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A Next-Generation Transport Simulator for the Waste Isolation Pilot Plant (WIPP) Performance Assessment

Jennifer M. Frederick, Michael A. Nole, and Heeho Park

IHLRWM 2022

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Disposal IV

This research is funded by WIPP programs administered by the Office of Environmental Management (EM) of the U.S. Department of Energy.



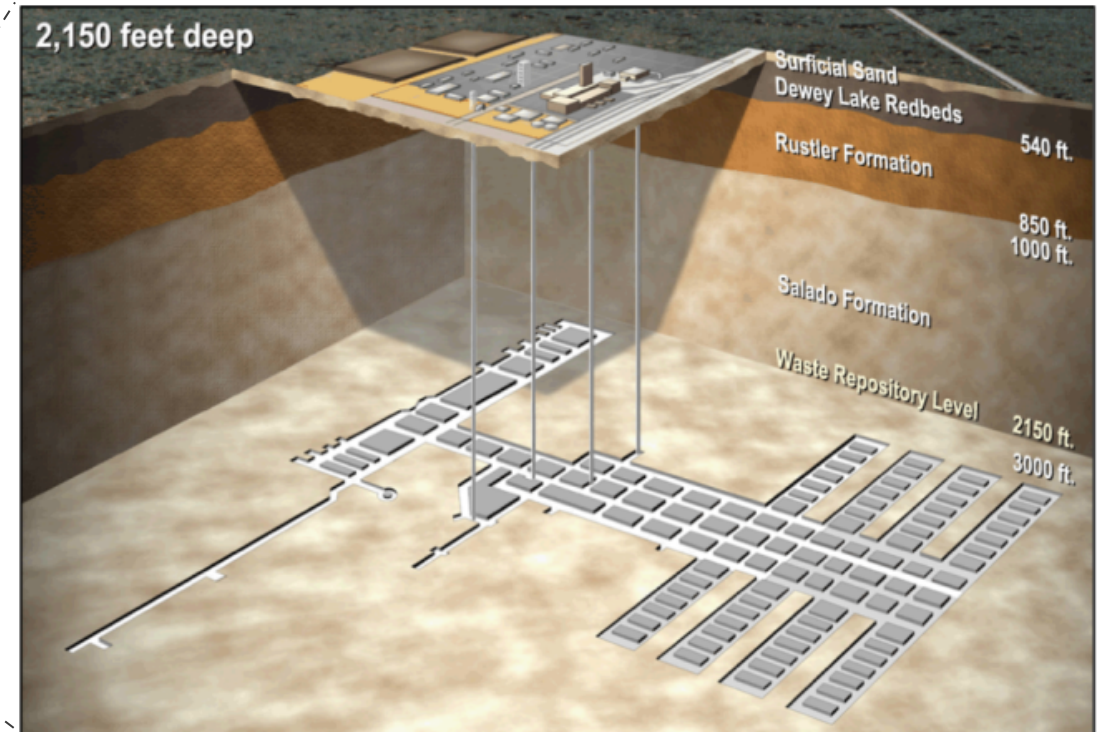
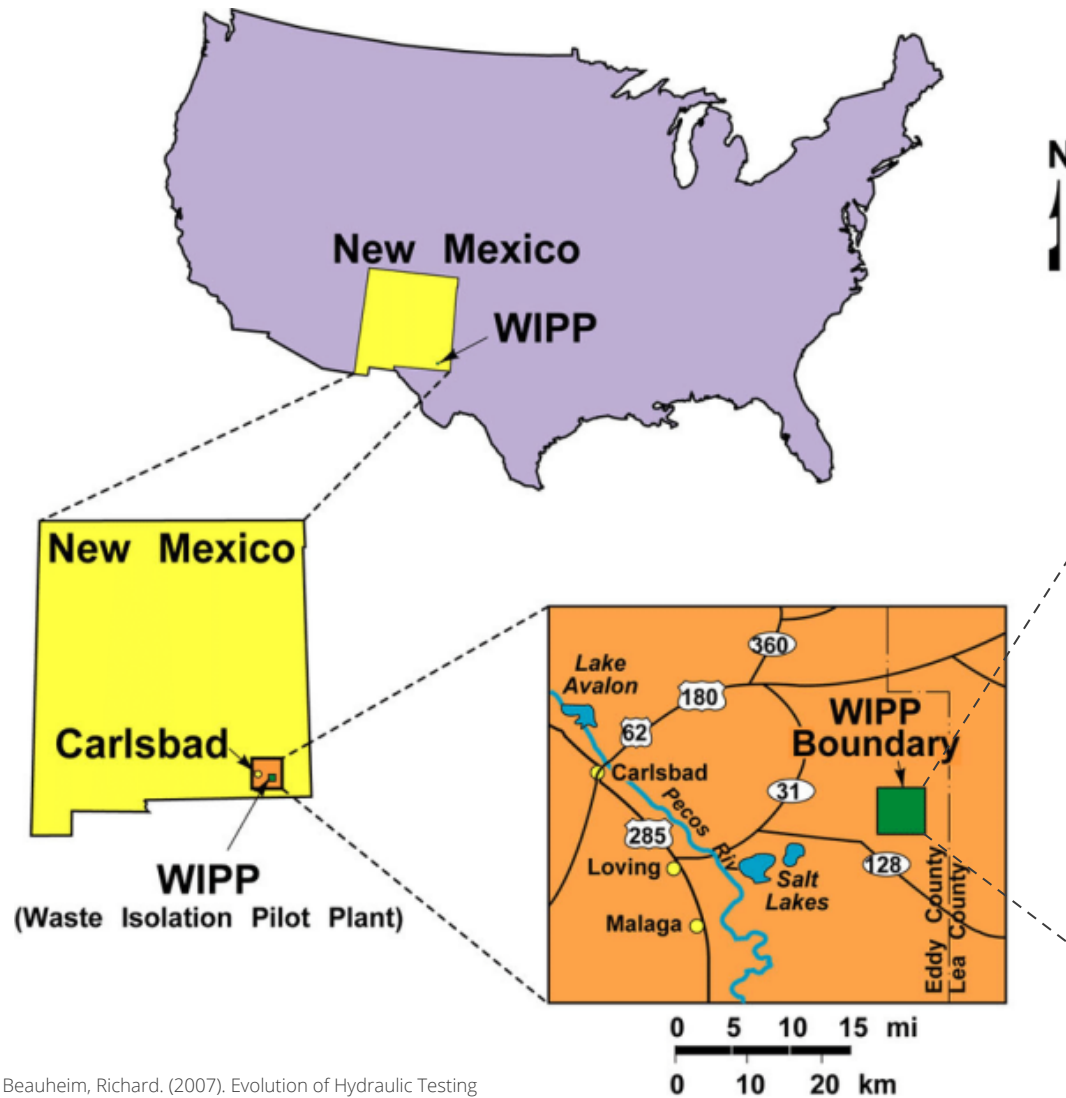
- Transport needs for WIPP performance assessment
- PFLOTRAN's Nuclear Waste Transport (NWT) Mode
 - Process model coupling
 - Governing equations
 - Solution technique





