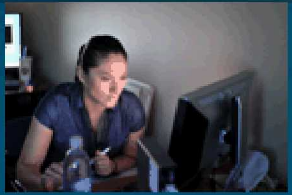
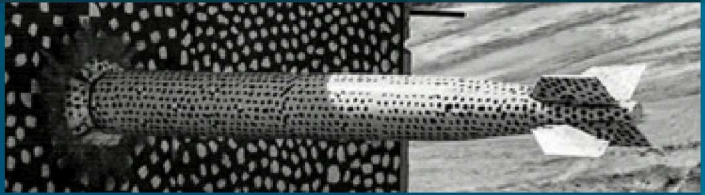
SAND2020-3017C

Development of PFLOTRAN Transport Capability for Use in the Waste Isolation Pilot Plant Performance Assessment





PRESENTED BY

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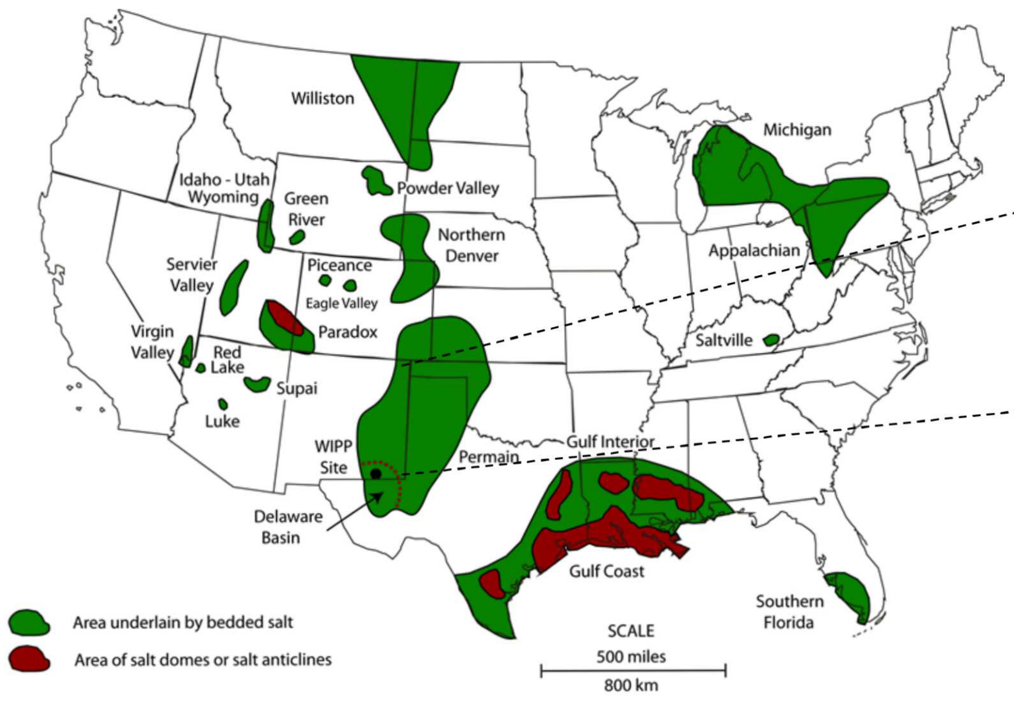
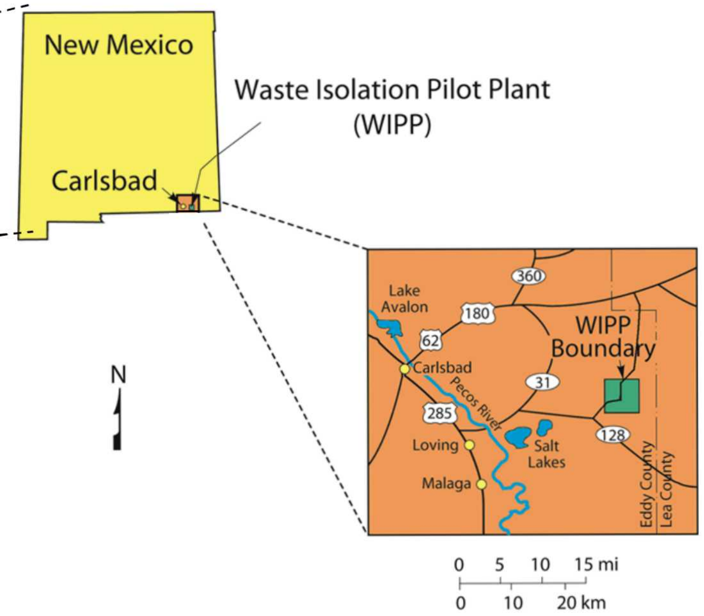
SAND2020-xxxx C

Waste Isolation Pilot Plant (WIPP)

- Transition to a 3-D model domain for Performance Assessment
  - Development of WIPP_FLOW mode in PFLOTRAN
  - Development of NUCLEAR_WASTE_TRANSPORT mode in PFLOTRAN

