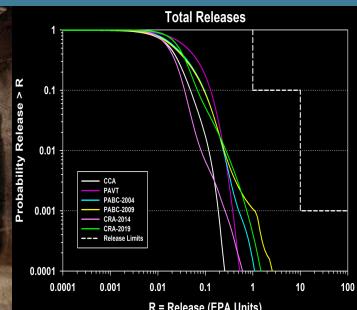
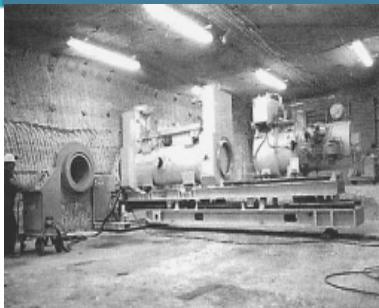




PFLOTRAN 3D Meshing and Modeling



Tara LaForce, Emily Stein, Cliff Hansen and
Heeho Park

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.



Objectives

Motivation: The proposed addition of new waste panels to the Waste Isolation Pilot Plant (WIPP) challenges the modeling assumptions inherent in the two-dimensional (2D) flared grid used in PA calculations.

Current objective:

Simulate repository with additional panels on the 3D grid to support the APPA peer review by corroborating flow calculations on 2D-flared grid

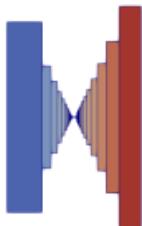
Create a fully 3D modeling domain that is representative of the repository

- Improved simulation and resolution of lateral flow
- Consistent with existing 2D-flared model and other WIPP modeling studies