Waste Isolation Pilot Plant (WIPP)

- The WIPP is the nation's only licensed deep geologic repository for defense-related transuranic waste
- Operated by U.S. Department of Energy (DOE)
- Long-term performance regulated by U.S. Environmental Protection Agency (EPA)



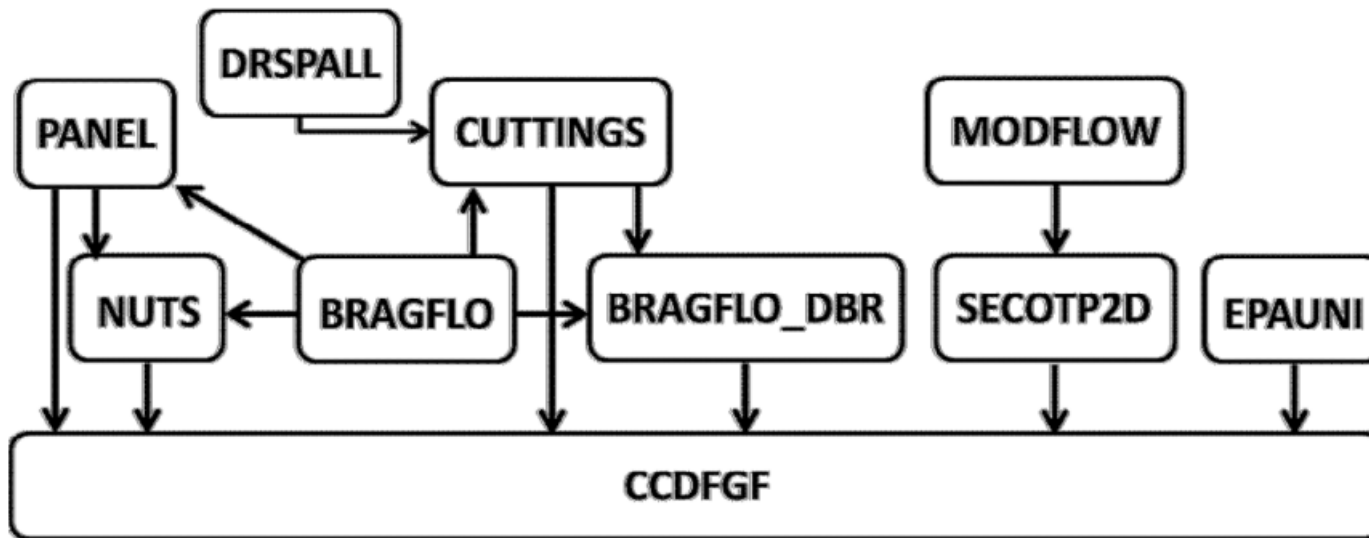
Beauheim, Richard. (2007). Evolution of Hydraulic Testing at the Waste Isolation Pilot Plant.

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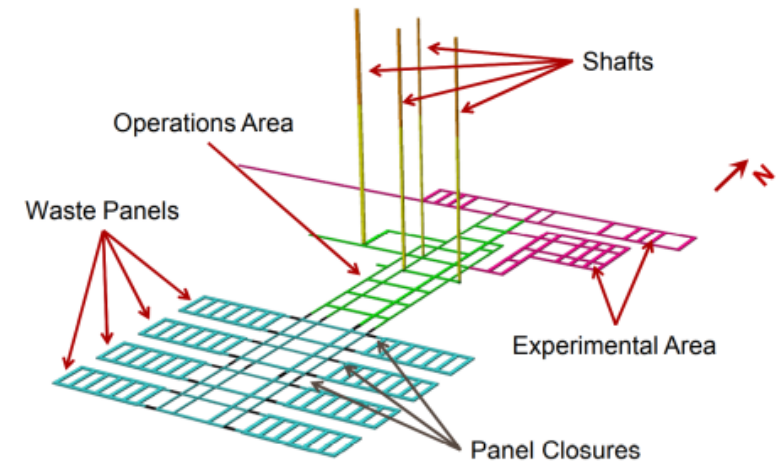


WIPP Performance Assessment

- Performance assessment (PA) calculations cover 24 peer-reviewed conceptual models.
- PA computations include 10 principal codes and many utility codes.



Long-term regulatory compliance is demonstrated via Performance Assessment (PA) undertaken by Sandia National Laboratories, Carlsbad.



