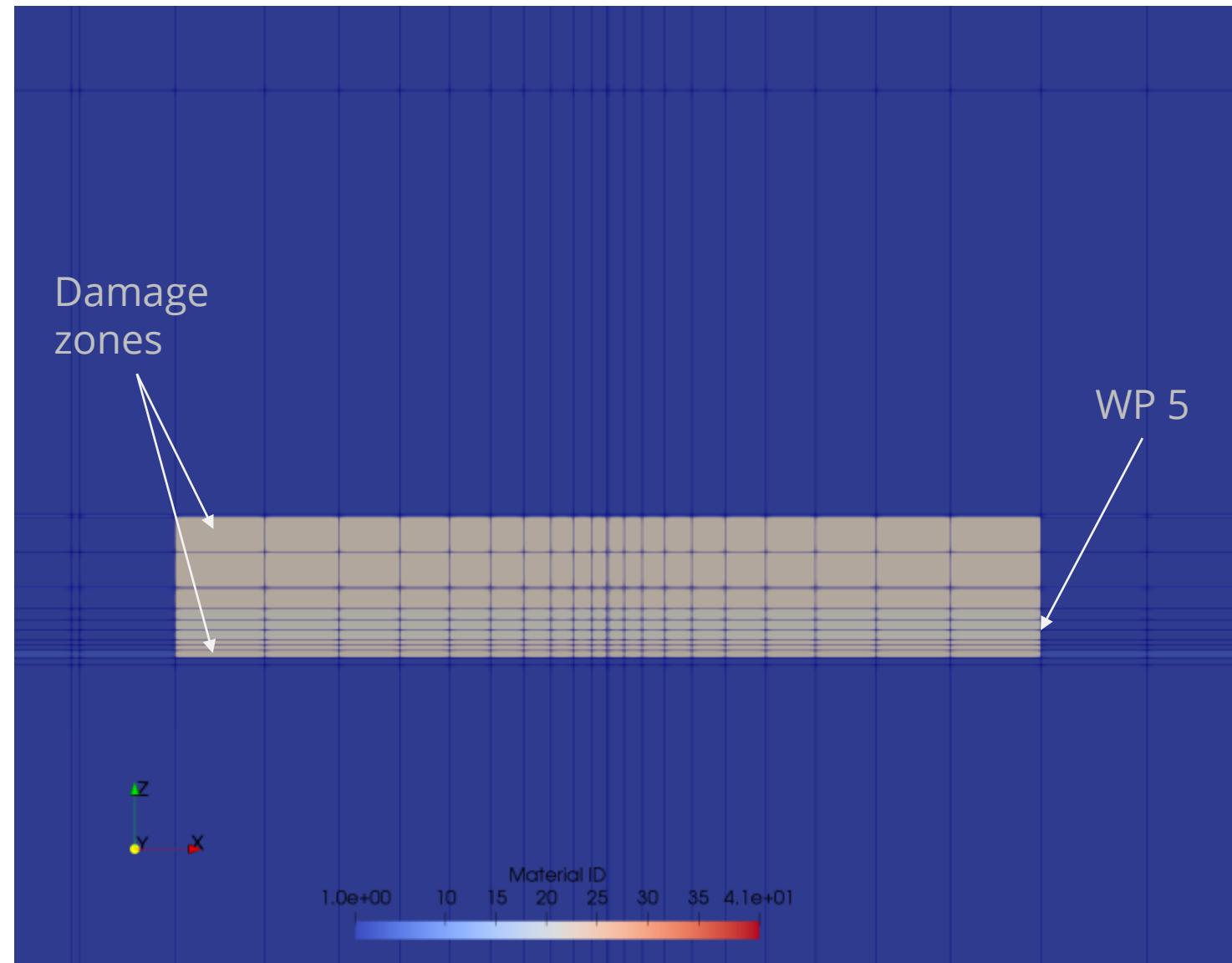
Red = damage zone over W OPS

Light blue = W OPS

