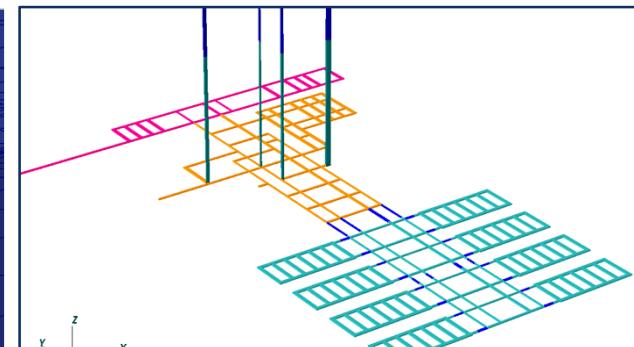
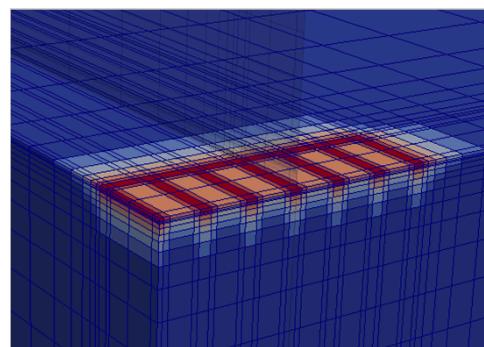
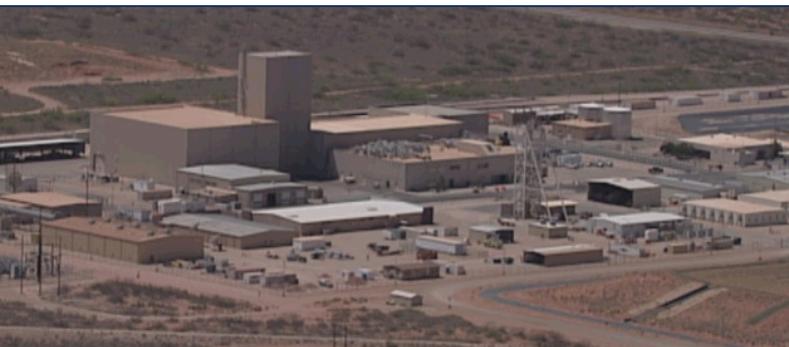


Exceptional service in the national interest



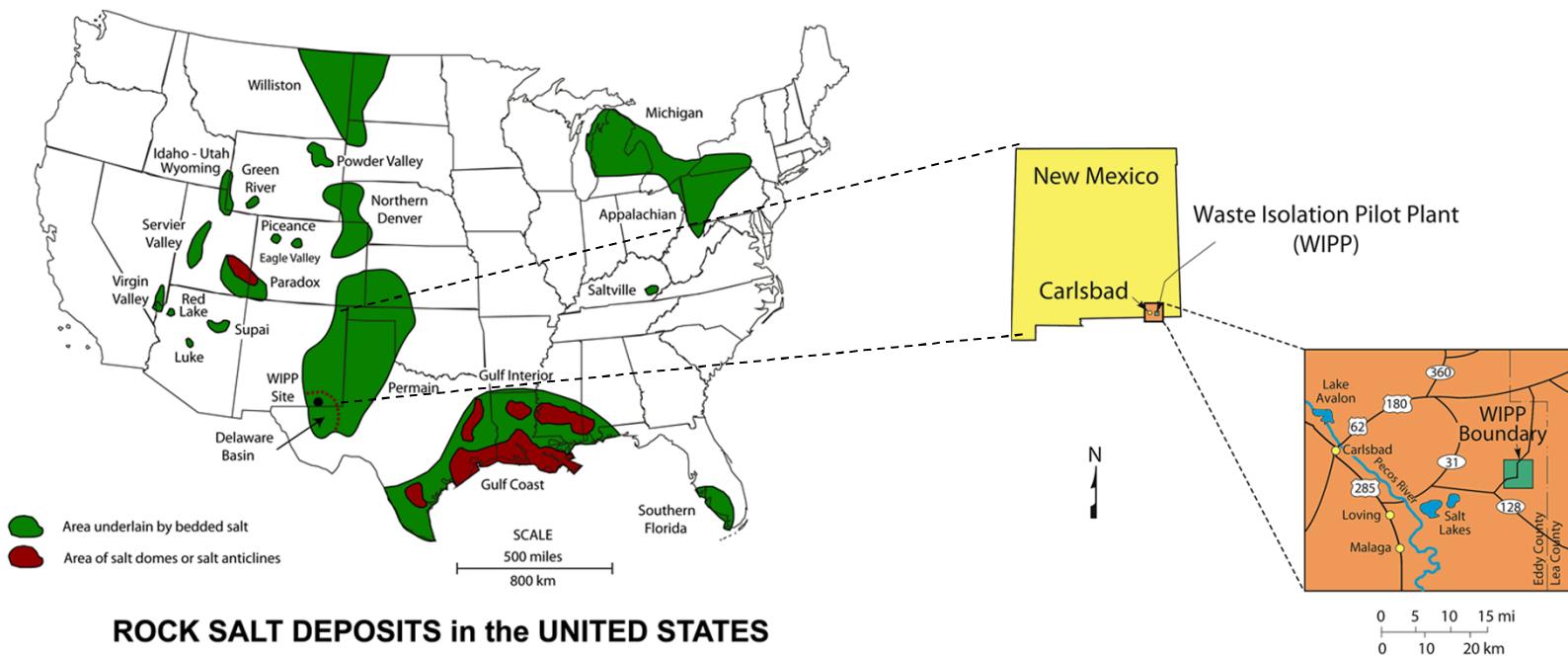
PFLOTRAN Simulation of Waste Isolation Pilot Plant Single Waste Panel

Heeho Park, Glenn Hammond
12/14/2015

WHAT IS THE WASTE ISOLATION PILOT PLANT?

Waste Isolation Pilot Plant (WIPP)

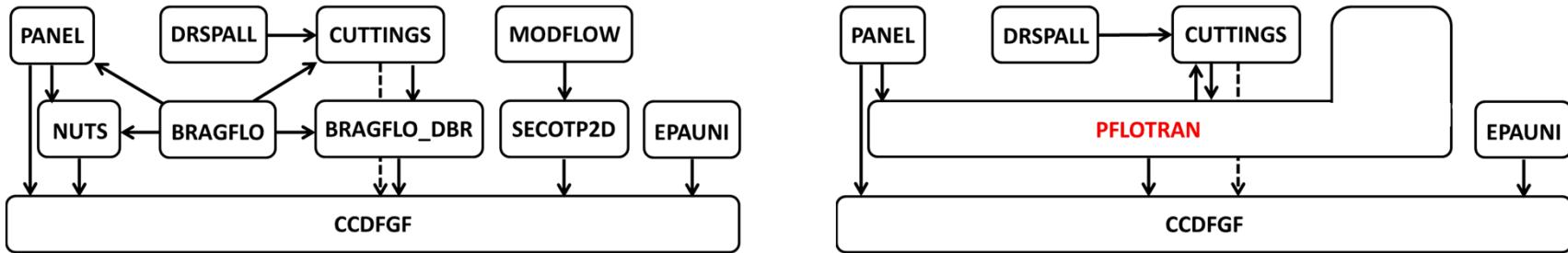
The Waste Isolation Pilot Plant (WIPP), located in southeastern New Mexico, has been developed by the U.S. Department of Energy (DOE) for the deep geologic disposal of transuranic (TRU) waste.