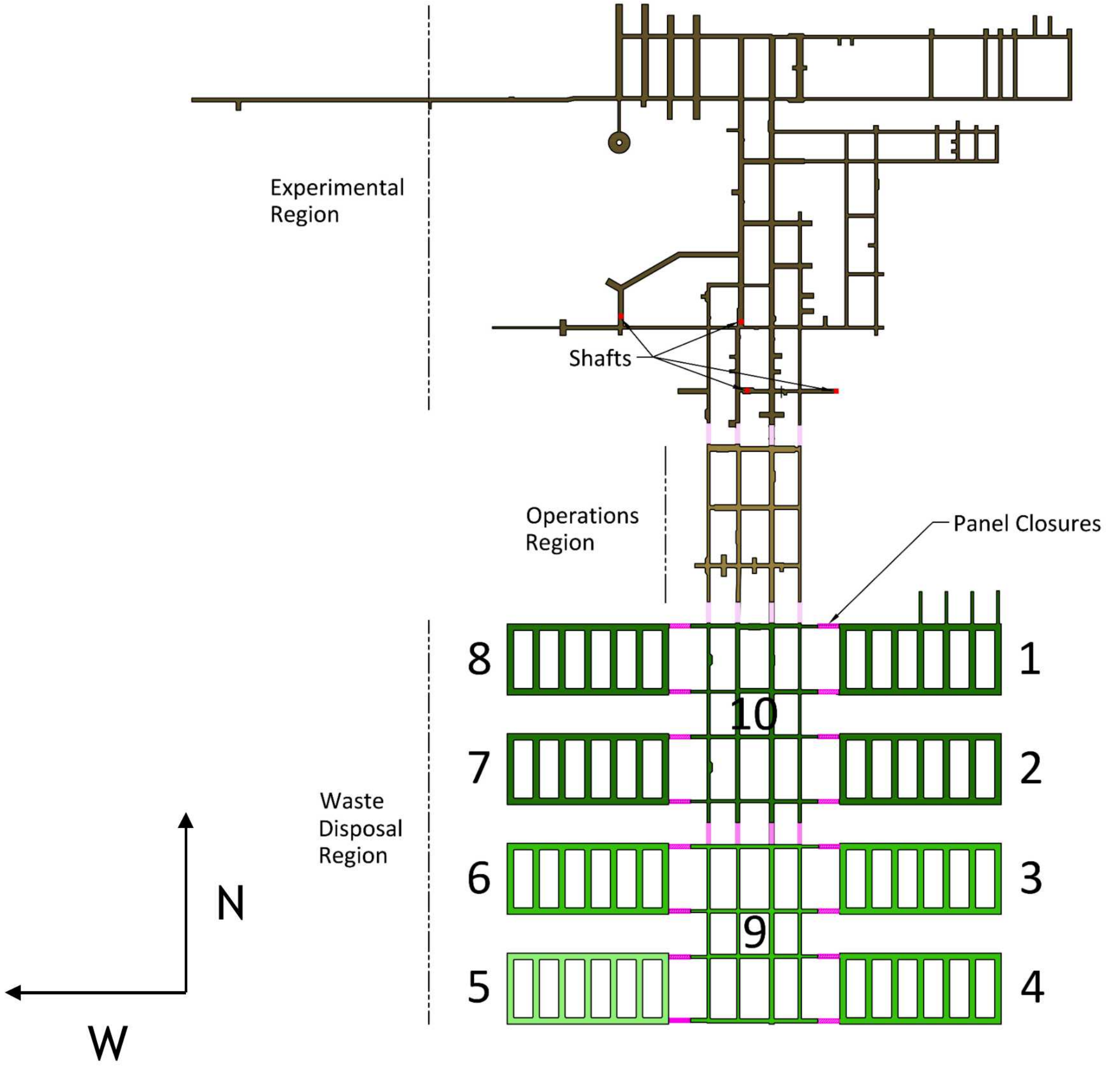


ROCK SALT DEPOSITS in the UNITED STATES

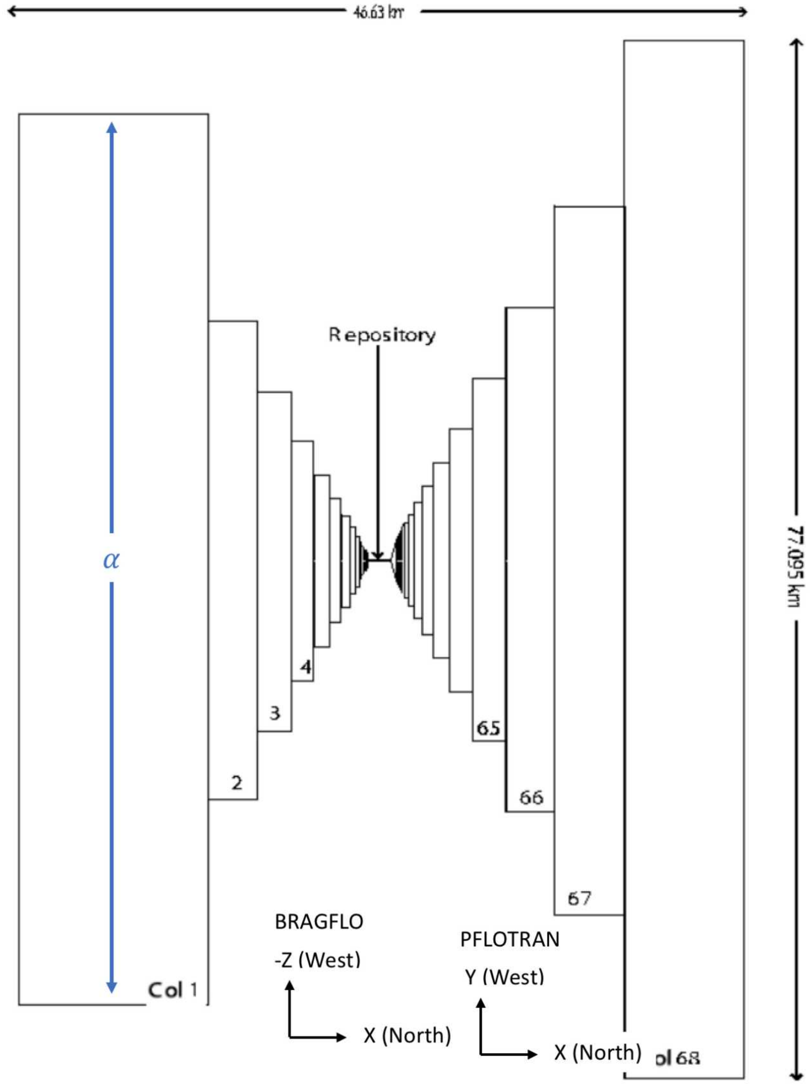


Need for a 3-D Model Domain

Repository Layout



2-D Flared Grid



Current WIPP Recertification PA Codes

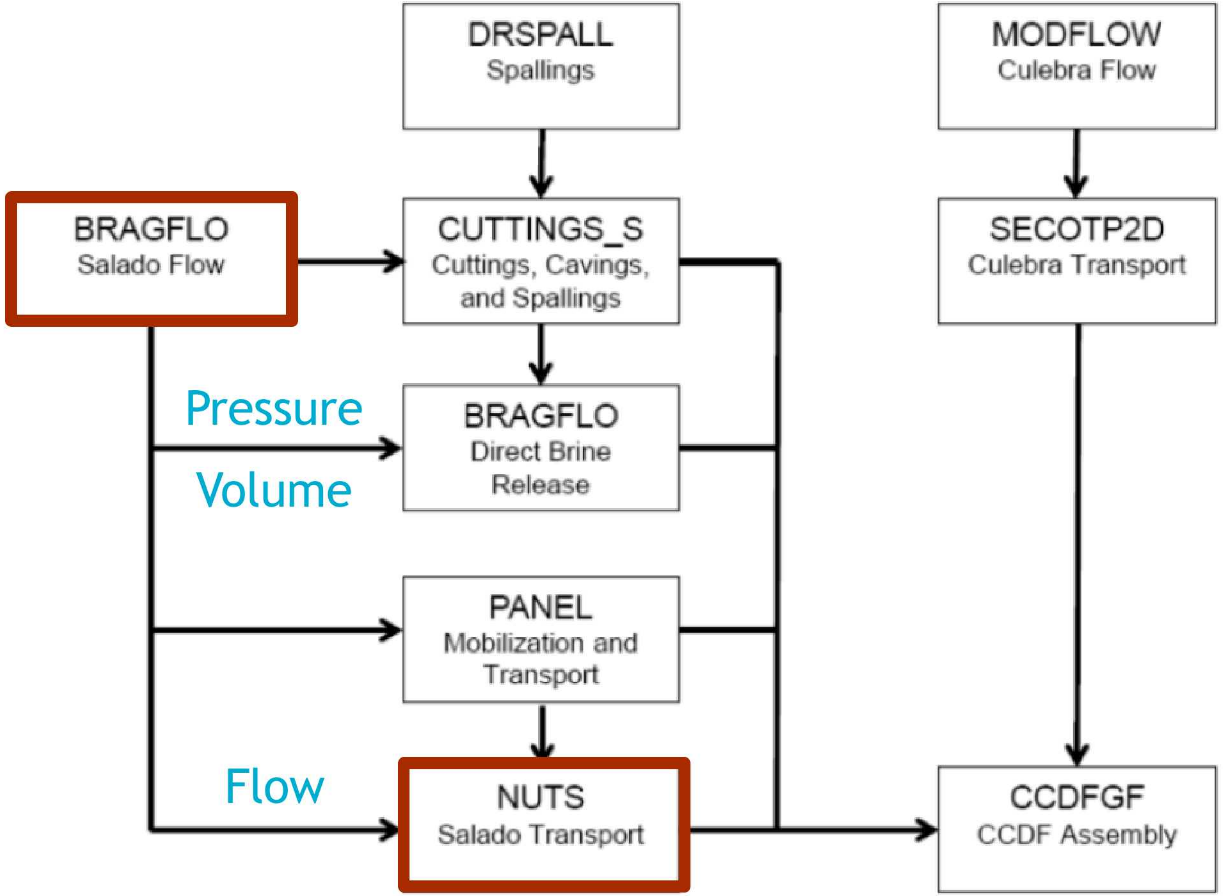
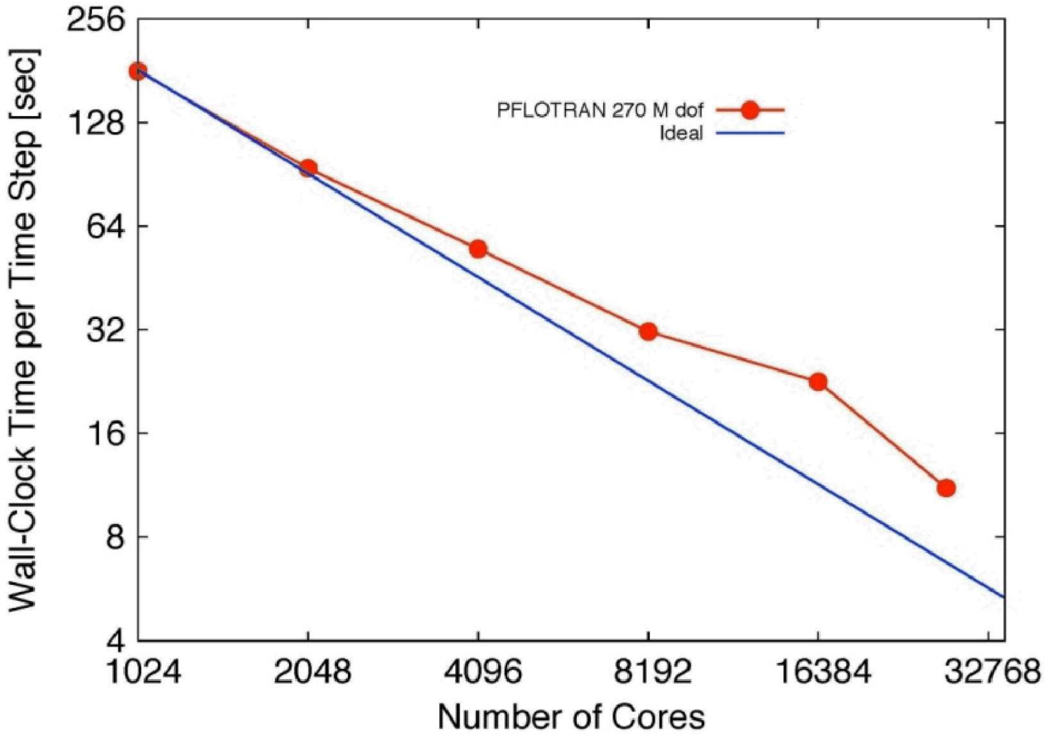


Figure PA-1. Computational Models Used in PA

PFLOTRAN (https://www.pflotran.org)

- Open source, state-of-the-art, massively parallel subsurface flow and reactive transport
- 3-D domain decomposition with PETSc (https://www.mcs.anl.gov/petsc/) Argonne NATIONAL LABORATORY
- Strong scaling to over 10,000 cores

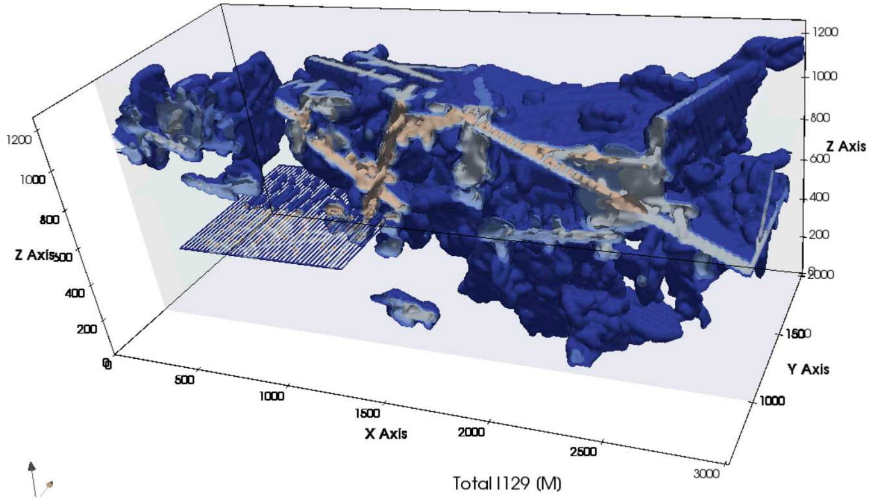


BERKELEY LAB · Los Alamos NATIONAL LABORATORY EST. 1943 · OAK RIDGE National Laboratory · OFM Research · Pacific Northwest NATIONAL LABORATORY · Sandia National Laboratories · PFLOTRAN

PFLOTRAN Usage