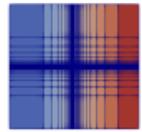
Meshes with identical repository



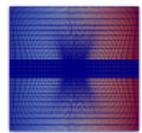
Full meshes



2D

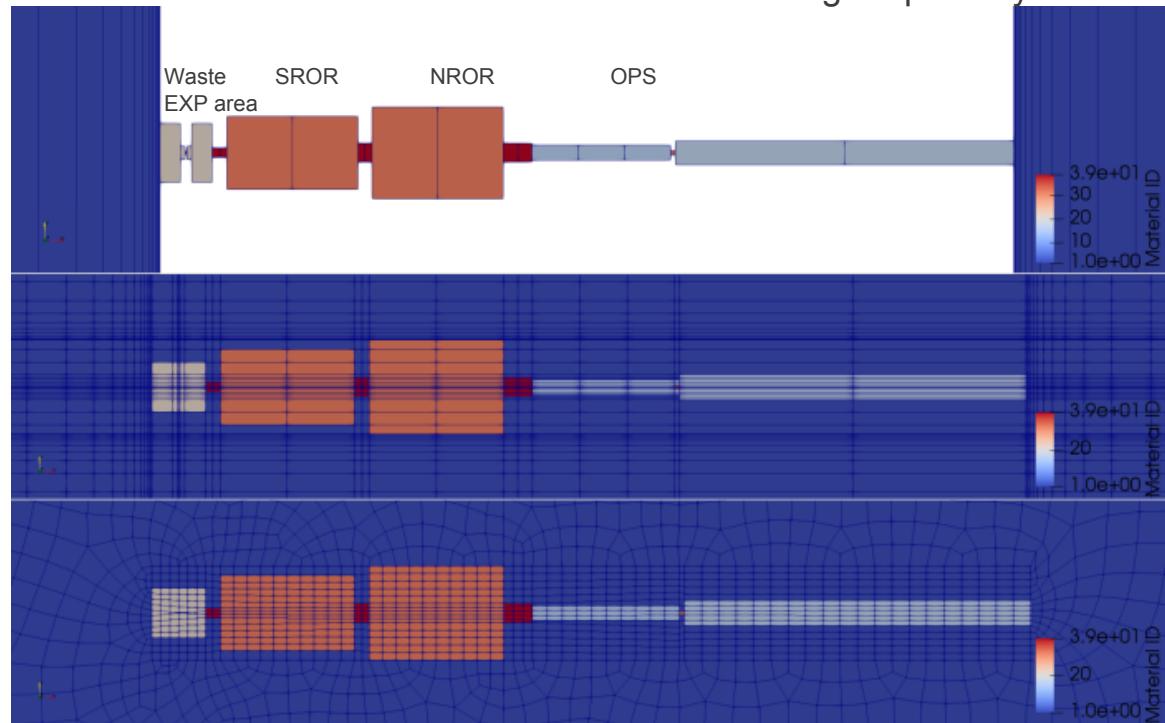


Explicit
unstructured



Spider

Slice at $z=382.5$ through repository



Top figures: after Stein et al 2018



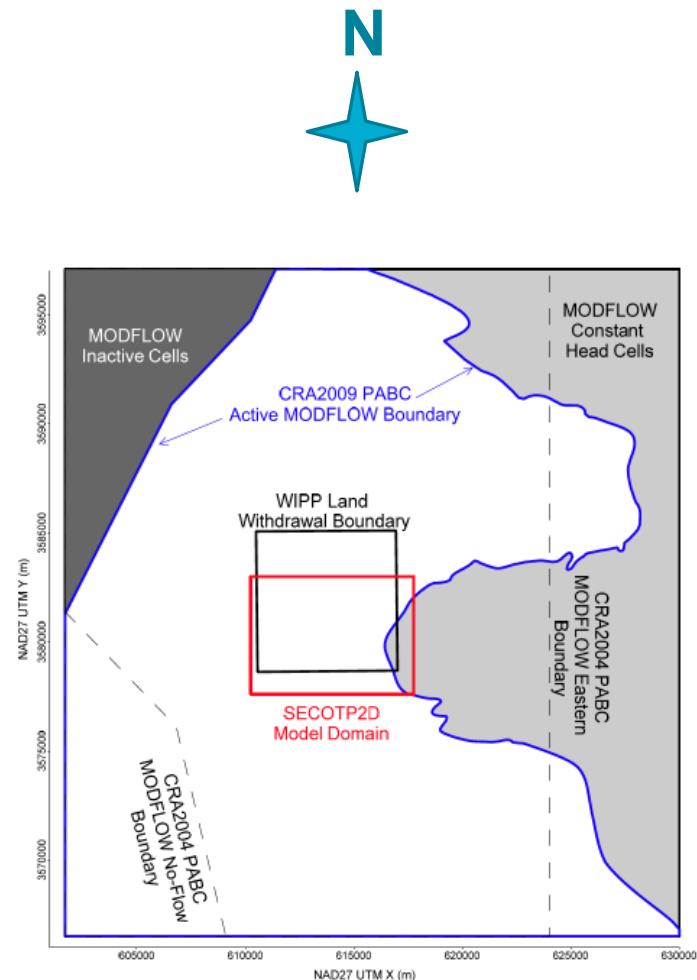