- The DOE demonstrates compliance with Environmental Protection Agency (EPA) containment requirements by means of performance assessment (PA) calculations conducted by Sandia National Laboratories (SNL).
 - Computer codes incorporating 24 peer-reviewed conceptual models
- WIPP PA calculations estimate the probability and consequence of potential radionuclide releases from the repository to the accessible environment for a regulatory period of 10,000 years after facility closure.
- To date, WIPP PA calculations have employed multiple 2D numerical models requiring simplification of the conceptual model (meshing, physical/chemical process models, etc.).

WHERE IS PFLOTRAN USED IN WIPP PA?

PFLOTTRAN Implementation



Codes	Description
BRAGFLO	Simulates porous media flow in and surrounding the repository over 10,000 years
NUTS	Calculates radionuclide transport in the Salado Formation including the repository
BRAGFLO-DBR	Predicts release from the repository to the environment via borehole intrusion
MODFLOW	Used to calculate flow field away from the repository in the Culebra member of the Rustler Formation
SECOTP2D	Computes radionuclide transport in fractured porous media (Culebra)

Current PA vs PFLOTRAN

Codes	Current PA	PFLOTRAN
BRAGFLO (Flow)	<ul style="list-style-type: none"> - Immiscible - Isothermal - Two-phase flow 	<ul style="list-style-type: none"> - Miscible/Immiscible - Anisothermal - Multiphase Flow - Diffusion
NUTS (Transport)	<ul style="list-style-type: none"> - Multicomponent transport - Single porosity - Constant sorption - Single continuum model 	<ul style="list-style-type: none"> - Biogeochemical Transport - Dissolution/precipitation - Multi-rate sorption - Multi-continuum model
General Comparison	<ul style="list-style-type: none"> - 2D - Structured grid - Parallel with single core simulations - Limitations on simulation size - Many I/O interfaces required - Network of coupled 2D simulations - Simplified process models and coarse mesh for less total CPU time. 	<ul style="list-style-type: none"> - 3D - Unstructured/structured grid - Massively parallel - Simulation size only depends on hardware capability - WIPP-specific functionalities implemented - Detailed process models and high mesh resolution for more total CPU time.

Other Advantages of PFLOTRAN

- **Open source development**
 - A broad research community that leverages innovation in subsurface and computational sciences
- In-house code development expertise
 - **Multiple Sandians are PFLOTRAN developers with authorization to commit changes to the code**
- Managed under a modern support infrastructure
 - **Distributed source control management through Mercurial**
 - **Central, open source repository resides on Bitbucket**
 - Comprehensive regression and unit testing using Python
- PFLOTRAN HDF5 file formats
 - **Compatible with open source visualization tools** (i.e. VisIt and Paraview)
- Managed under QA if PFLOTRAN is accepted to be used for PA
 - Automated building and testing through Buildbot
 - Frozen version housed in Sandia's HPC environment

PFLOTRAN VERIFICATION

Fundamental Process Testing

- PFLOTRAN (vs TOUGH2, vs BRAGFLO)

vs BRAGFLO (Brine and Gas Flow) - 100%

- Test Case #B1: Pressure drawdown with radial grid
- Test Case #B2: Horizontal one-dimensional infiltration
- Test Case #B3: Horizontal one-dimensional infiltration with Dirichlet BC
- Test Case #B4: Two-dimensional infiltration
- Test Case #B5: Two-dimensional, two-phase flow with gas injection
- Test Case #B8: Well production at specified bottom hole pressure
- Test Case #B9: Heterogeneous reservoir conditions
- Test Case #B10: No flow boundary conditions
- Test Case #B11: Pressure and density of water column in equilibrium

Testing WIPP Specific Functionalities

- PFLOTRAN (vs BRAGFLO)

vs BRAGFLO - 91%

- Test Case #B6_a: Gas (hydrogen) generation in two-phase flow
- Test Case #B6_b: Change in porosity due to creep closure
- Test Case #B6_c: Fractures
- Test Case #B6_d: Klinkenberg effect
- Test Case #B6_e: RKS equation of state for gas density
- Test Case #B6_f: Material map change due to creep closure and human intrusion
- Test Case #B6_g: One-Dimensional WIPP initial condition two-phase flow
- Test Case #B6_h: Gas (air) injection in two-phase flow
- Test Case #B6_i: LHS interface with PFLOTRAN
- Test Case #B6_j: WIPP well production with constant bottom hole pressure
- Test Case #B6_k: Direct Brine Release

A VERIFICATION EXAMPLE

Two-Dimensional Infiltration

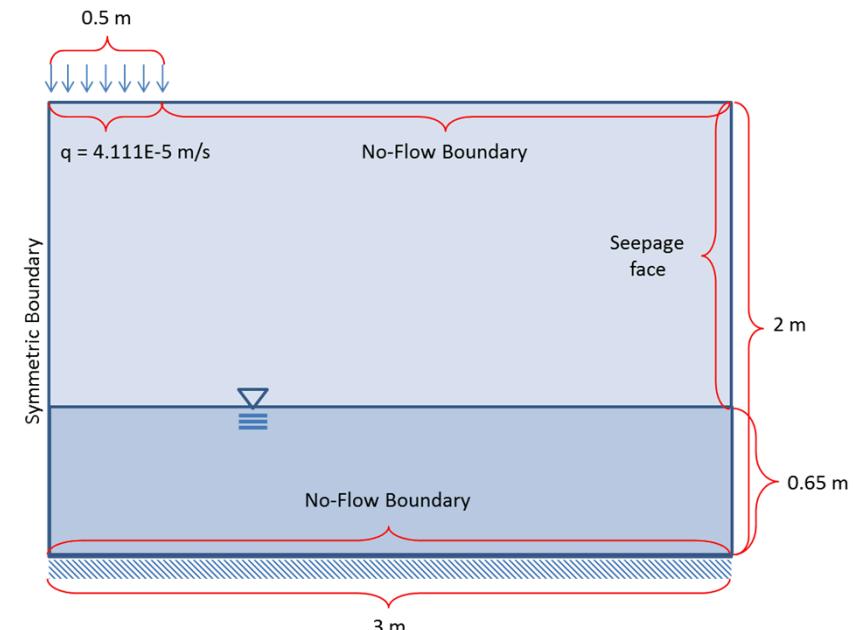
- The original experimental setup was done by Vauclin et al.
- Seepage face only allows outflow
- Capillary/Relative Permeability relations:

$$S_e = \frac{1 - S_w}{S_w}$$

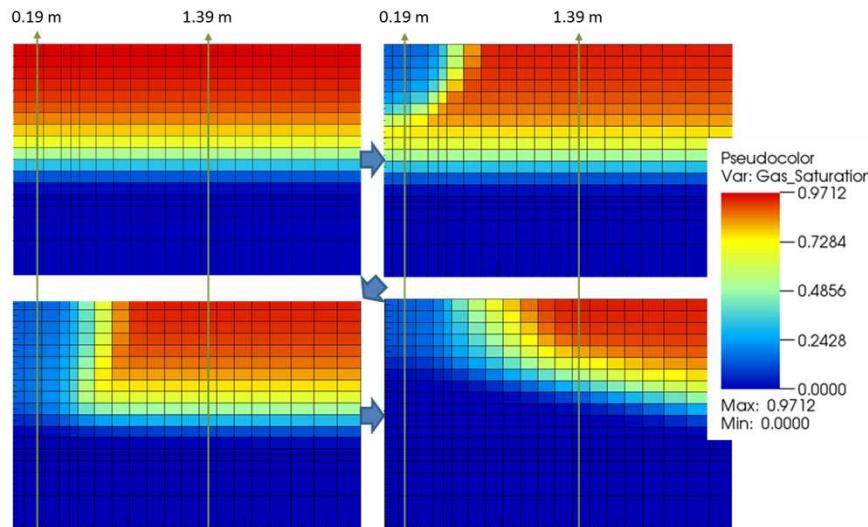
$$k_{rw} = \frac{1}{1 + 28.768353 S_e^{1/0.58}}$$