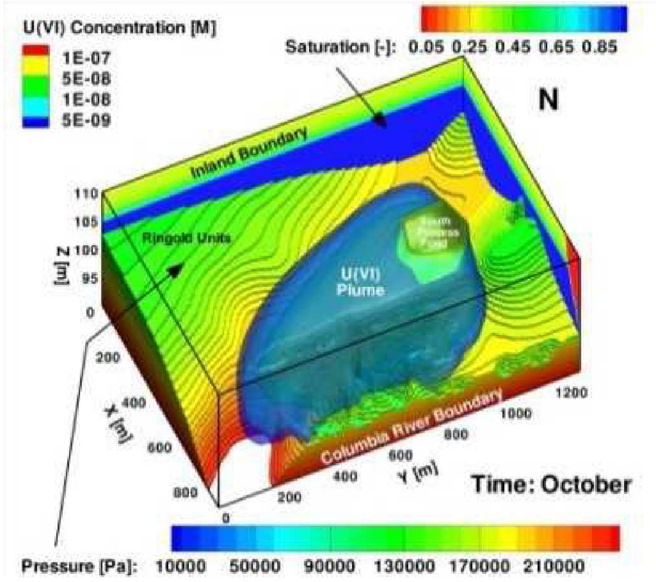
Agriculture
Apatite reactive barrier
Behind-casing pressure development in well annulus
Biogeochemical hot spots/hot moments
Biogeochemistry in groundwater-river exchange zones
CO_2 sequestration
Coupled surface/subsurface land mode
Geothermal systems
Groundwater age
Groundwater management
Interpretation of in-situ through-diffusion experiments
Modelling of enhanced oil recovery (using CO_2 as solvent)
Modelling of oil and gas reservoirs
Mountain block recharge beneath soil mantled hill slopes
Multicomponent transport of trace gases
Nuclear waste repository performance assessment
Nuclear waste repository near-field models
Permafrost modeling
pH sweep and water quality data analysis
Radionuclide transport
Redox gradients within hyporheic zones
Remediation design
Species specific diffusion and Donnan equilibrium in clays
Surface/hill slope hydrology