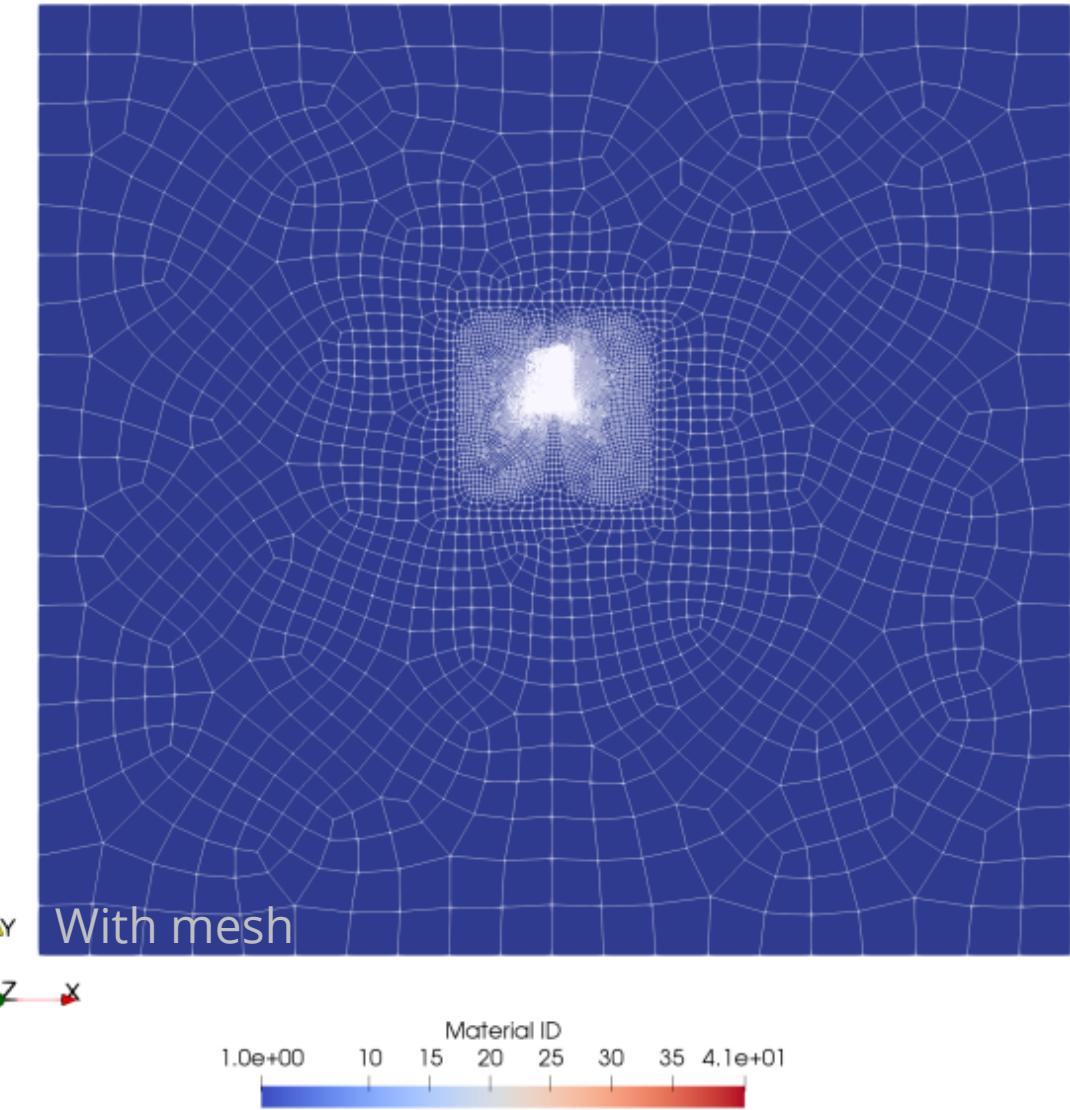
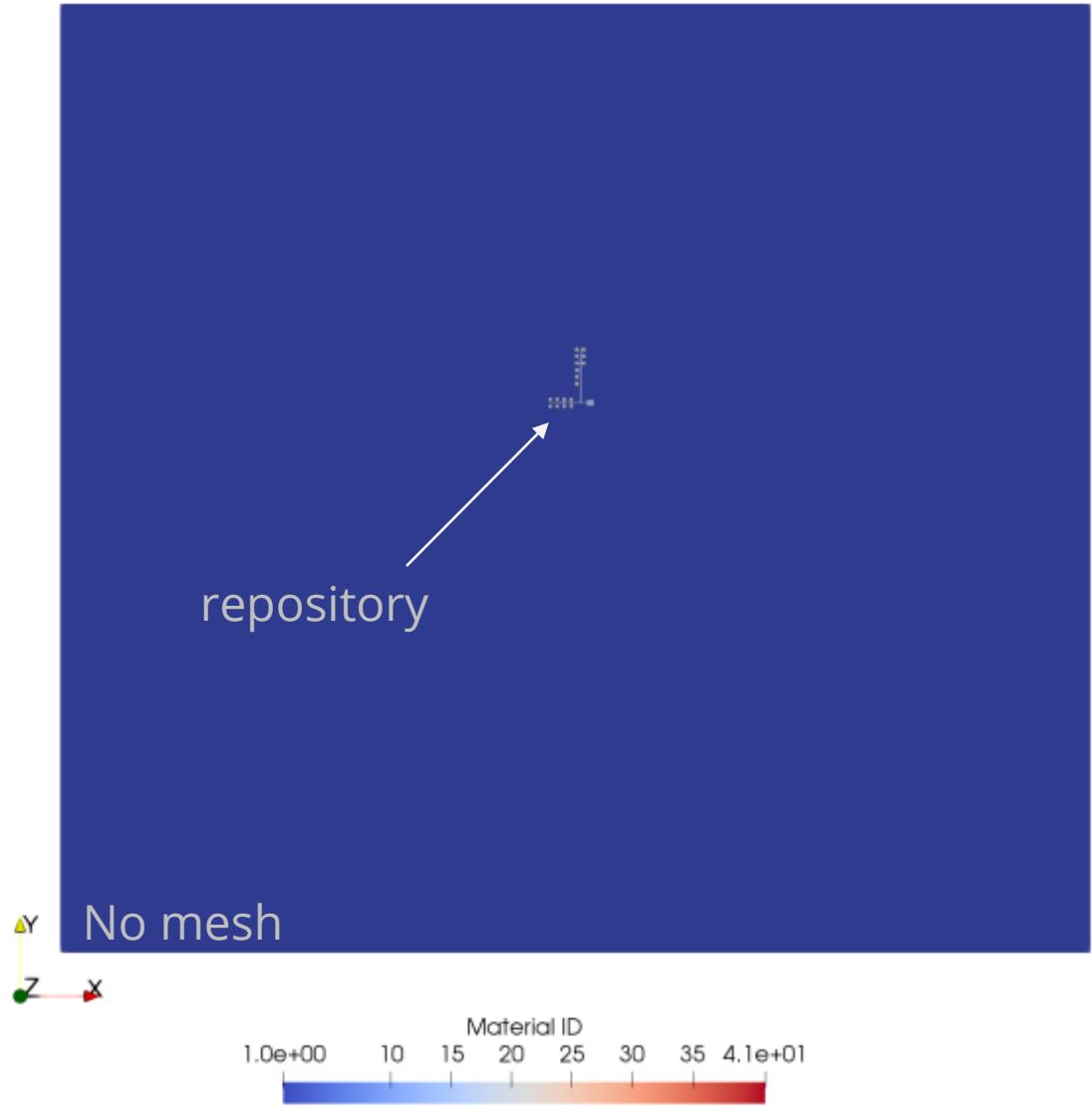