$$k_{rmw} = 1 - k_{rw}$$

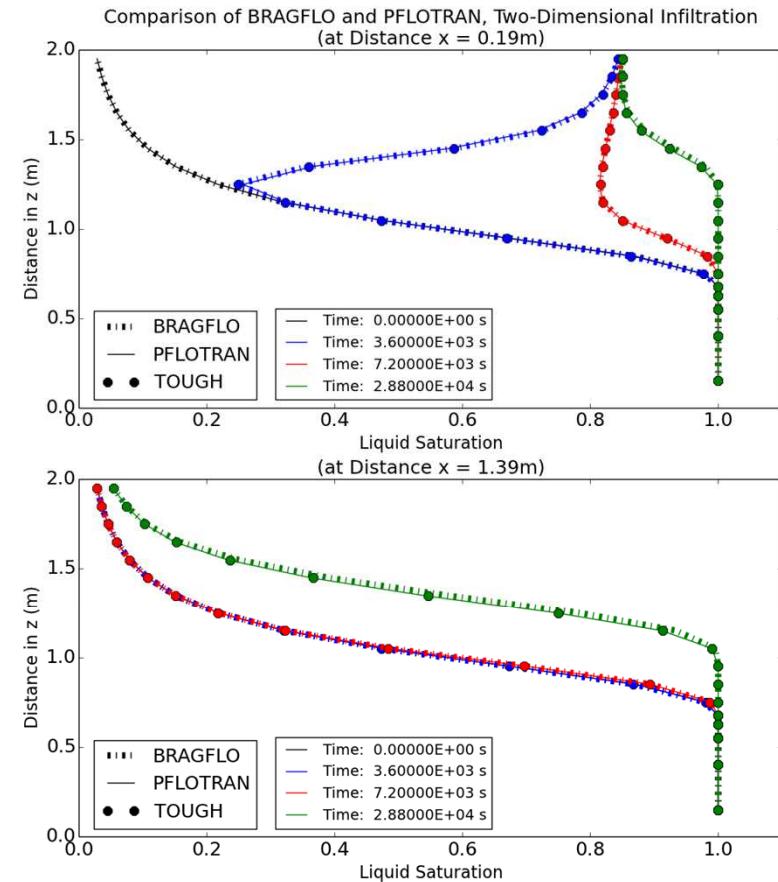
$$P_c = 3783 .0145 S_e^{(1/2.9)}$$



Two-Dimensional Infiltration

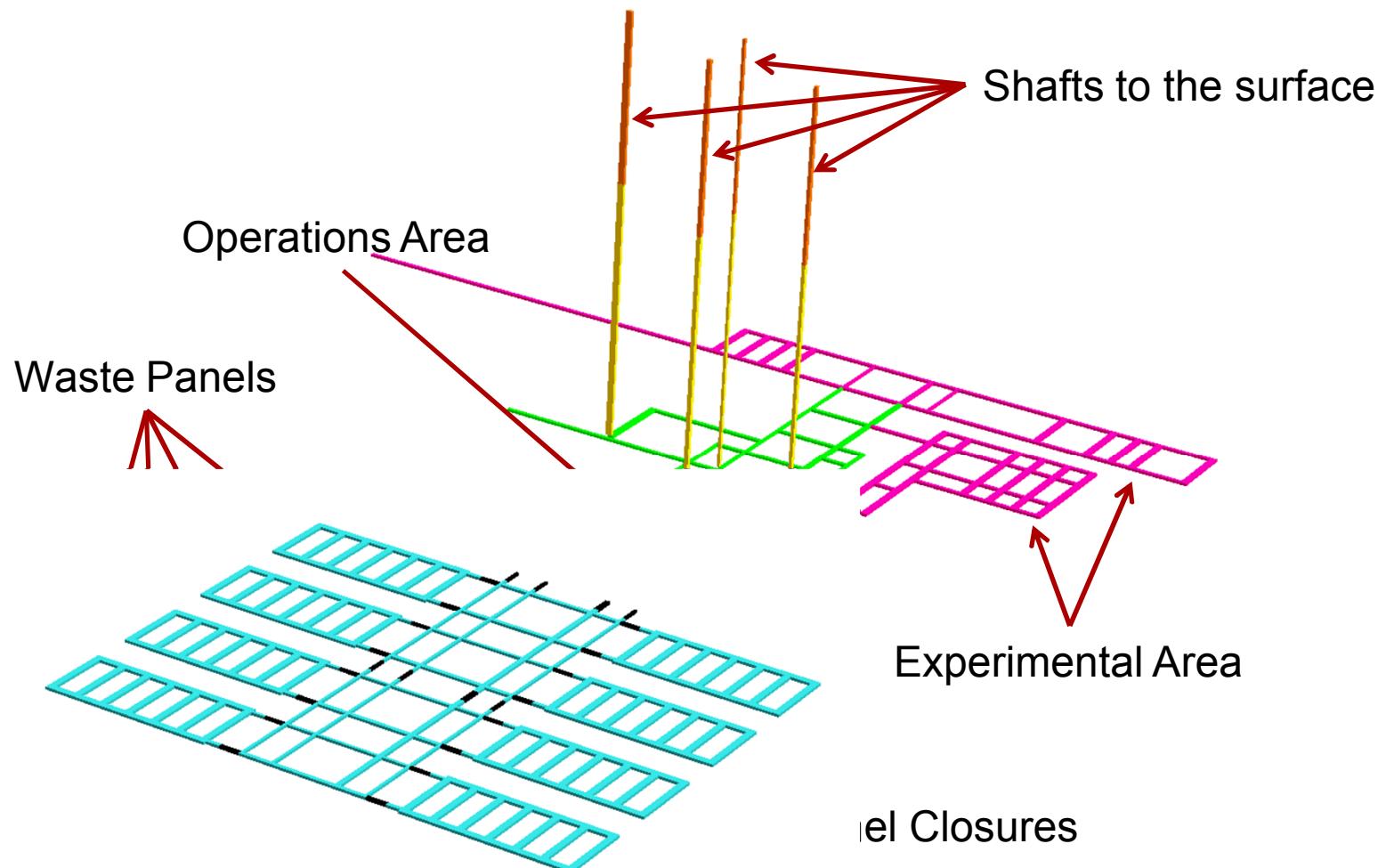


Water is being injected into the four left most cells in the top row. Gas saturation of the domain at 0 hour, 1 hour, 2 hours, and 8 hours from simulations of PFLOTTRAN