DOE NE's Geologic Disposal Safety Assessment Framework



Mariner et al. 2016

Uranium migration (Hanford 300 Area)



Hammond and Lichtner, 2010

WIPP PA Flow and Transport Scenarios

S1 – Undisturbed

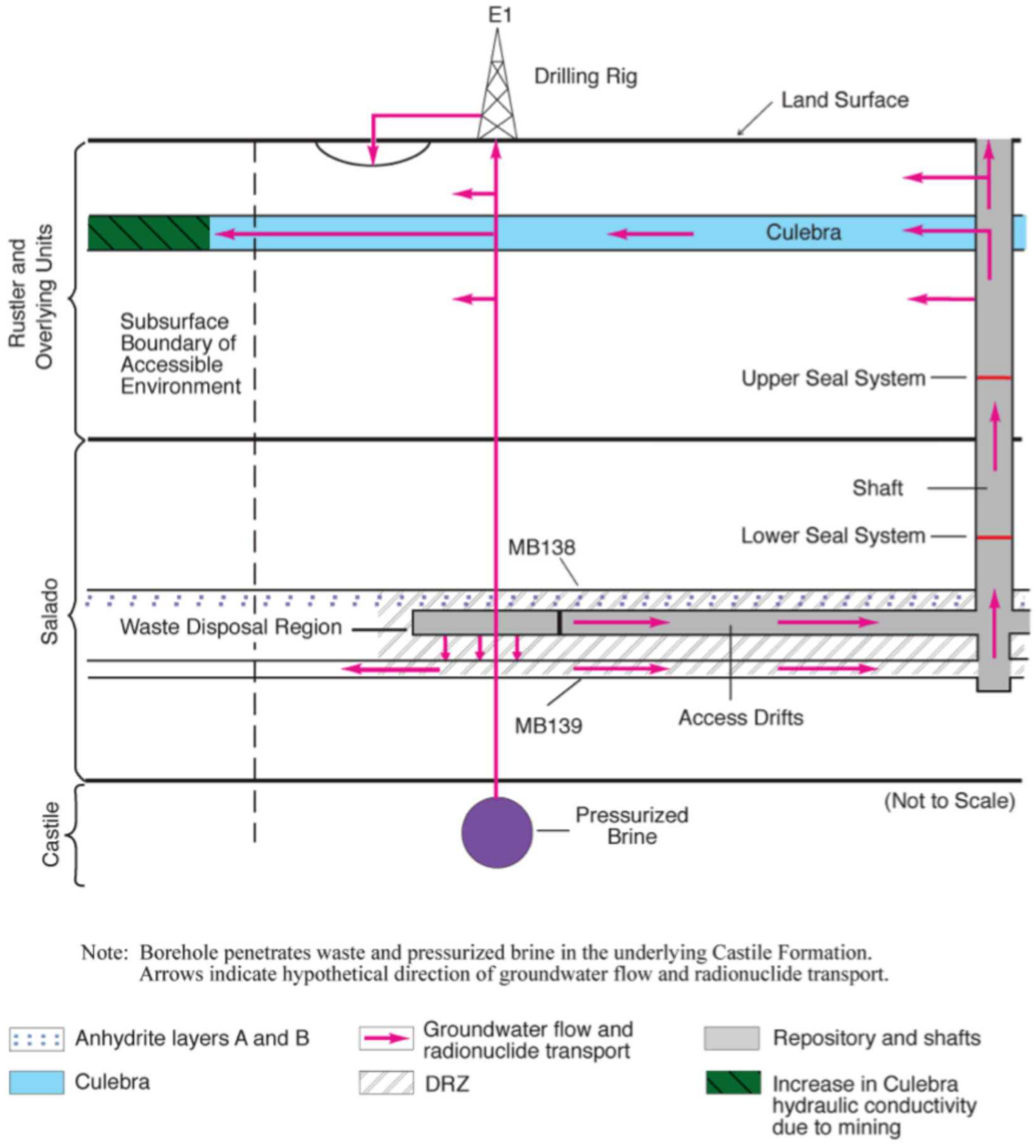
S2 – Intrusion 350 y into pressurized brine pocket

S3 – Intrusion 1000 y into pressurized brine pocket

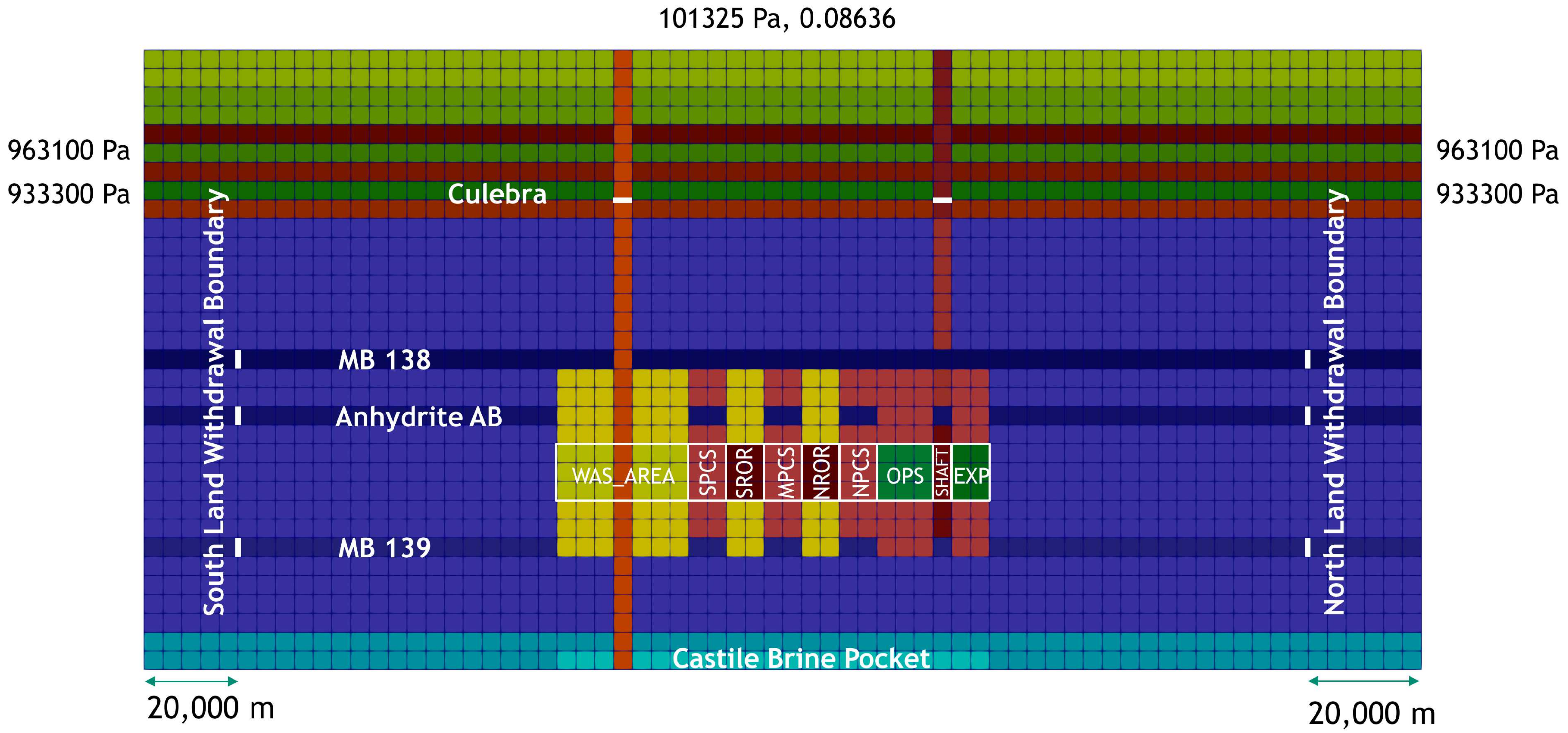
S4 – Intrusion 350 y

S5 – Intrusion 1000 y

S6 – Intrusion at 1000 y, second intrusion at 2000 y into pressurized brine pocket