Outer domain boundary

No unique way to go from 2D flared to 3D boundary

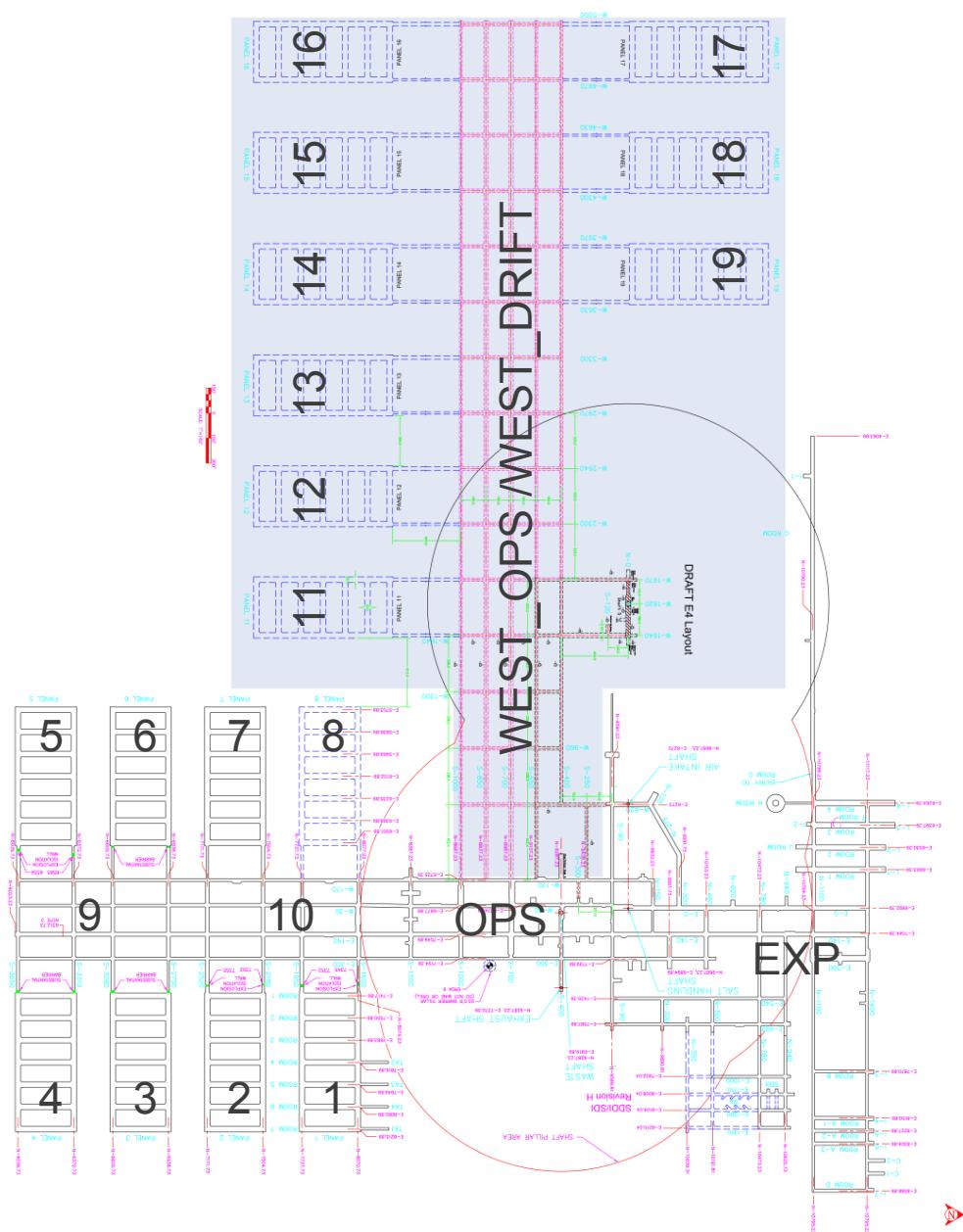
3D Culebra flow modelling offers a solution
(Kuhlman, 2010)

- 28.3 x 30.7km
- Extends to the east where Culebra permeability goes to near zero (light gray area)
- Extends to west at Nash Draw flow boundary (dark gray area)

