Verification of PFLOTRAN for 3-D WIPP Performance Assessment: PFLOTRAN-BRAGFLO Benchmark

PRESENTED BY
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Waste Isolation Pilot Plant (WIPP)

- Transition to a 3-D model domain for Performance Assessment
- Development of WIPP_FLOW mode in PFLOTRAN
- PFLOTRAN-BRAGFLO benchmark
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/)
- Strong scaling to over 10,000 cores

**Flow Modes**

- RICHARDS – single phase variably saturated
- TH (Thermo-Hydro) – Richards equation + Energy
- GENERAL – Multiphase Air-Water-Energy
- MPHASE – Supercritical CO$_2$-Water-Energy
- IMMIS – Immiscible CO$_2$-Water-Energy
- MISCIBLE – Miscible Water-Glycol
- FLASH2 – Supercritical CO$_2$-Water-Energy
PFLOTRAN Usage

- Agriculture
- Apatite reactive barrier
- Behind-casing pressure development in well annulus
- Biogeochemical hot spots/hot moments
- Biogeochemistry in groundwater-river exchange zones
- CO₂ 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 CO₂ 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

Uranium migration (Hanford Area 300)

Hammond and Lichtner, 2010
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

Scope

• Development of WIPP_FLOW mode in PFLOTRAN

• PFLOTRAN-BragFLO comparison on suite of 0-D, 1-D, and 2-D test problems

• PFLOTRAN-BragFLO comparison on suite of 1800 PA simulations
Development of WIPP_FLOW mode in PFLOTRAN

• Two-phase immiscible flow

• Fully coupled WIPP-specific process models and constitutive relationships
  • Gas generation, brine consumption/generation
  • Creep closure
  • Fracturing of marker beds and DRZ
  • Soil compressibility
  • Characteristic curves (capillary pressure, relative permeability)
  • Klinkenberg effect (gas permeability)
  • Redlich-Kwong-Soave Gas Equation of State

• Material Changes
  • Evolution of DRZ and Shaft
  • Borehole Intrusion and Evolution
## Development of WIPP_FLOW mode in PFLOTRAN

<table>
<thead>
<tr>
<th>BRAGFLO Variable</th>
<th>BRAGFLO Label</th>
<th>PFLOTRAN Keyword</th>
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WIPP PA Flow Comparison – 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 Comparison – 2-D Flared Grid

- 101325 Pa, 0.08636
- 963100 Pa
- 933300 Pa
- Culebra
- Anhydrite AB
- MB 138
- MB 139
- South Land Withdrawal Boundary
- North Land Withdrawal Boundary
- Castile Brine Pocket

- WAS_AREA
- SPCS
- SROR
- NPCS
- NNROR
- NPCS
- OPS
- SS
- EXP
Borehole is the only potential release pathway with liquid fluxes (away from the repository) large enough to advect radionuclides to the accessible environment.

Such fluxes occur only Scenarios 2, 3, and 6, in which the borehole penetrates the pressurized brine pocket.

Focus on comparison of WAS_AREA Pressure and Borehole/Culebra Flow in Scenarios 2, 3, and 6.

- Quantify time-integrated differences
- Compare uncertainty distributions at discrete times
Quantification of Time-Integrated Differences

Liquid Pressure and Saturation

Abs. Diff. = \( \int_0^{10000} \frac{\text{abs}(\text{BRAGFLO} - \text{PFLOTRAN})}{10000} \, dt \)

Rel. Diff. = \( \frac{\int_0^{10000} \text{abs}(\text{BRAGFLO} - \text{PFLOTRAN}) \, dt}{\int_0^{10000} \text{BRAGFLO} \, dt} \)

Liquid Flow

Abs. Diff. = \( \int_0^{10000} \text{abs}(\text{BRAGFLO} - \text{PFLOTRAN}) \, dt \)

Rel. Diff. = \( \frac{\int_0^{10000} \text{abs}(\text{BRAGFLO} - \text{PFLOTRAN}) \, dt}{\int_0^{10000} \text{abs}(\text{BRAGFLO}) \, dt} \)
Time-Integrated Differences – WAS_AREA Pressure R1S2

![Graph showing time-integrated differences in WAS_AREA pressure R1S2](image)

- **X-axis**: Time [y] ranging from 0 to 10,000
- **Y-axis**: Liquid pressure [Pa] ranging from 0 to 1.6
- **Legend**: PFD r1_s2 WAS_AREA PRESBRIN nonviolators

![Graph showing relative difference area between curves](image)

- **X-axis**: Difference: Area Between the Curves / Time
- **Y-axis**: Relative Difference Area Between the Curves / Area Under B养老o Curve

The graphs illustrate the time-integrated differences in WAS AREA pressure for different time periods, highlighting variations and patterns over time.
Time-Integrated Differences – WAS_AREA Liquid Pressure

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<th>Relative Difference</th>
<th>Absolute Difference (Pa)</th>
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<td>3</td>
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<td>6</td>
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Time-Integrated Differences – Borehole/Culebra Liquid Flow

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<th>Absolute Difference (kg)</th>
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<tr>
<td>Scenario 3</td>
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<tr>
<td>Scenario 6</td>
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</table>
Uncertainty Distribution v. Time – WAS_AREA Pressure R1S2
Uncertainty Distribution – Borehole/Culebra Cumulative Flow at 10 ky
Summary

• Comparison to BRAGFLO demonstrates that 2-phase immiscible flow and WIPP-specific process models are implemented correctly in PFLOTRAN

• PFLOTRAN performs robustly over the entire sample space used in WIPP PA

• Differences between BRAGFLO and PFLOTRAN flow solutions are sufficiently small that the transition to PFLOTRAN (for flow calculations) should have minimal impact on PA

• Next steps:
  • Similar comparison underway for radionuclide transport (PFLOTRAN-NUTS)
  • 3-D problem under development


Uncertainty Distribution – Shaft/Culebra Flow

Cumulative Flux Stats for shaft culebra

Toward repository

Replicate/Scenario

Cumulative Flux at 100,000 y [Kg]
Uncertainty Distribution – Marker Bed Flow

Cumulative Flux Stats for lwb_south_anhydrite

Toward repository

Away from repository

Replicate/Scenario

Cumulative Flux at 10000 y [kg]