WIPP PA Flow and Transport – 2-D Flared Grid

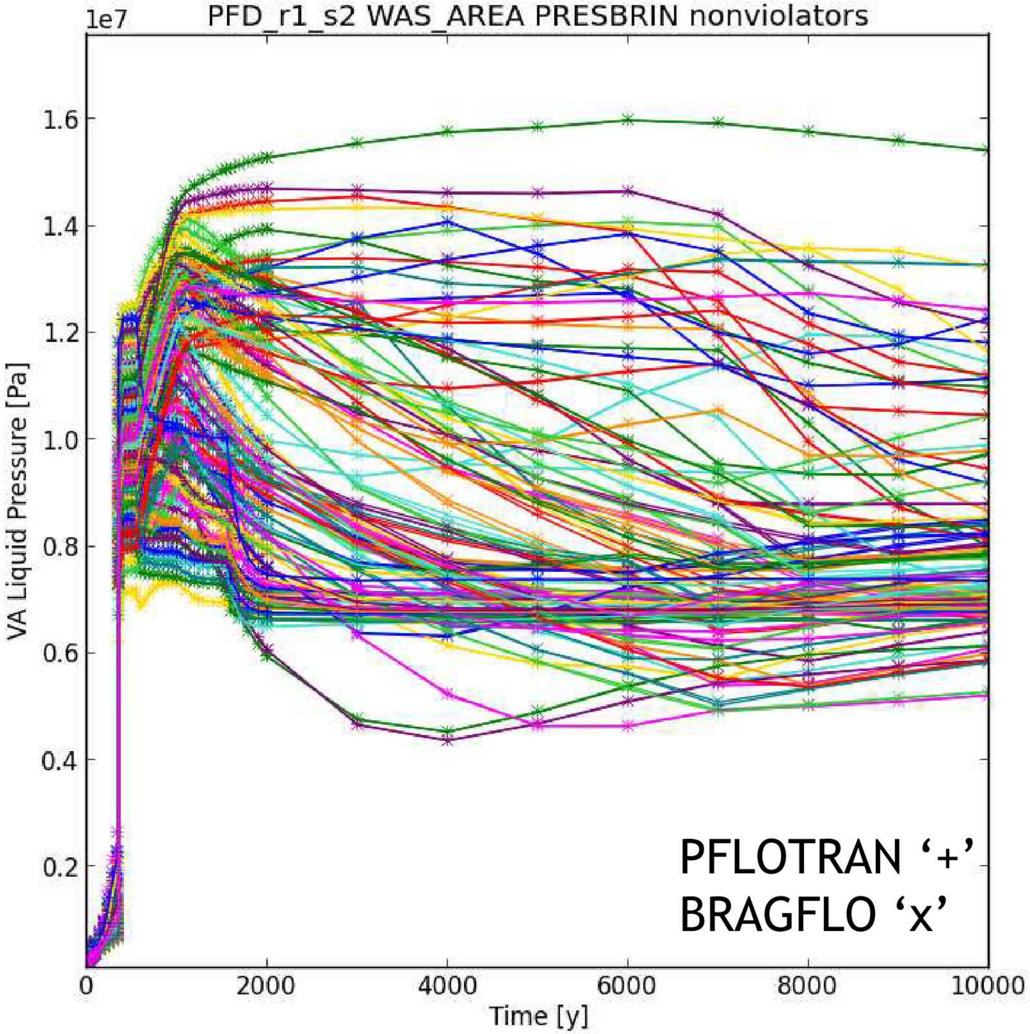


PFLOTRAN-BRAGFLO Comparison

Objectives

- Verify that 2-phase immiscible flow and WIPP-specific process models are implemented correctly in PFLOTRAN
- Verify that PFLOTRAN performs robustly over the entire sample space used in WIPP PA
- Quantify differences between BRAGFLO and PFLOTRAN flow solutions

Replicate 1, Scenario 2
Volume-weighted average brine pressure in the waste area



PFLOTRAN-NUTS Comparison

Objectives

- Verify that WIPP-specific transport capabilities are implemented correctly in PFLOTRAN
- Verify that PFLOTRAN performs robustly over the entire sample space used in WIPP PA
- Assess differences between NUTS and PFLOTRAN transport solutions

Scope

- Development of NUCLEAR_WASTE_TRANSPORT mode in PFLOTRAN
- PFLOTRAN-NUTS comparison on suite of 0-D, 1-D, and 2-D test problems
- PFLOTRAN-NUTS comparison on suite of 1500 PA simulations (S1-S5)

PFLOTRAN Nuclear Waste Transport (NWT) Mode

WIPP-specific transport capabilities

- Handles dry-out (formulation and discretization of governing equations is robust at 100% gas saturation)
- Conservation of species mass at step change in porosity (e.g., borehole intrusion)
- Calculation of advective fluxes on flared grid (comparison to existing baseline)

Other

- Phase partitioning (solid, aqueous, sorbed)
- Decay and ingrowth (in all phases)
- Advection in liquid phase (which may coexist with a mobile gas phase)
- Diffusion in liquid phase (neglected in WIPP PA)

Mass Conservation Equations

SUBSURFACE_TRANSPORT

Ψ_j = mol j / L fluid

$$\underbrace{\frac{\partial}{\partial t}\left(\varphi \sum_{\alpha} s_{\alpha} \Psi_j^{\alpha}\right)}_{\text{Change in mass in fluid phase(s)}} + \overbrace{\nabla \cdot \sum_{\alpha} \Omega_j^{\alpha}}^{\text{Flux (advection \& dispersion)}} = \underbrace{Q_j}_{\text{Source/sink}} - \overbrace{\sum_m \nu_{jm} I_m}^{\text{Rate-controlled mineral precipitation and dissolution}} - \underbrace{\frac{\partial S_j}{\partial t}}_{\text{Change in sorbed concentration}},$$

NUCLEAR_WASTE_TRANSPORT

$\sum \mathcal{M}_j^{\alpha}$ = mol j / m³ bulk

$$\underbrace{\frac{\partial}{\partial t}\left(\mathcal{M}_j^A + \mathcal{M}_j^P + \mathcal{M}_j^S\right)}_{\text{Change in total mass in bulk material}} + \overbrace{\mathcal{F}_j^A}^{\text{Flux (advection \& dispersion)}} = \underbrace{Q_j}_{\text{Source/sink}} + \overbrace{R_j}^{\text{Decay \& Ingrowth}},$$