LWB not in center of domain and repository is not in the center of the LWB



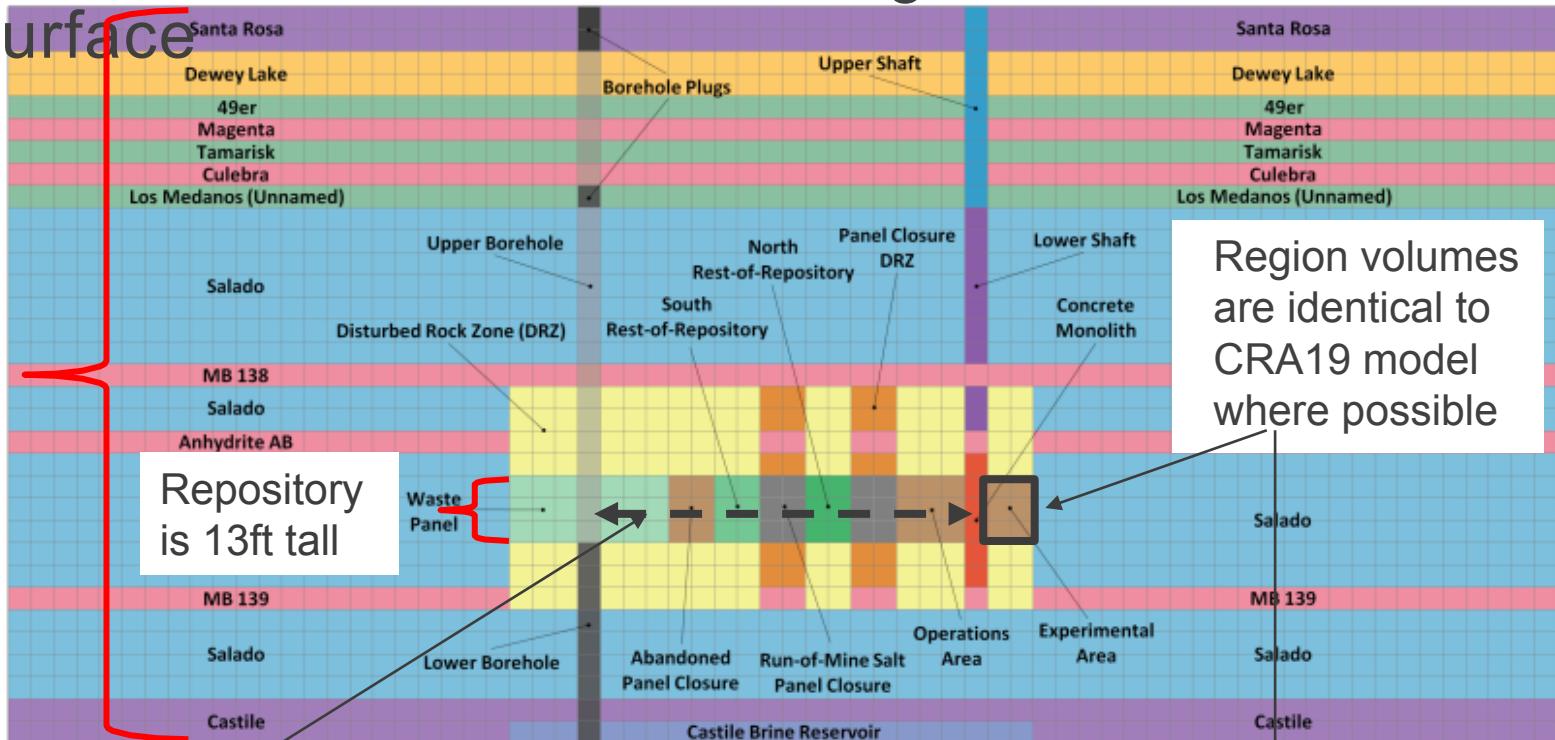
Footprint with Additional Panels



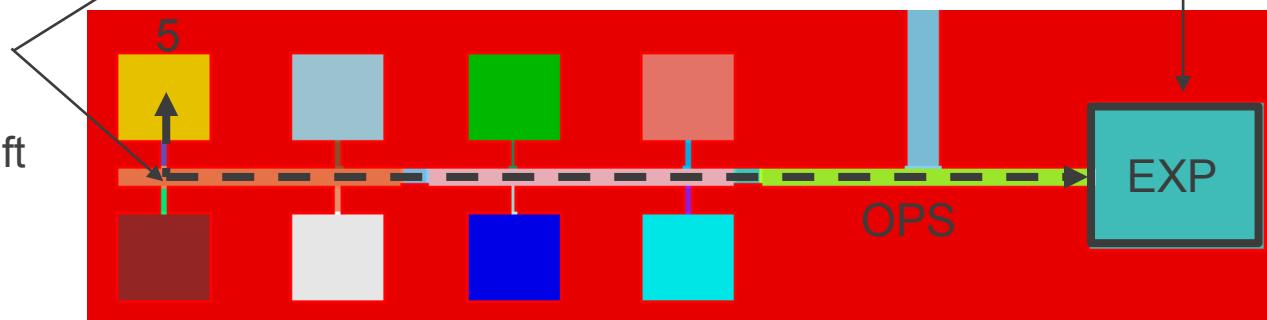
3D simulation model: Consistent with BRAGFLO models and current understanding of the subsurface



Vertical
mesh
spacing is
preserved



Distance from
borehole to shaft
is identical to
CRA19 model





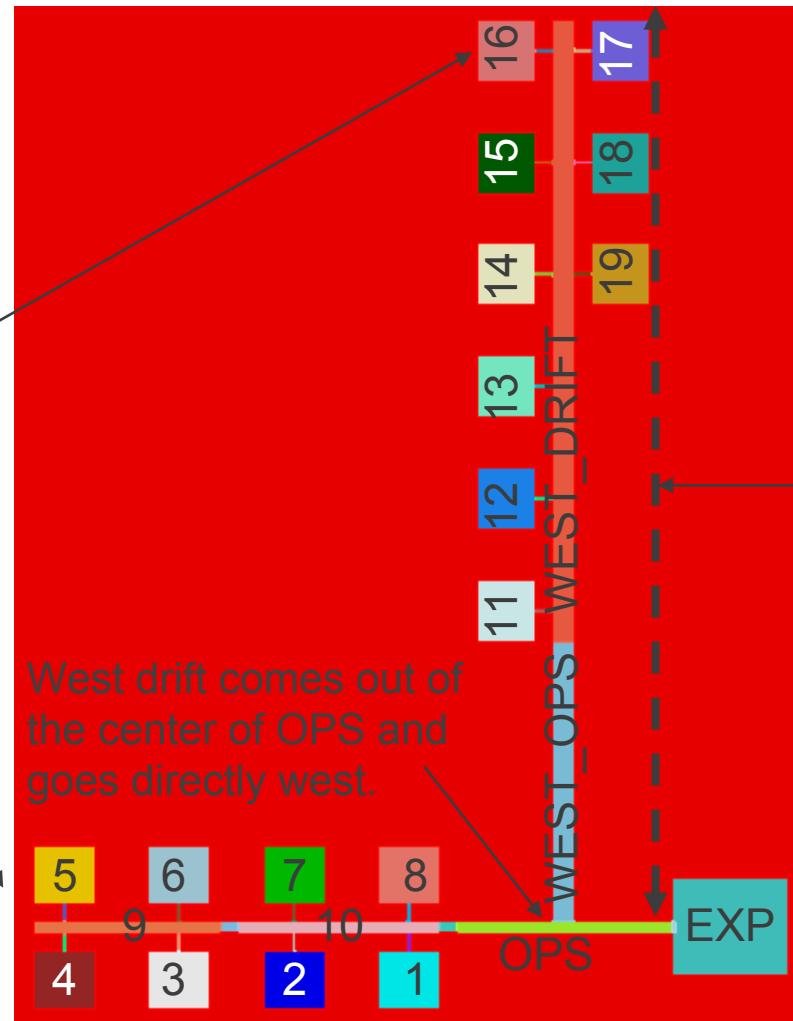
3D simulation model: Consistent with BRAGFLO models and current understanding of the subsurface

- Repository is 13ft tall everywhere and vertical mesh spacing is preserved
- Distance from borehole to shaft is identical to CRA19 model
- Length of panel closures is preserved
- Region volumes are identical to CRA19 model where possible
- Dip is north/south and identical to CRA19

3D simulation model: other considerations



Dimensions of waste panel (WP) 11-19 and panel closure systems (PCS) 11-19 are identical to WP 1-8 and PCS 1-8.