# Slice $y = 16497.5$ through borehole and WP 5-8: WP 5 only

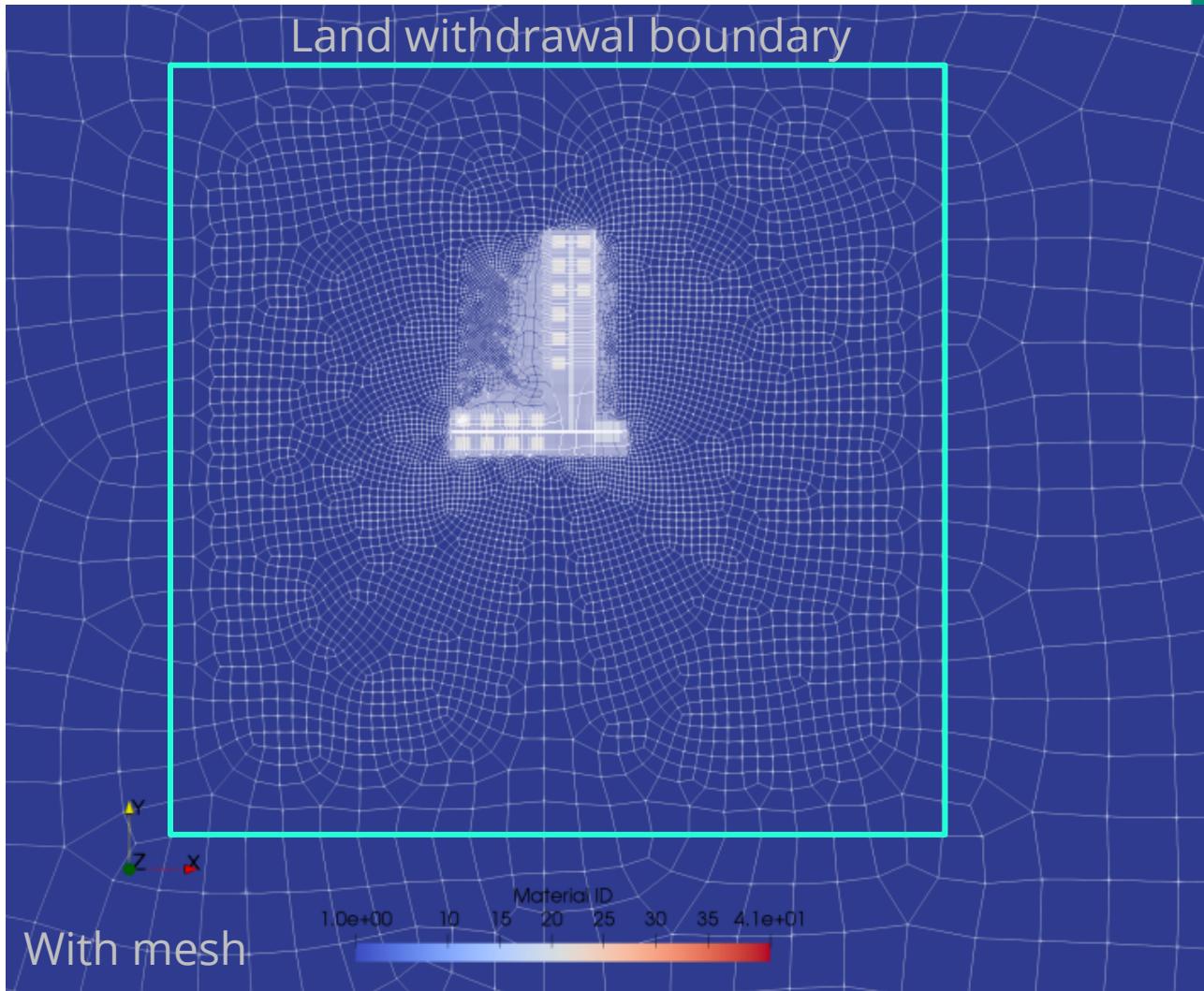