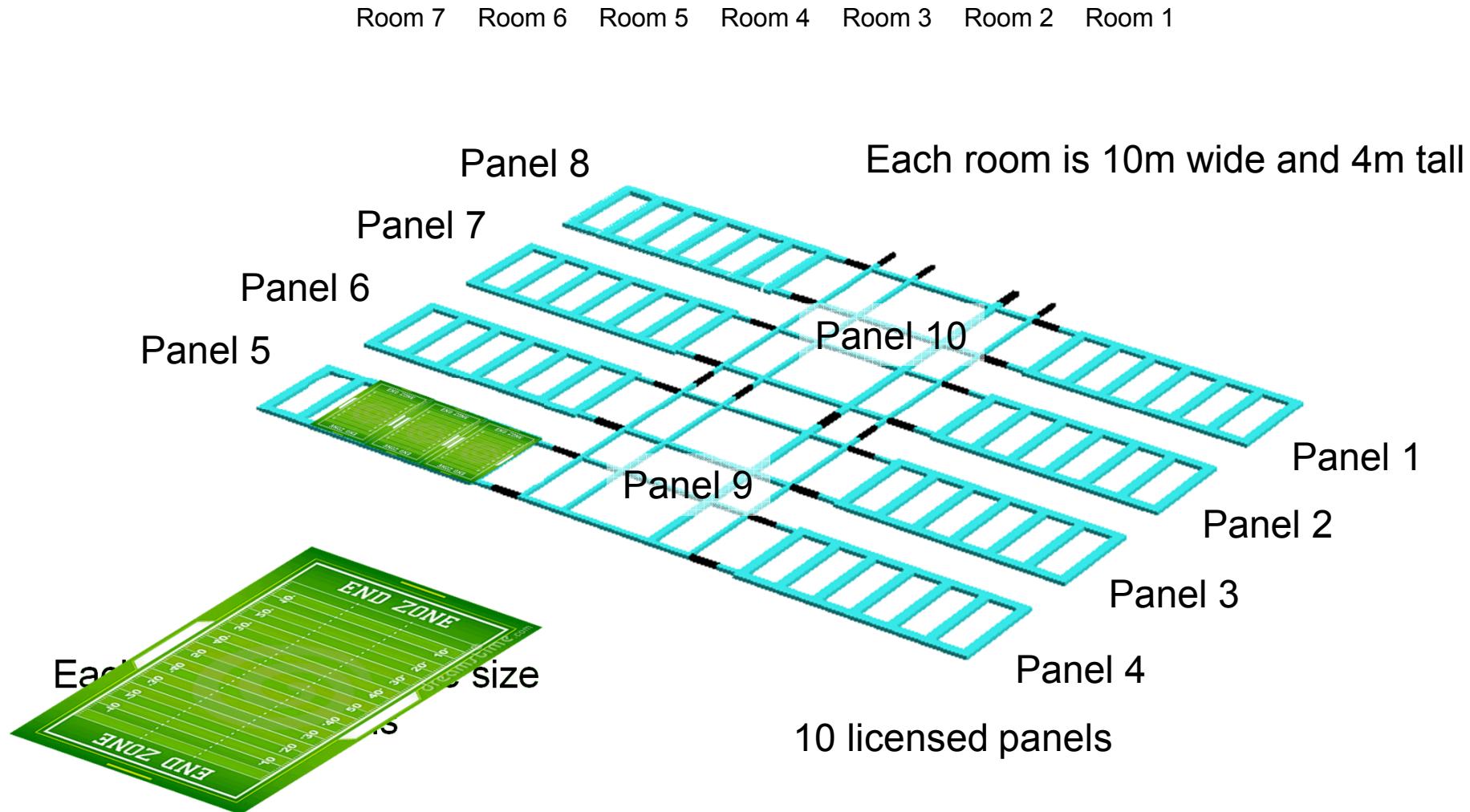


WIPP DESCRIPTION

WIPP Underground Structures



Panels and Rooms



3D MODELING WITH PFLOTTRAN

3D One Panel Model

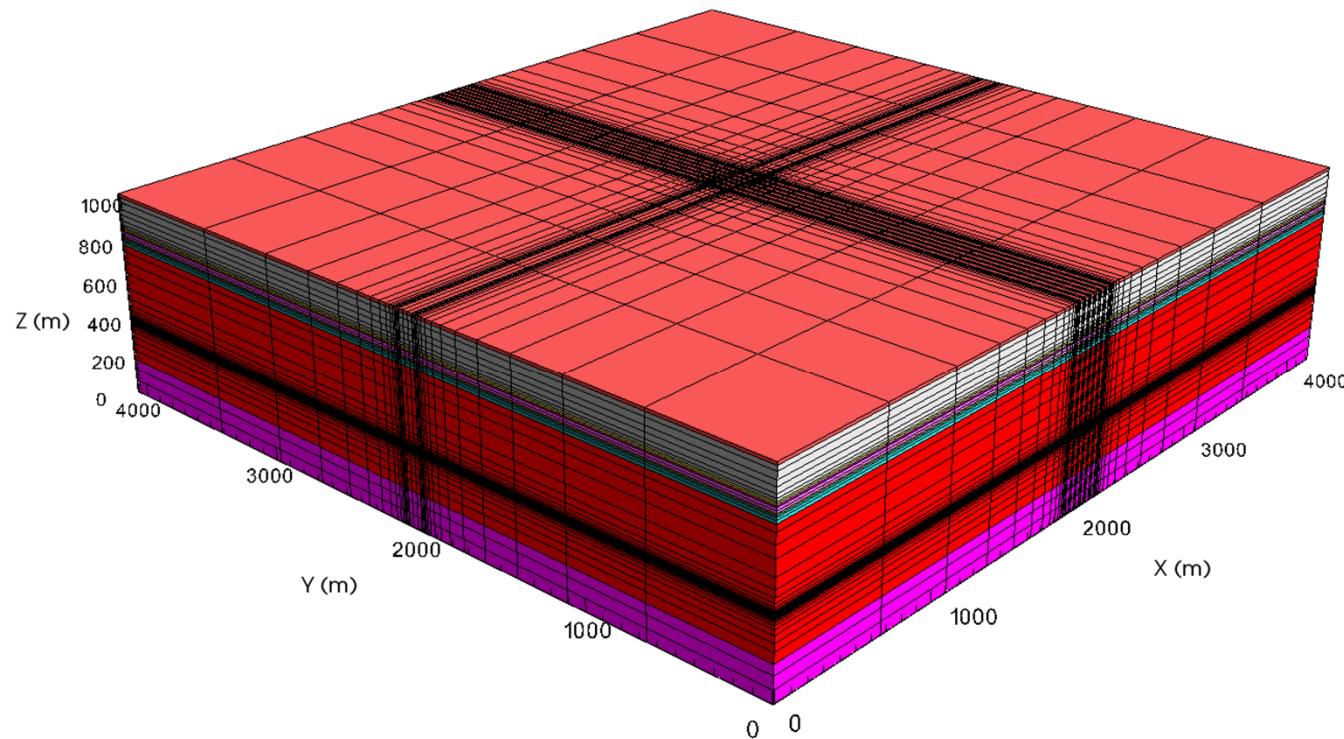
- Flow model
 - Uses two-phase general mode (hydrogen, brine)
 - Initial Conditions
 - Excavated waste panel is unsaturated
 - Disturbed rock zone (DRZ) is 40% saturated due to mechanical opening
 - Rest of the domain is saturated
 - Boundary Condition
 - No-Flow Boundary condition at the Land Withdrawal boundary (3.2 km)