Distance from panel closure to the end of WP 16 and 19 is identical to BRAGFLO APPA model



3D simulation model: other considerations

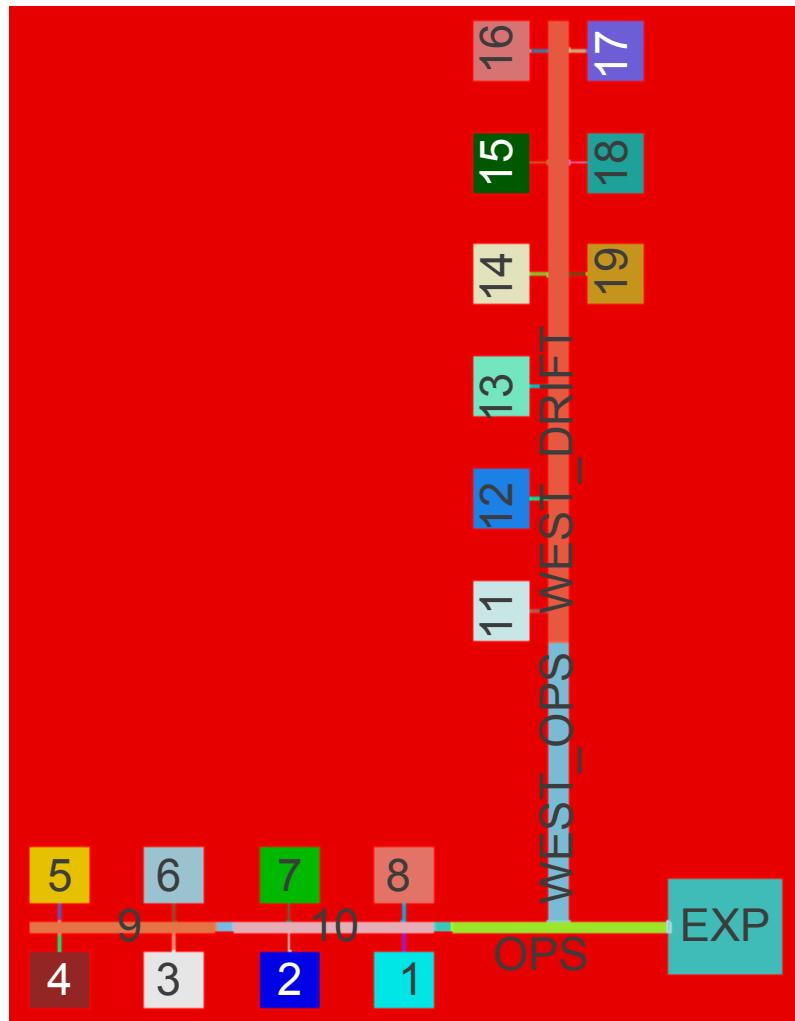