Test Suite

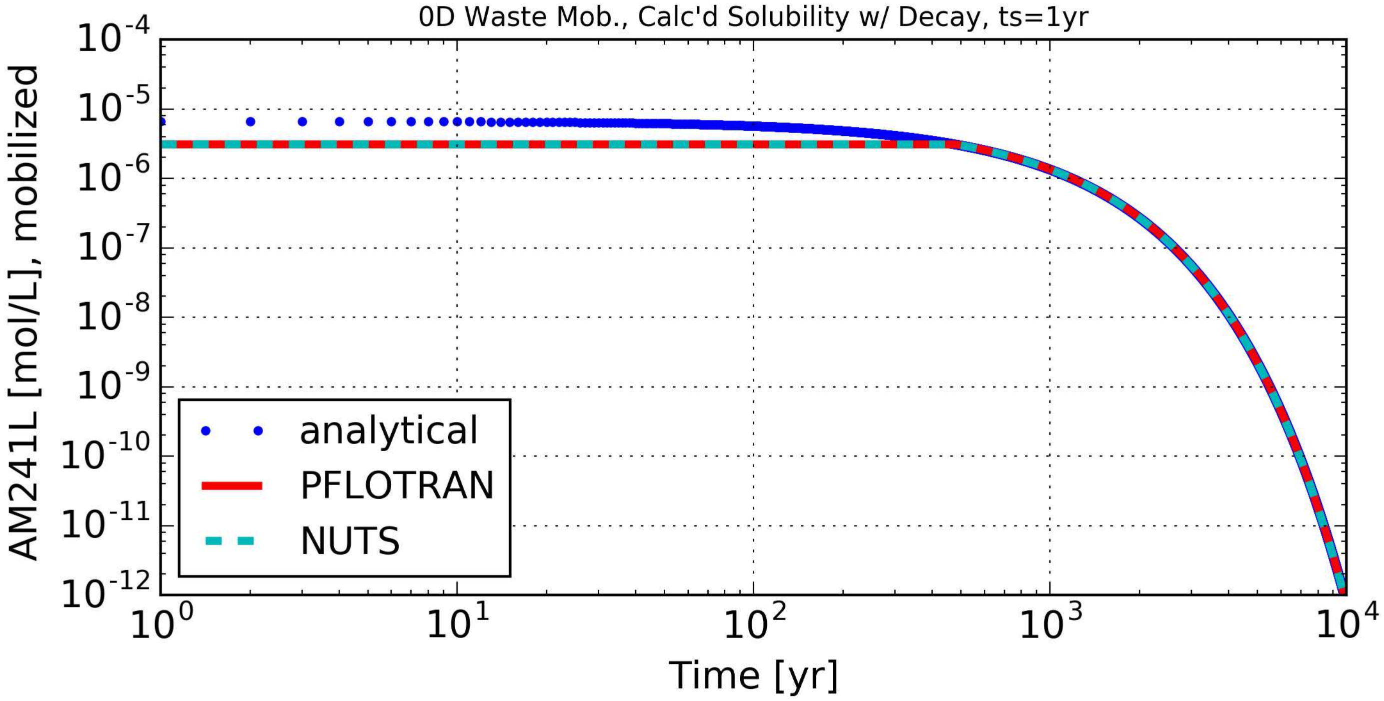
Test problems

- 70 test problems
- 0-D, 1-D, 2-D regular cartesian
- 1-D and 2-D flared grid

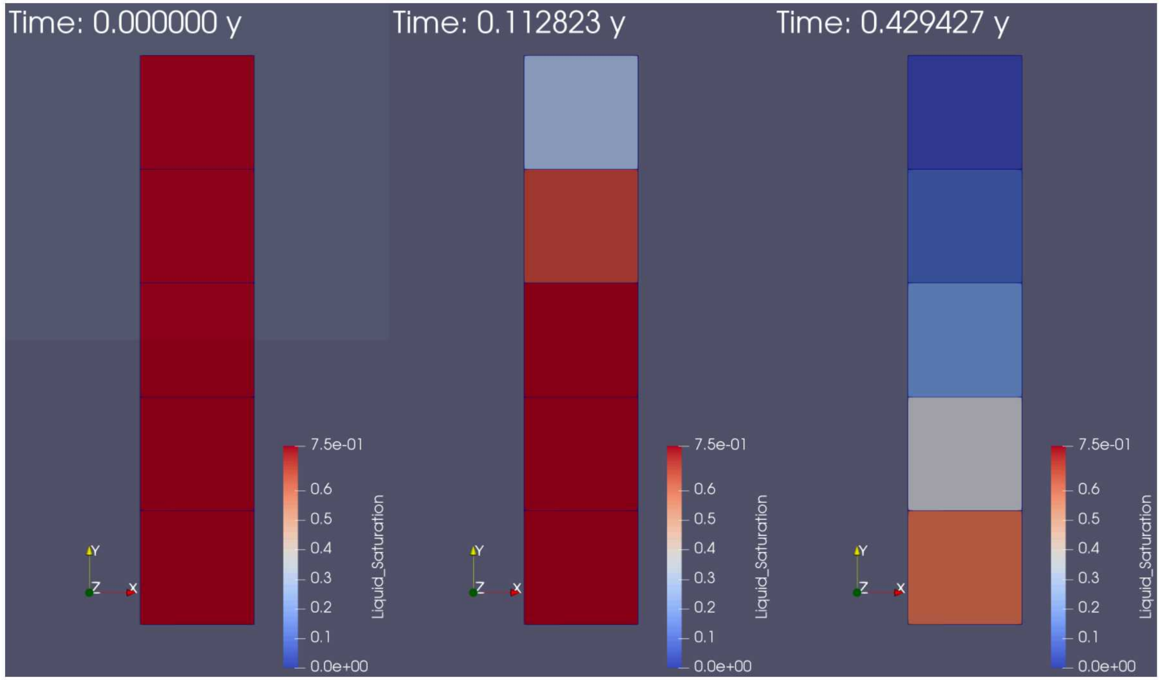
Comparison

- To NUTS solutions
- To analytical solutions