 - Waste area generates gas (hydrogen) for 10,000 years

3D One Panel Model

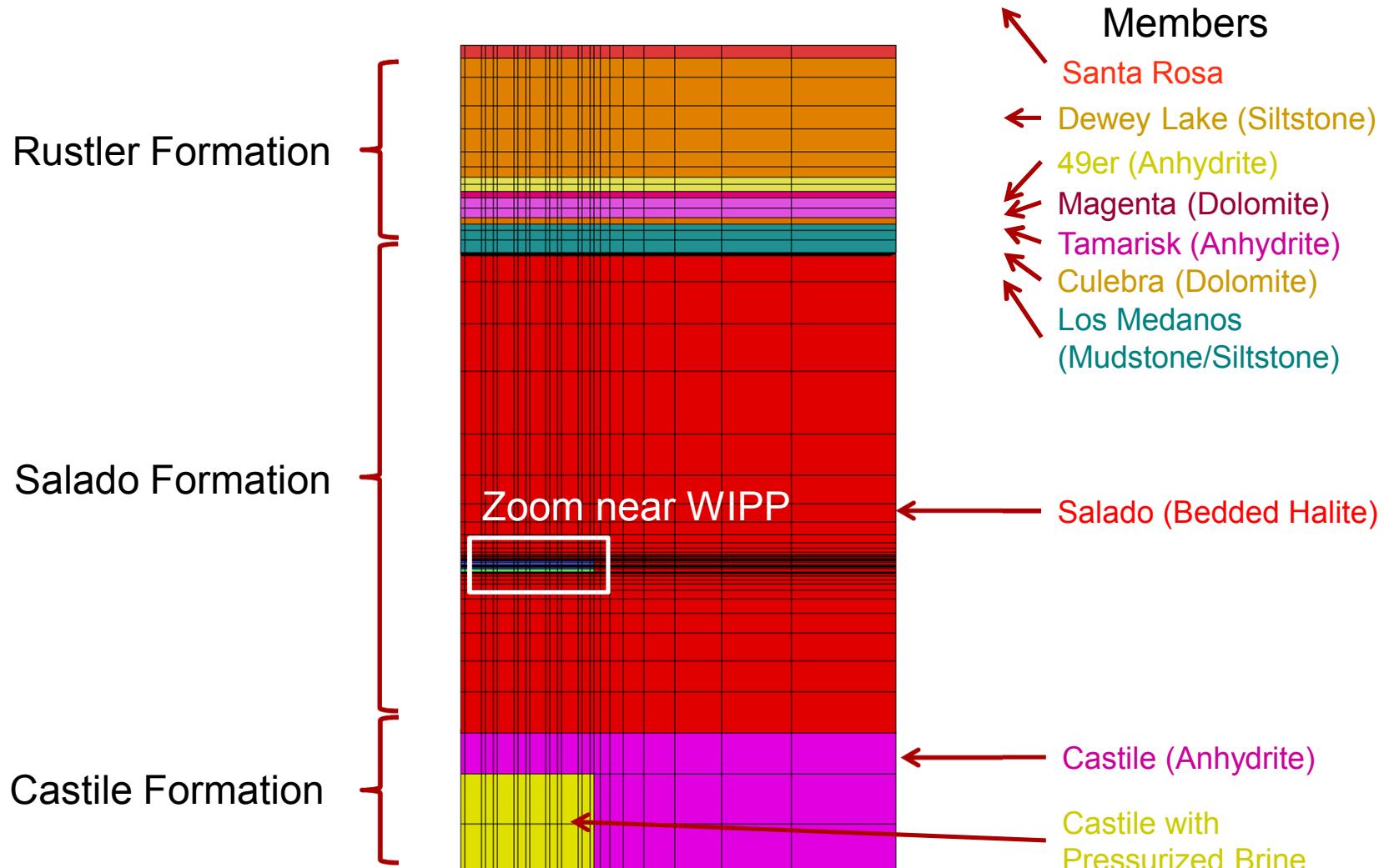
- Transport model
 - Tracking tracer; Am-241, Pu-239, Pu-238, U-234, Th-230;
 - Radioactive decay reaction
 - Pu-238 ($t_{1/2}=84\text{yr}$) \rightarrow U-234 ($t_{1/2}=2.46\text{E}5\text{yr}$) \rightarrow Th-230
 - Sorption
- Undisturbed condition (no human borehole intrusion)
 - Creep closure
 - DRZ fractures
 - RKS equation of state for gas
 - Klinkenberg
 - Latin Hypercube sampled parameters