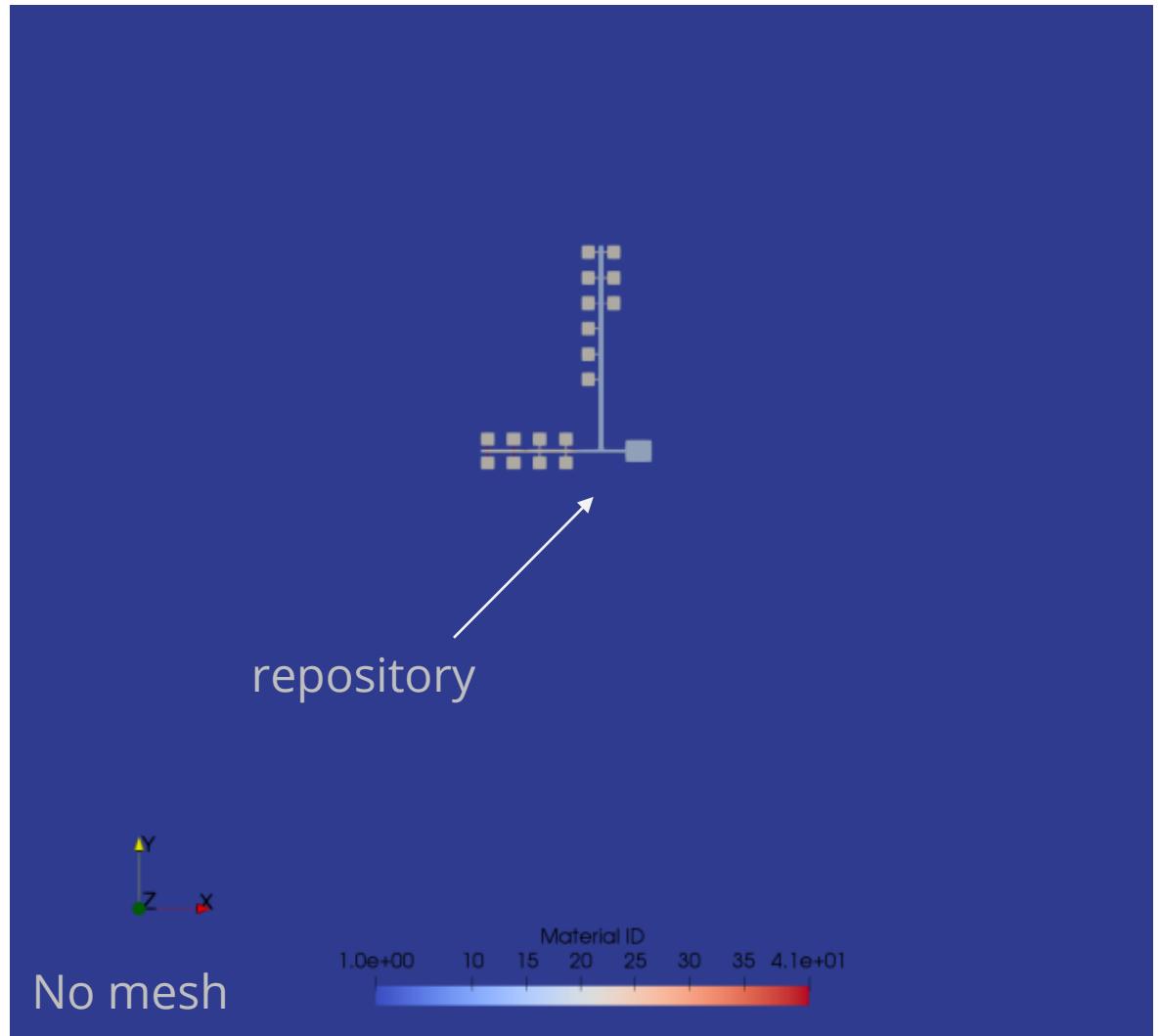
Area near WP only  
Dark blue = Salado  
Pink/gray = Damage zone over WP  
Light gray = WP