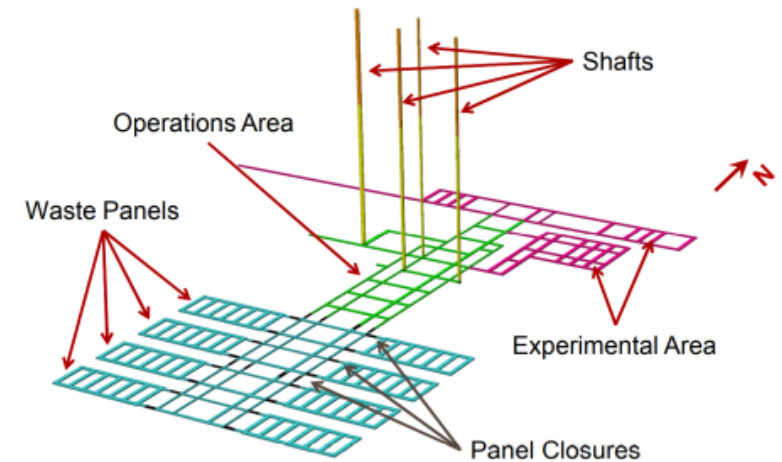
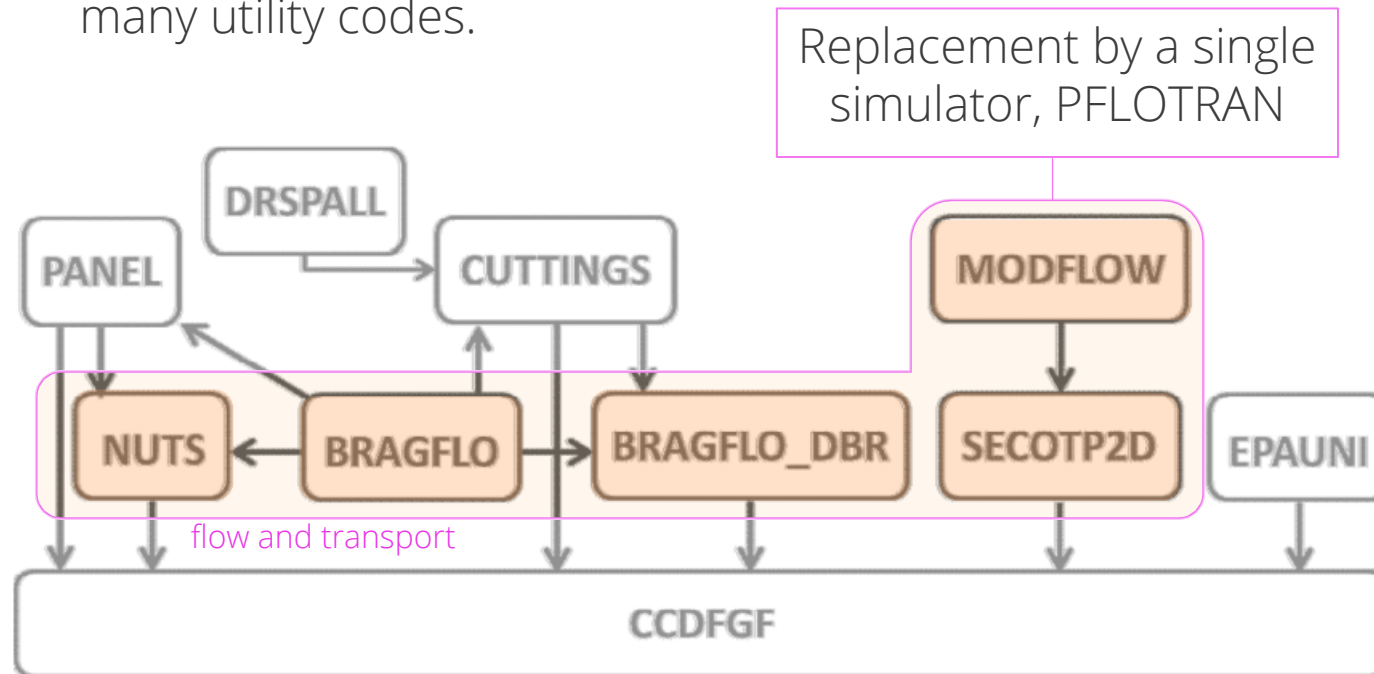
DOE is interested in reducing the number of principal codes to improve efficiencies for an asymmetric repository.