Mobilized concentration in 0-D domain with decay



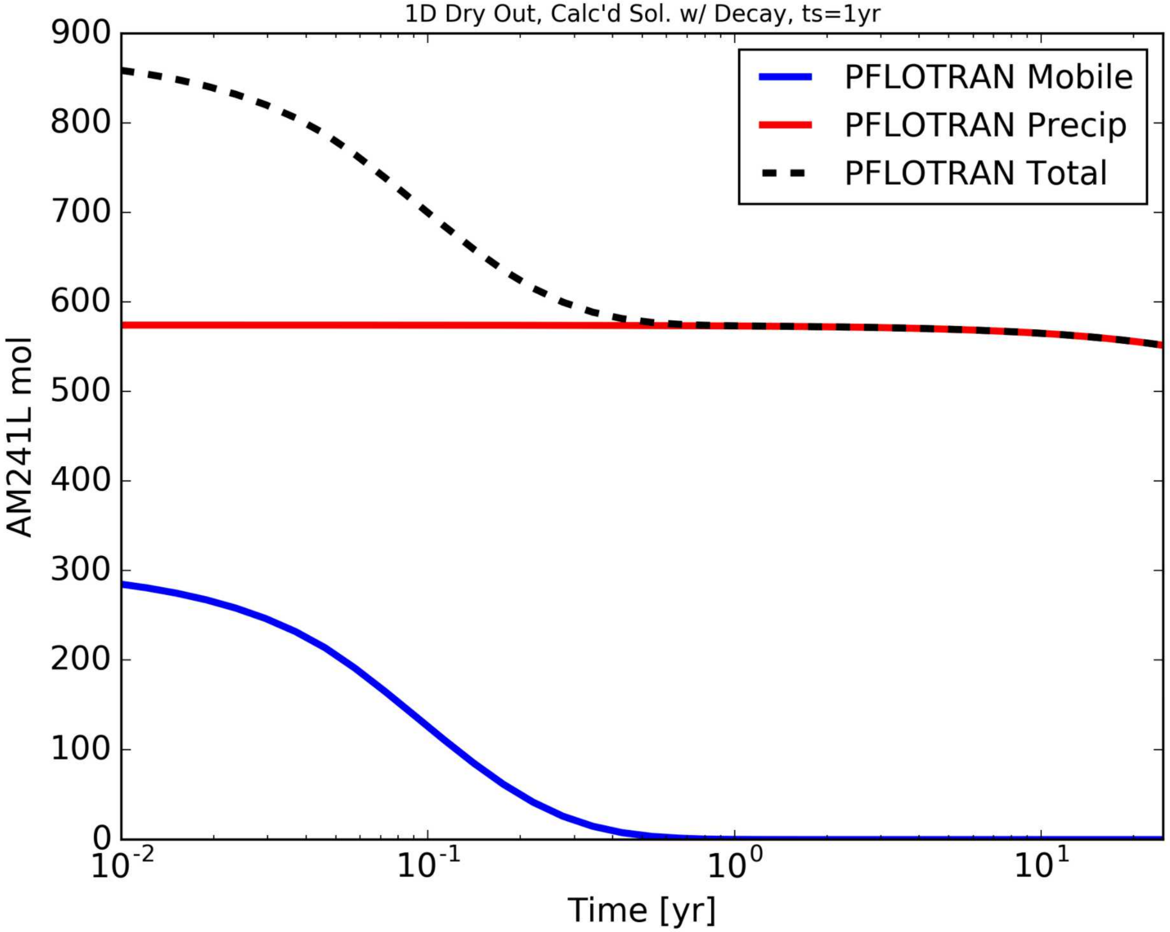
Partitioning of mass during dry-out



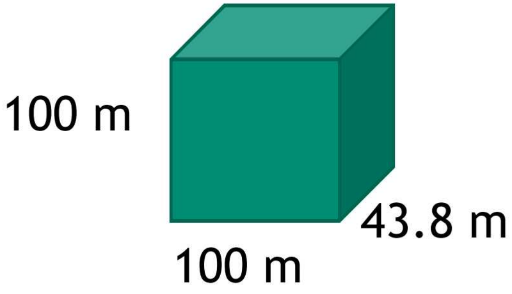
t = 0 y   t = 0.1 y   t = 0.4 y

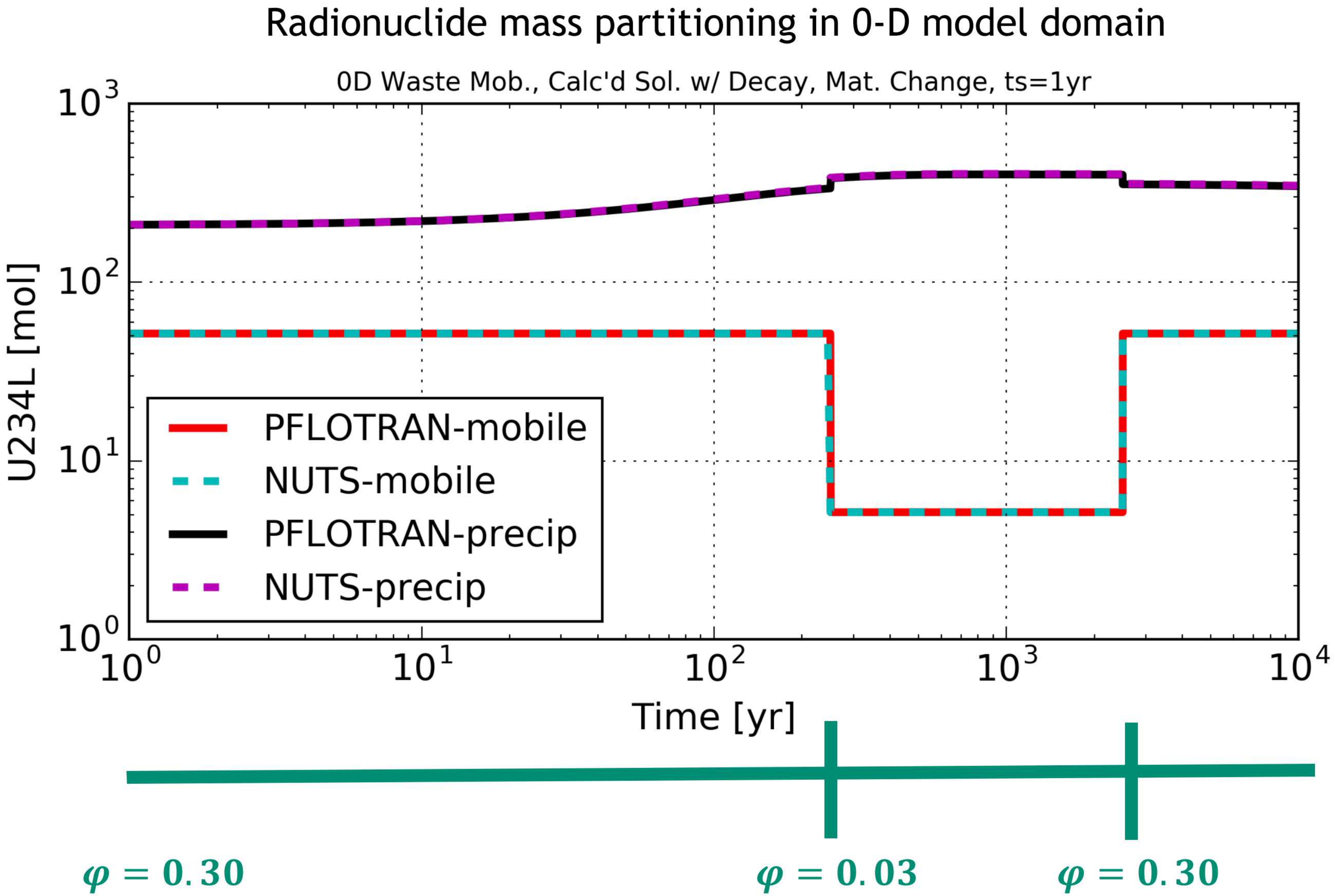
Liquid saturation in draining 1-D model domain