One Panel Model Domain

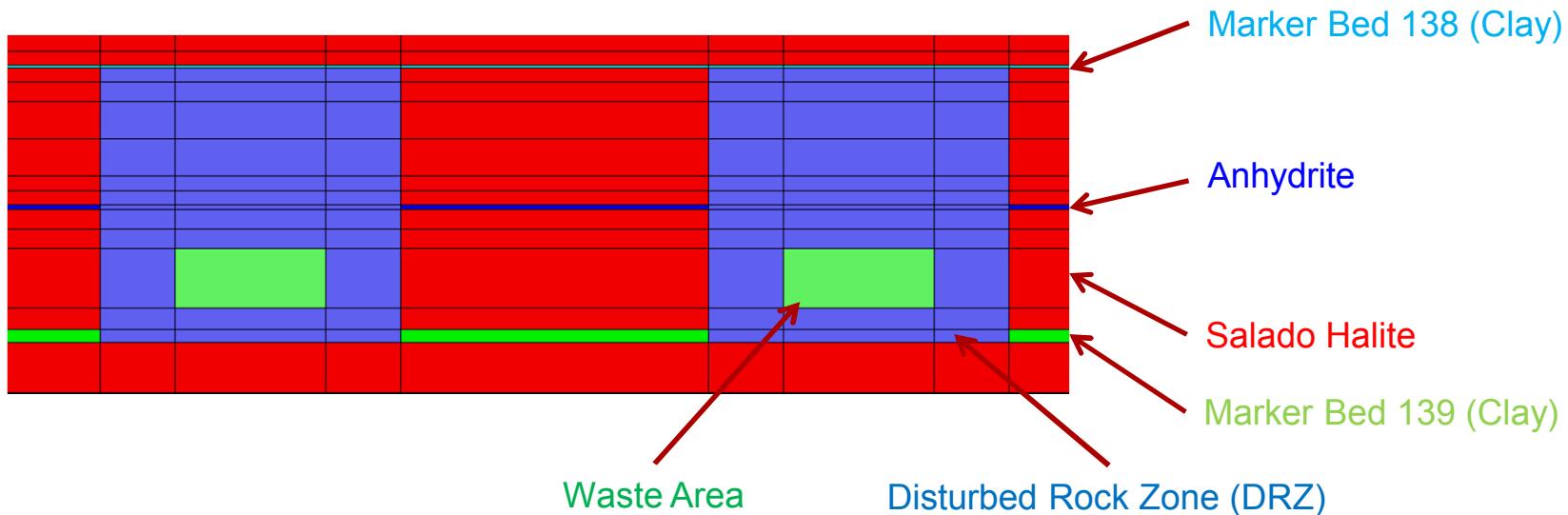
- 97,614 elements
- Domain spans out 2 km from the panel in all four directions



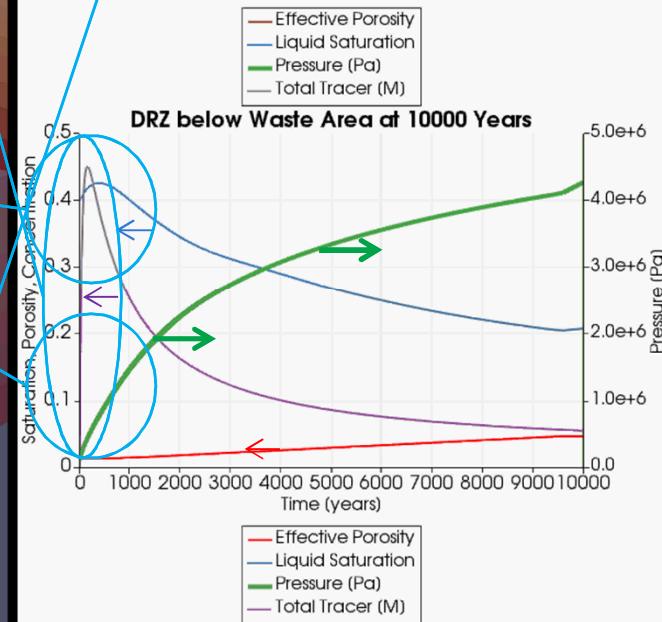
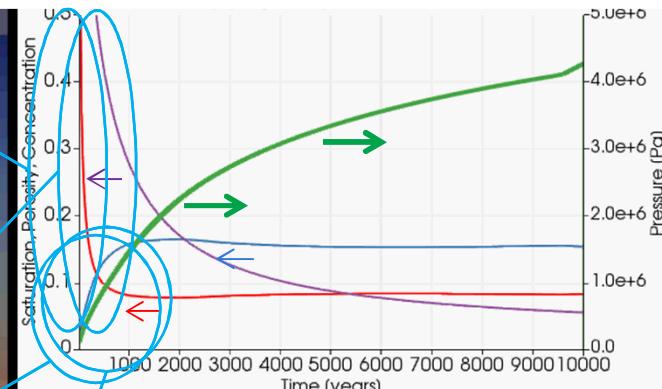
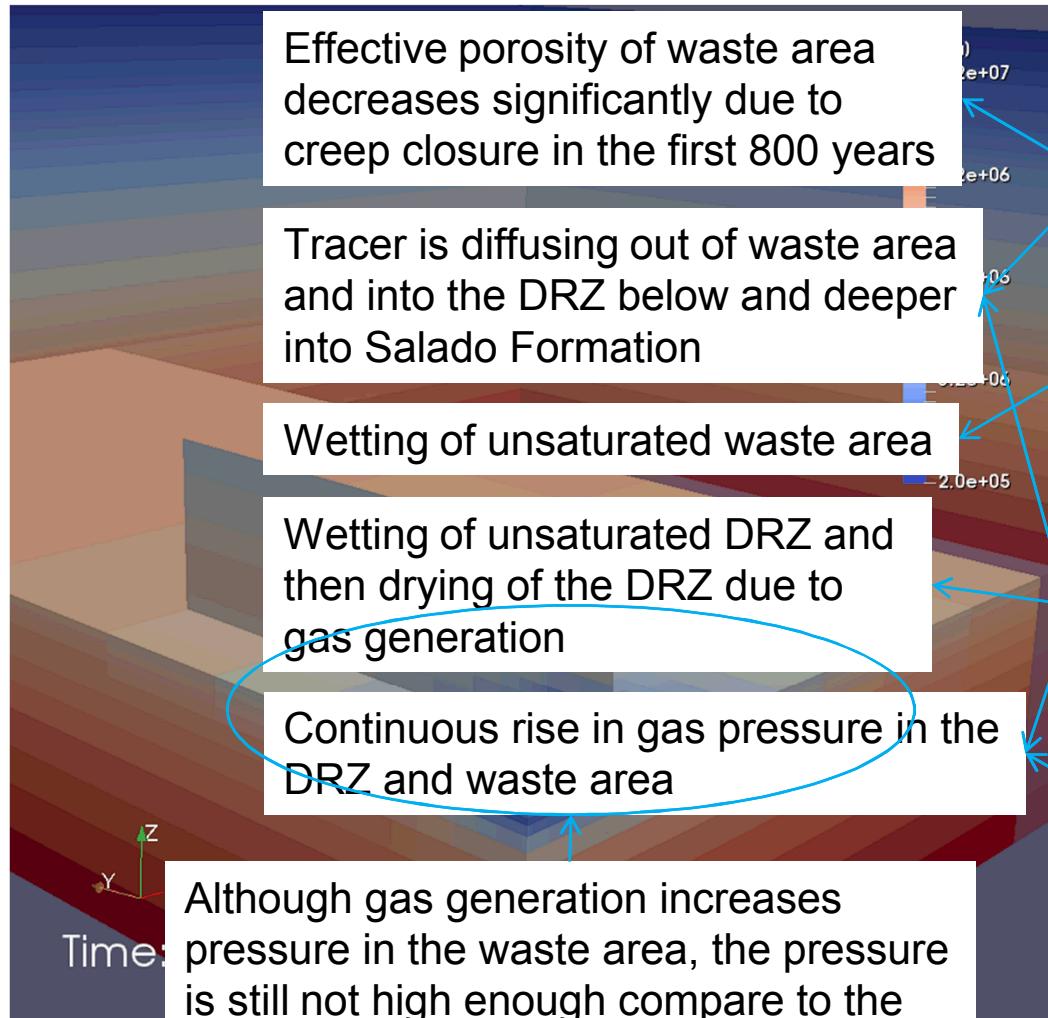
Geologic Structures at WIPP