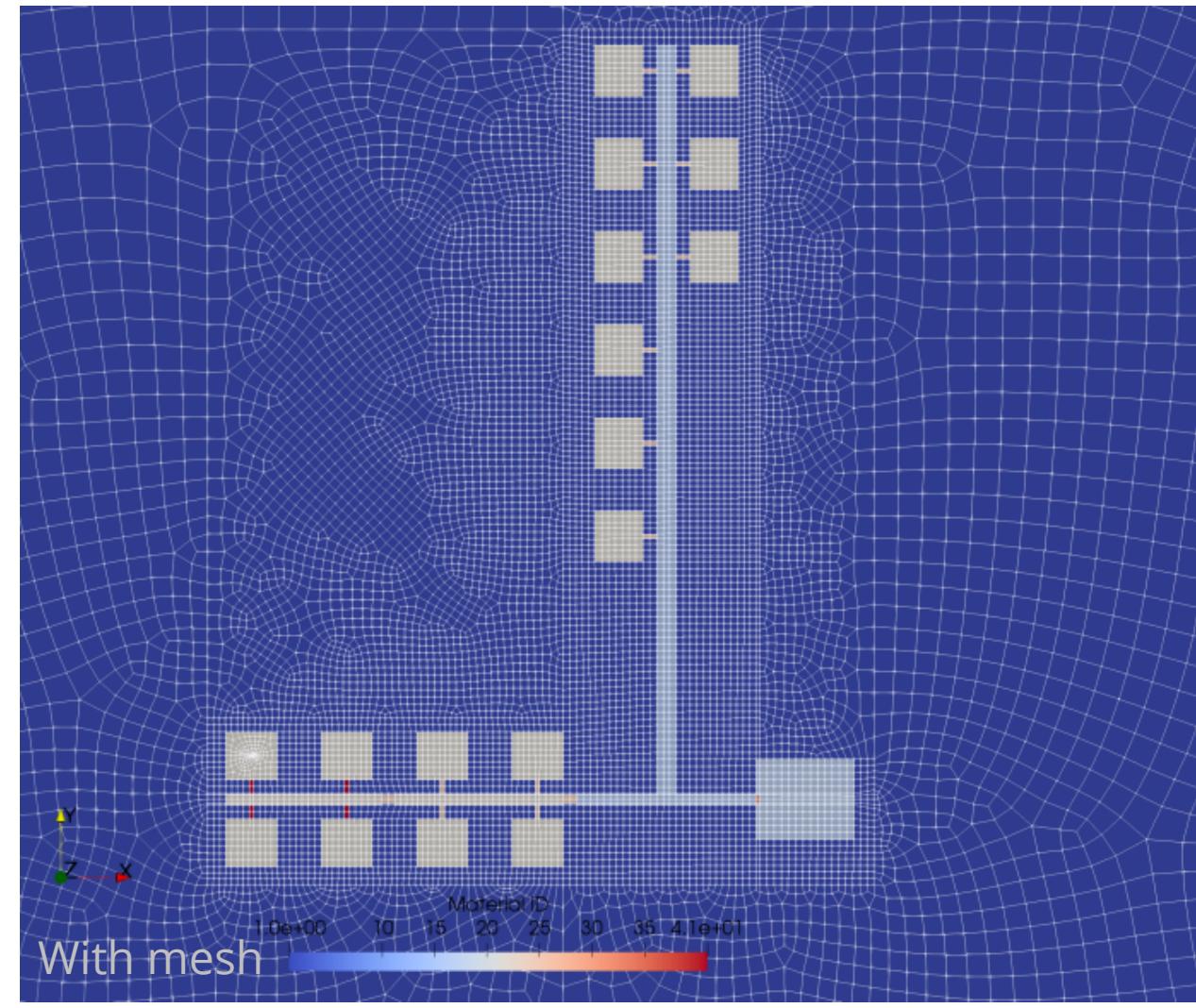
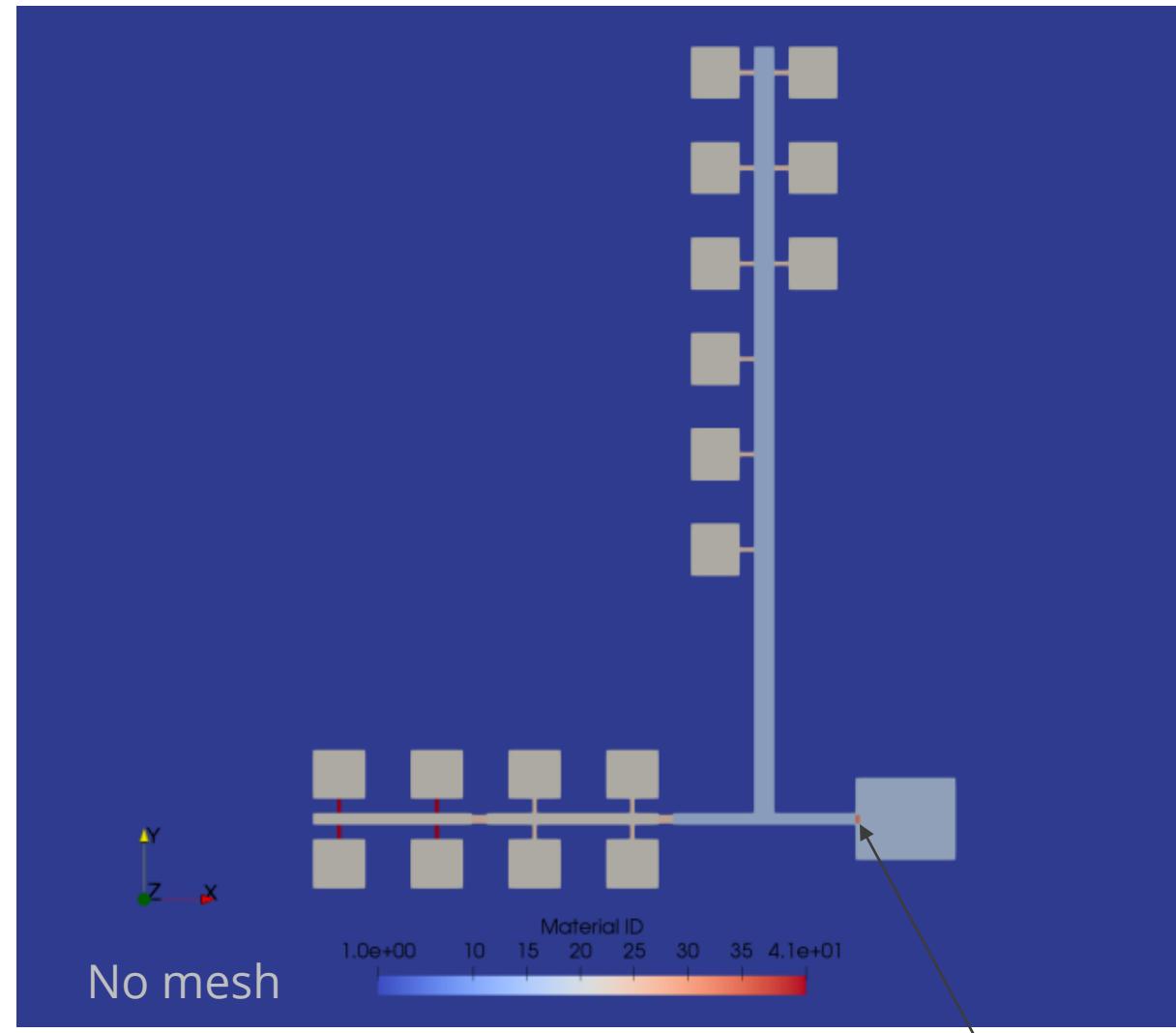
# Slice through top of repository at z=382.5: full model