Radionuclide mass partitioning in uppermost grid cell

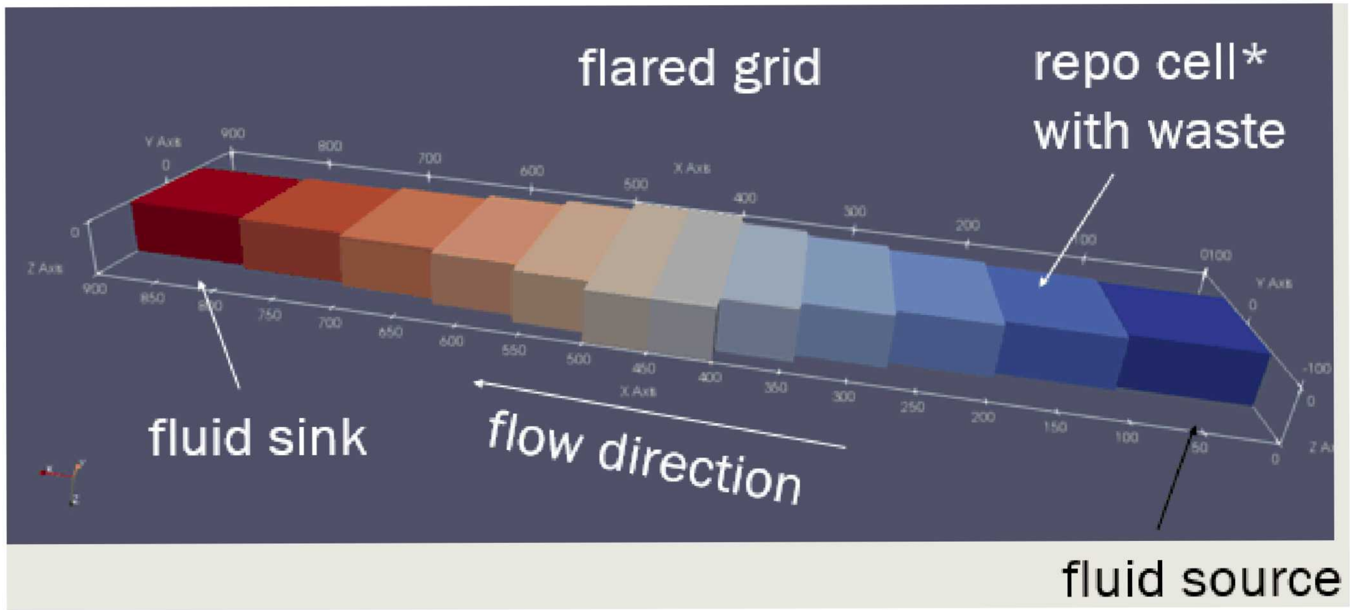


Partitioning of Mass During Step Change in Porosity (φ)

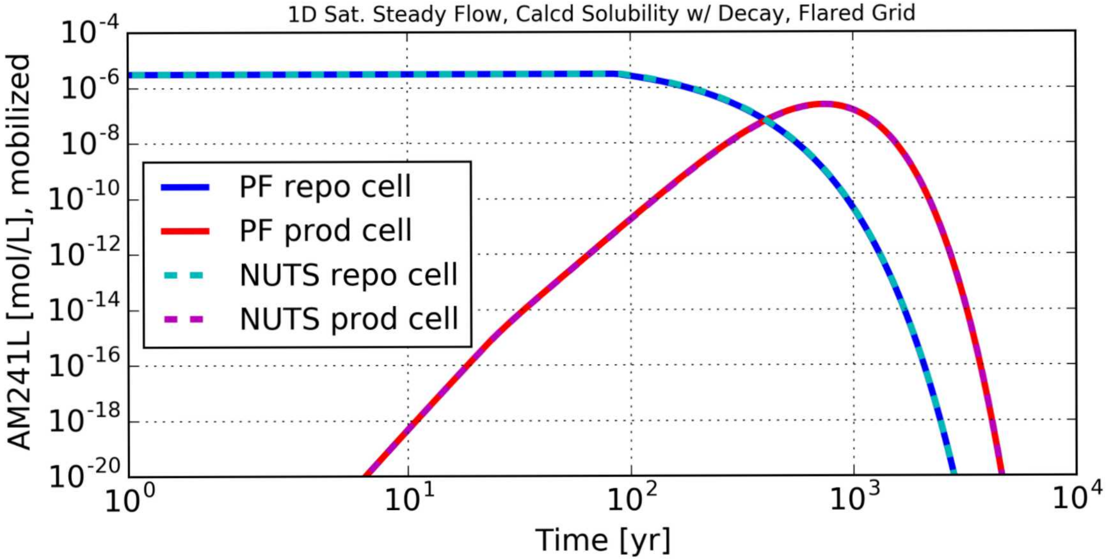




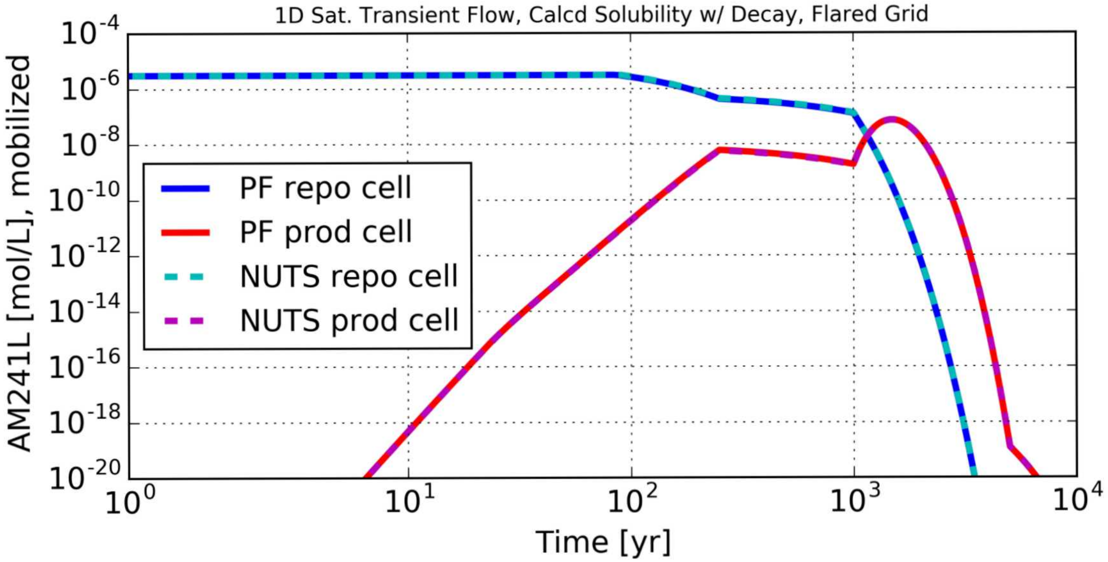
Flux Calculation on Flared Grid



Mobilized concentration w/ steady flow



Mobilized concentration w/ transient flow



Summary

Flow

- Comparison to BRAGFLO demonstrates that 2-phase immiscible flow and WIPP-specific process models are implemented correctly in PFLOTRAN
- WIPP_FLOW mode performs robustly over the entire sample space used in WIPP PA

Transport

- Comparison to NUTS demonstrates that WIPP-specific transport capabilities are implemented correctly in PFLOTRAN

Next

- PFLOTRAN-NUTS comparison on 1500 WIPP PA realizations
- Development and demonstration of 3-D problem

References

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