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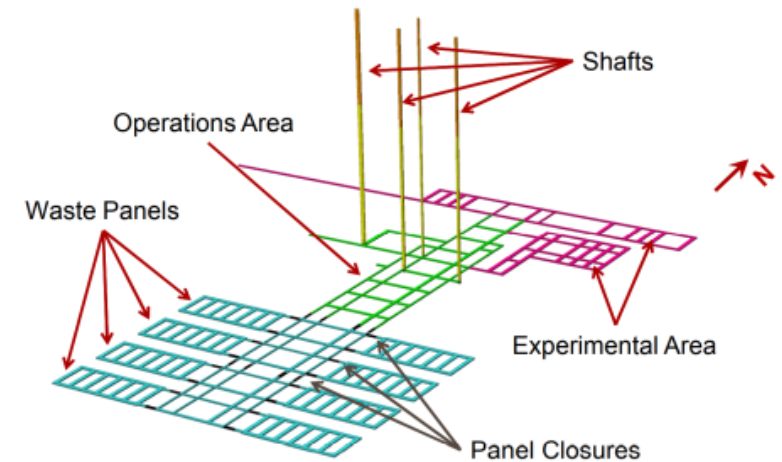
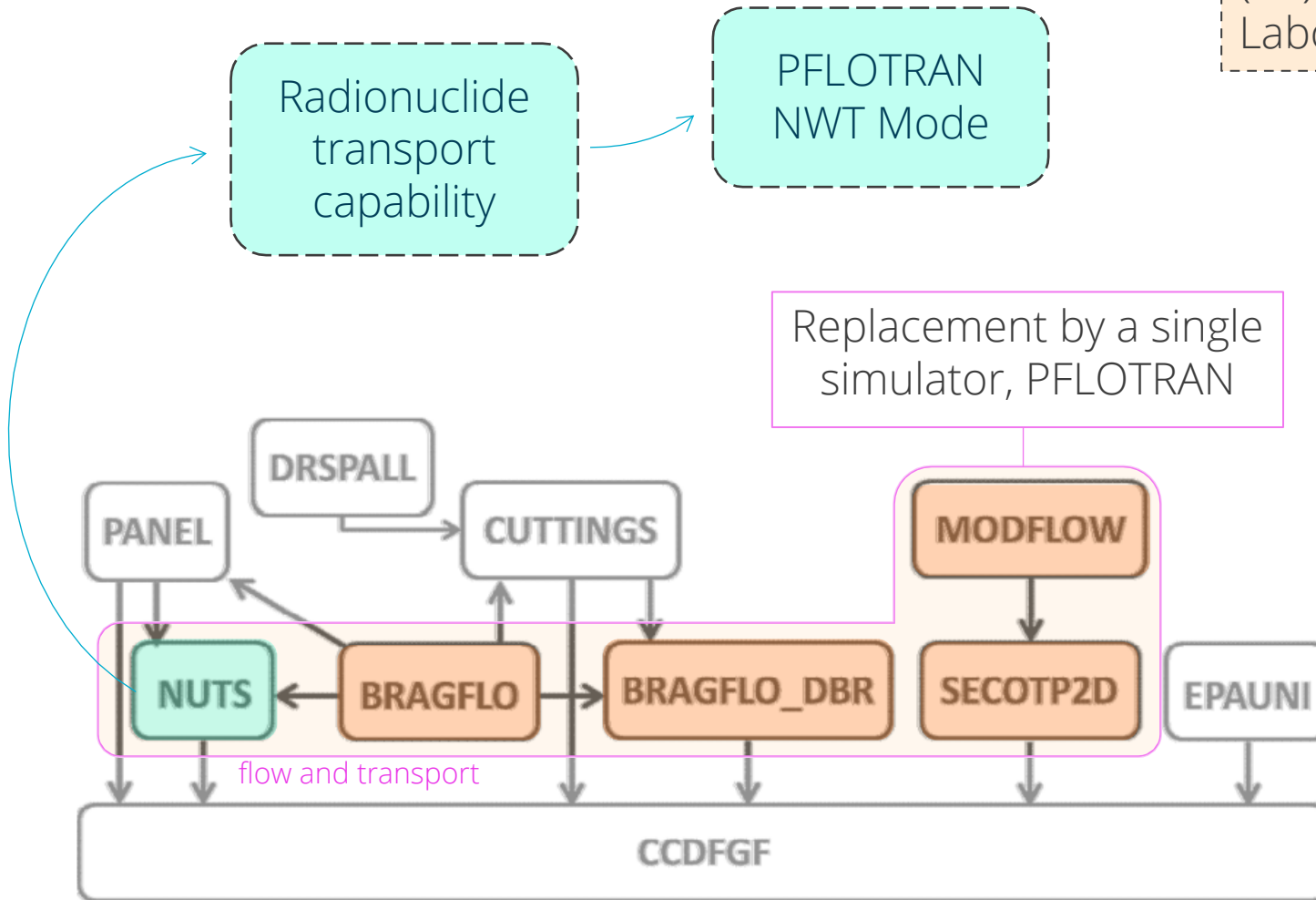