# Slice through top of repository at z=382.5: LWB

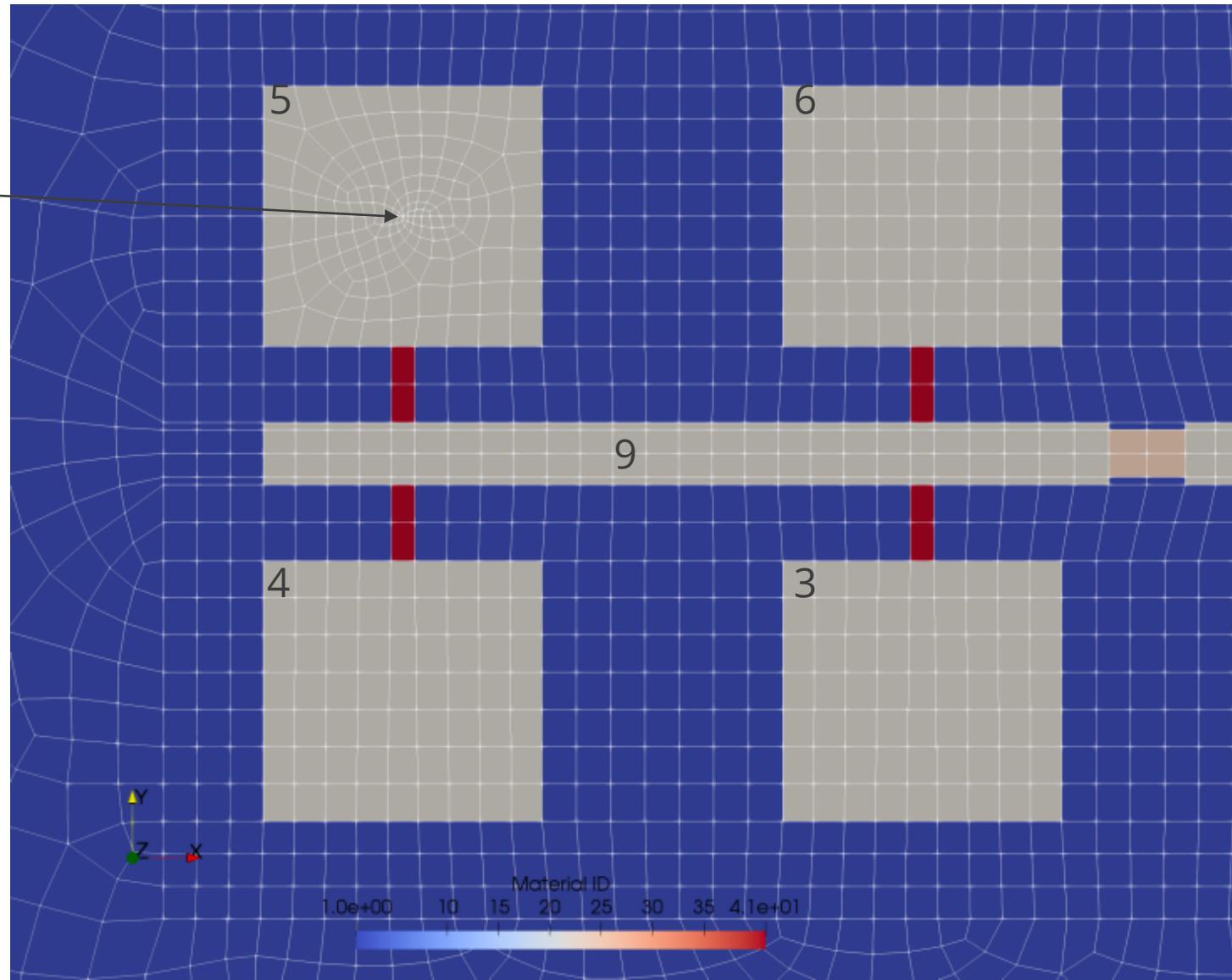


# Slice through top of repository at z=382.5: repository



# Slice through top of repository at z=382.5: WP 3-6 and 9

Borehole



Blue = Salado  
Gray = Waste Panels  
Red = Abandoned Panel Closures  
Pink = Panel Closures (PCS)

# Peer Review Panel follow up question



4. Please provide the Sandia definitions for Eulerian and Lagrangian grid deformation and specify which is being used in the above.

Response:

Grid deformation happens in the rock mechanics modeling used to generate the porosity surface. The outputs of the rock mechanics modeling are reported in terms of Eulerian porosity. The Salado flow model does not employ any grid deformation, simply a dynamic porosity that is a function of time and pore pressure. The porosity from the rock mechanics model is translated into a Lagrangian porosity (current pore volume divided by original room volume) for use in BRAGFLO. When the porosity is reported from the BRAGFLO model it is in terms of the Lagrangian porosity.

See Appendix PORSURF of the CRA-2014 submittal for more information on the rock mechanics model:

DOE(2014) CRA-2014 Appendix-PORSURF - [https://wipp.energy.gov/library/CRA/CRA-2014/CRA/Appendix\\_PORSURF/Appendix\\_PORSURF.htm](https://wipp.energy.gov/library/CRA/CRA-2014/CRA/Appendix_PORSURF/Appendix_PORSURF.htm)



## Peer Review Panel follow up question

6. Please provide a technical description and/or references for the details of the numerical methods used in BRAGFLO. This should include:

A. Spatial and temporal discretization methods

The numerical methods used in BRAGFLO are described in Chapter 4 of the User's Manual.

B. Linearization method (e.g., Newton-Raphson method, etc.)

The numerical methods used in BRAGFLO are described in Chapter 4 of the User's Manual.

C. Linear algebra solution method(s)

The numerical methods used in BRAGFLO are described in Chapter 4 of the User's Manual. The banded LU solver is used for WIPP PA calculations.