All defined volumes are lumped into boxes of equivalent volume

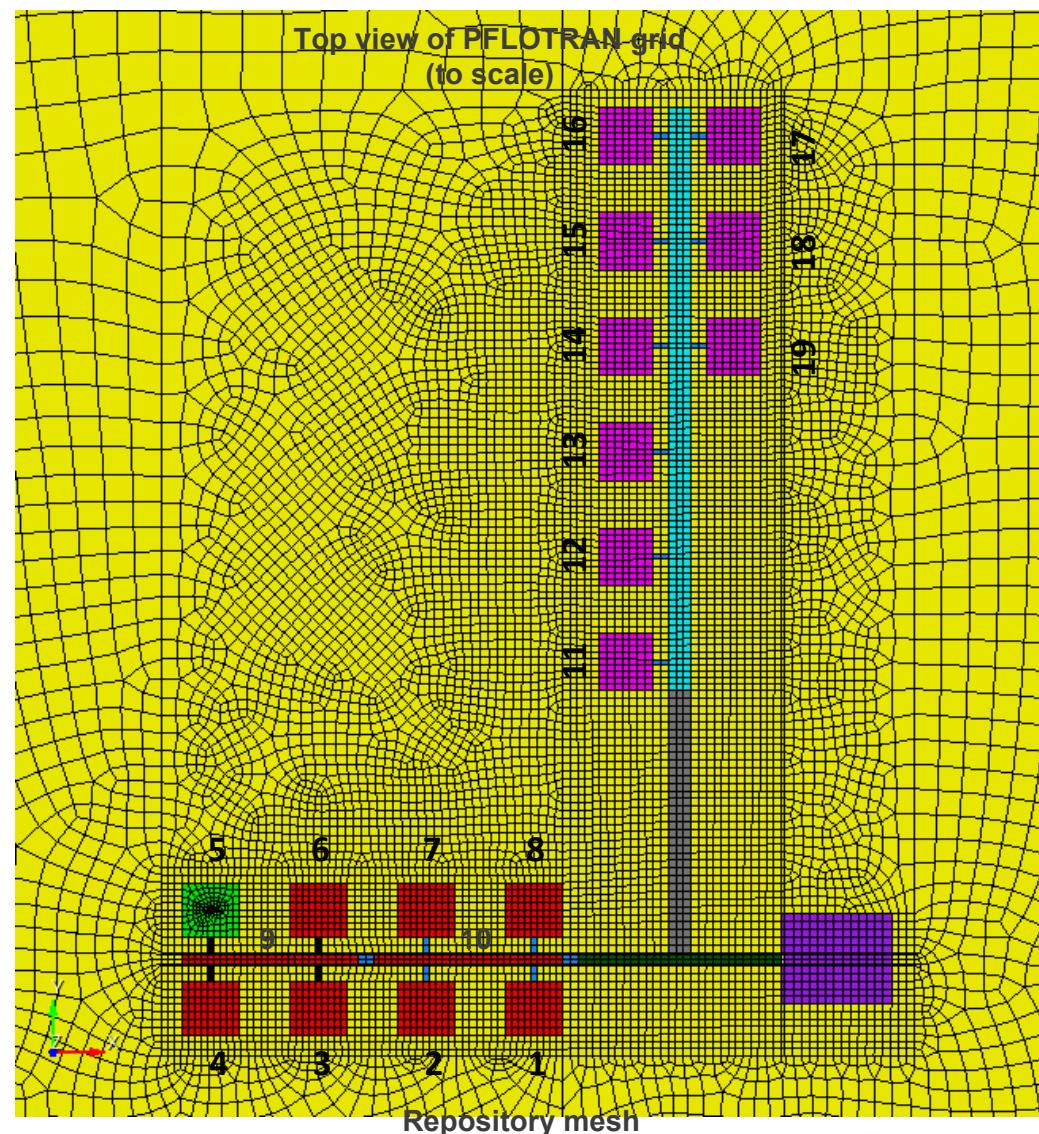
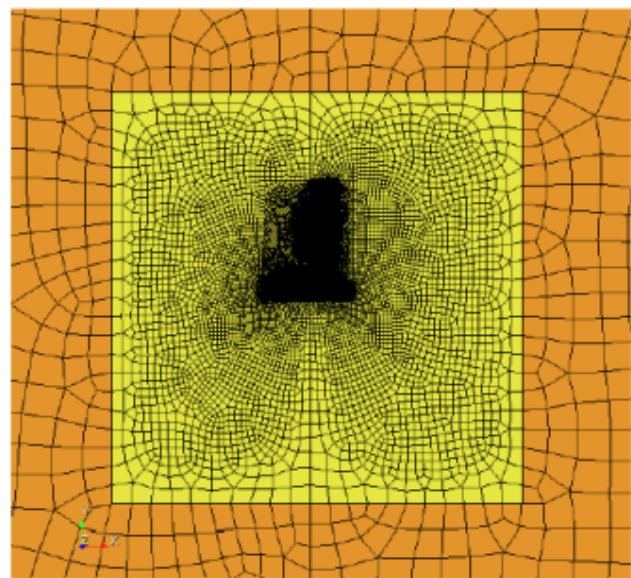
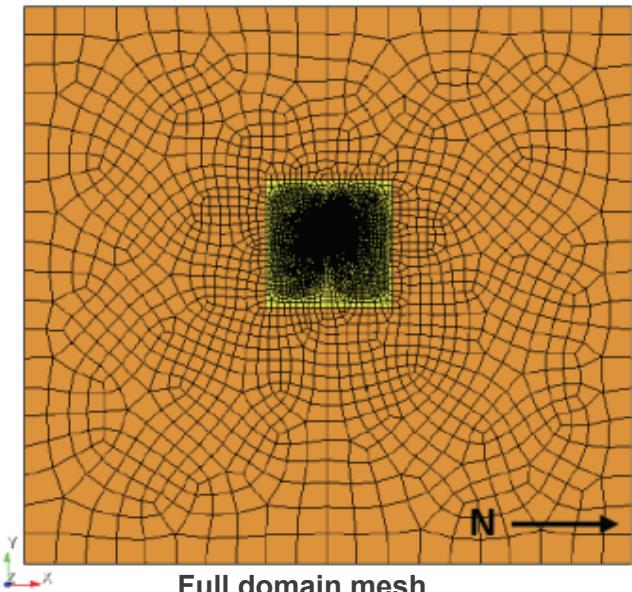
Additional waste panels:

- Dimensions of WP 11-19 and PCS 11-19 are identical to WP 1-8 and PCS 1-8.
- West drift comes out of the center of OPS and goes directly west.
- Distance from panel closure to the end of WP 16 and 19 is identical to new BRAGFLO model

3D simulation model



Additional panels grid: 531,894 cells



Observations and Conclusions



- A 3D model suitable for Salado flow calculations has been built that is
 - Physically realistic in 3D
 - Conceptually consistent with 2D flared model
- Simulations completed so far (LaForce et al, 2021)
 - 97% of 1800 simulations (3 replicates of 100 vectors for 6 scenarios) finished on the first attempt
 - S1 scenarios were the fastest and S3 the slowest based on both mean and median clock times
- Simulation results are very similar to BRAGFLO results, particularly for intrusion cases as shown in the next presentation

References



- Kuhlman, K. 2010. *Analysis Report for CRA-2009 PABC Culebra Flow and Transport Calculations*. AP-144/ERMS 552951 Sandia National Laboratories, Carlsbad, NM. (<https://wipp.energy.gov/library/CRA/CRA-2019/I%20-%20M/Kuhlman%20%202010%20%20ERMS%20549013.pdf>)
- LaForce and Park, 2021, *3D grid demonstration and simulation times on 1800 simulations*. ERMS 574946 Sandia National Laboratories, Albuquerque, NM.
- LaForce, T., C. Hansen, E. Stein, 2020. *Development of 3D model of the WIPP with proposed additional panels*. ERMS 573646 Sandia National Laboratories, Albuquerque, NM.
- Stein, E., J. Frederick, G.E. Hammond, J.C. Bethune. 2018. *UPDATE to the PFLOTRAN-BRAGFLO Benchmark: Comparison of Test Cases and Simulations on the 2-D Flared Grid*. ERMS 570622 Sandia National Laboratories, Albuquerque, NM