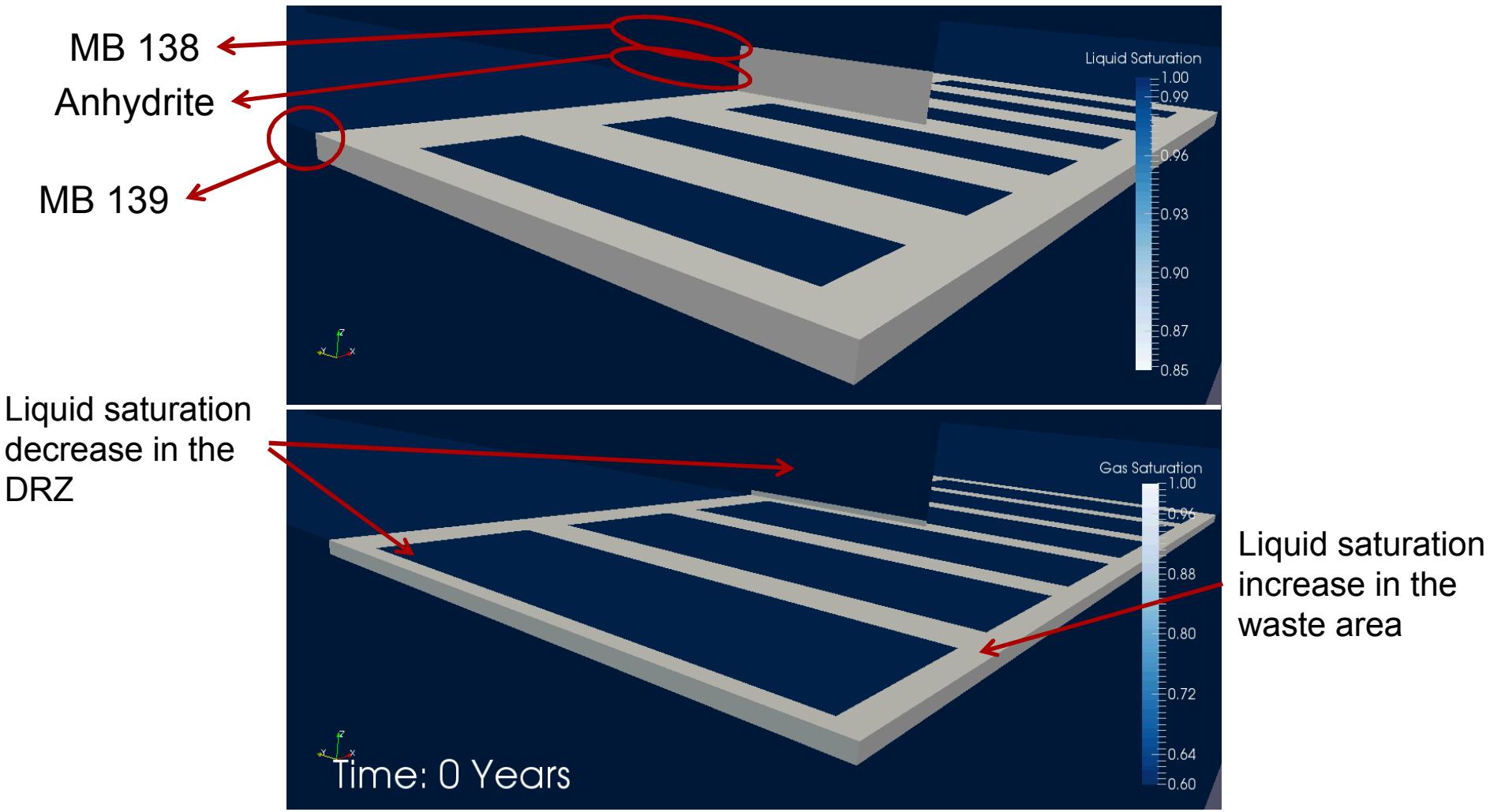
WIPP Surroundings



WIPP Specific Functions

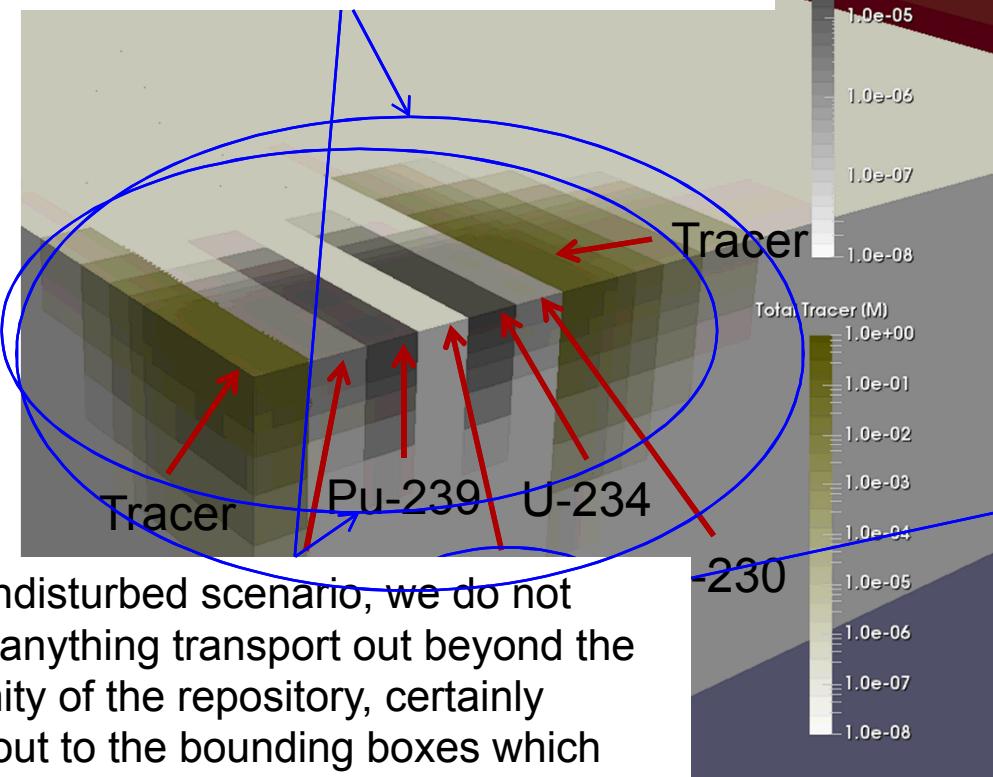


3D Flow

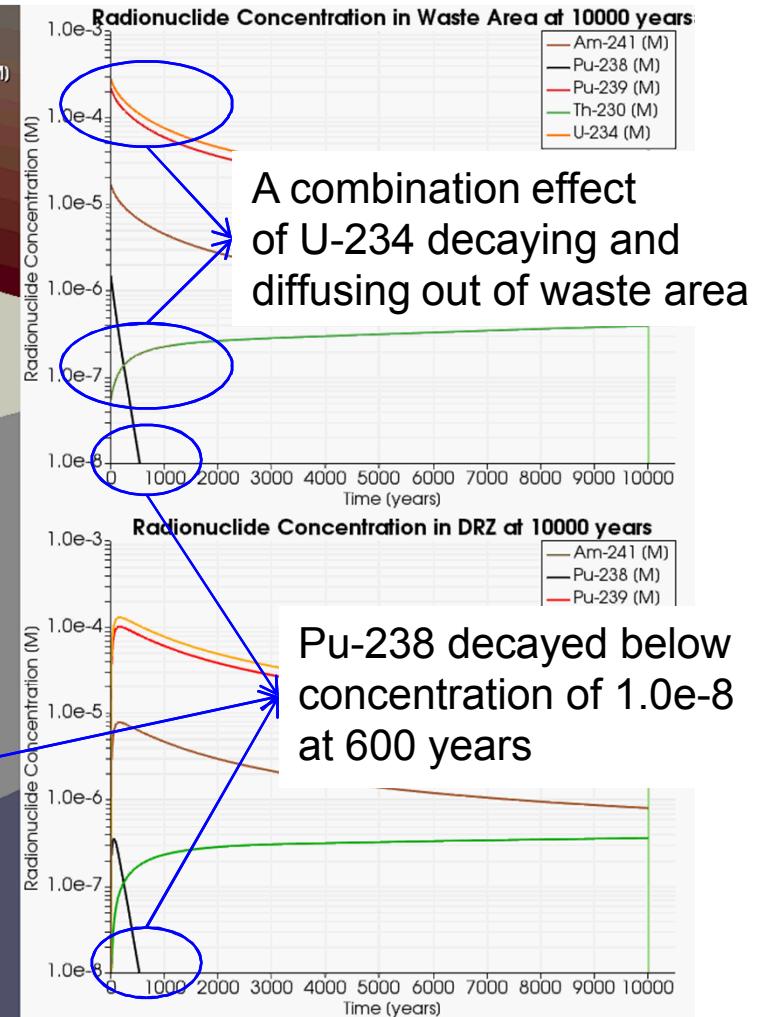


3D Transport

Also notice that major mode of transport in undisturbed scenario is diffusion as the pressure of the repository is lower than the hydrostatic pressure mentioned earlier

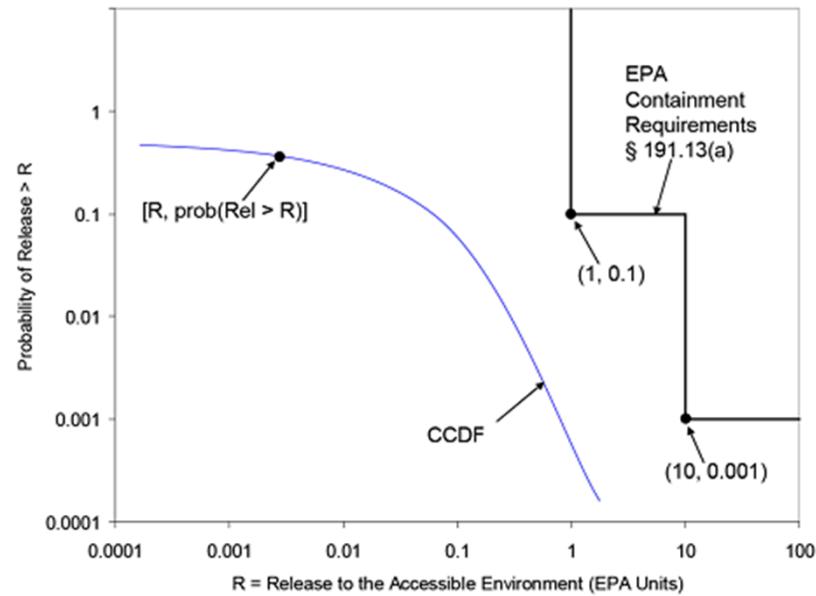


In undisturbed scenario, we do not see anything transport out beyond the vicinity of the repository, certainly not out to the bounding boxes which is within the Land Withdrawal Boundary



Future works

- One panel simulation with human borehole intrusion
- Direct Brine Release (DBR) simulation due to the intrusion
- Implementing PFLOTRAN into PA structures to generate Complementary Cumulative Distribution Function (CCDF) curves
- Full WIPP model



Questions? (References)

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