(Continued)



## Peer Review Panel follow up question

6. Please provide a technical description and/or references for the details of the numerical methods used in BRAGFLO. This should include:

D. Numerical convergence criteria and values used during time-stepping

Numerical Controls are described in Section 7.2.7 of the BRAGFLO User's Manual. Number of digits of accuracy to the right of the decimal in the change in gas saturation (EPSNORM(1)) is 3.0. Maximum relative change in brine pressure allowed over a time step (EPSNORM(2)) is 0.01. The minimum normalized gas saturation residual (FTOLNORM(1)) is set to 0.01, the minimum normalized brine pressure residual (FTOLNORM(2)) is set to 0.01. Both convergence criteria need to be satisfied (ICONVTEST=1).

(Continued)

# Peer Review Panel follow up question



6. Please provide a technical description and/or references for the details of the numerical methods used in BRAGFLO. This should include:

**E. Details of adaptive time-stepping (if used)**

Time stepping controls are described in section 7.2.2 of the BRAGFLO User's Manual. The initial time step (DELT) is set to 8.64 s (0.001days). The minimum time step (DELTMIN) is 8.64e-04 s, the maximum time step (DELTMAX) is 3.1557e8 s. The maximum fractional increase in time step (DTIMEMAX) is set to 1.25. The time step reduction factor (DELTFACTOR) when non-convergence occurs is set to 0.5 (DELTFACTOR is defined in section 7.2.7 of the BRAGFLO UM).

**F. Methods used to recover from non-convergence during a time-step**

If a time-step iteration fails to converge the time step reduction factor is applied and the new time step is attempted. If the time step is at the minimum, or the maximum time steps has been reached, the simulation will fail. Two fall back simulations are defined. First both of the normalized residual tolerances are increased to 0.1. The second fallback is to require only one of the convergence criteria to be met at each timestep (ICONVTEST=0).