DOE is interested in reducing the number of principal codes to improve efficiencies for an asymmetric repository.



WIPP Performance Assessment

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PFLOTRAN

- Petascale reactive multiphase flow and transport simulator
- Open source license (GNU LGPL-2.1)
- Object-oriented modern FORTRAN
- Founded upon well-known (supported) open source libraries:
 - MPI, PETSc, HDF5, METIS/ParMETIS, CMAKE
- Demonstrated in high performance computing (massively parallel)
- Version control with regression testing and rigorous code reviews before new code is introduced

Open Source Repository (Bitbucket)

The screenshot shows the Bitbucket web interface for the PFLOTRAN repository. The left sidebar contains navigation links: Source, Commits (selected), Branches, Pull requests, Pipelines, Deployments, Issues, Jira issues, Security, Wiki, and Downloads. The main content area is titled 'PFLOTRAN / code / pflotran Commits' and includes a search bar and a dropdown for 'All branches'. A commit history table is displayed with columns for Author, Commit, Message, Date, and Builds. The table lists 15 commits, including updates, initializations, and merges, with build status indicators (green checkmarks or red diamonds) in the Builds column.

Author	Commit	Message	Date	Builds
Piyosh Jaysaval	4a4bcd8	Updating regr... piyosh/coupled-flow-ert	22 hours ago	✓
Piyosh Jaysaval	b889bd8	Initializing del... piyosh/coupled-flow-ert	yesterday	✗
Jenn Frederick	de58ff5	Added output for... jenn/wipp-well-model	2 days ago	✓
Glenn Hammond	eeacfc4	Added gas c... glenn/gas-conc-in-out-file	2 days ago	✓
Glenn Hammond	4f42d97	MERGED: Merged in glenn/add-vtk-acknowle...	2 days ago	✓
Alex Salazar	8df443f	MERGED: Merged in alex/mwt-wasteform-pm ...	2 days ago	✓
Rosie Leone	67581e6	MERGED: Merged in rosie/mc-variable-fix (pu...	2 days ago	✓
Alex Salazar	d4c2617	MERGED: Merge branch 'master' into alex/nw...	2 days ago	✓
Alex Salazar	7c9b305	DPC-58: Remove DEBUG statements and unu...	2 days ago	✓
Glenn Hammond	05d8f92	added card to allow VTK output for unstruct...	2 days ago	✓
Glenn Hammond	9ed53e3	MERGED: Merged in glenn/merge-adjoint-ba...	2 days ago	✓
Glenn Hammond	c6f65e3	refacted adjoint, merging backward and forw...	3 days ago	✓
Glenn Hammond	dc3700b	removed ... glenn/cleanup-inverse-adjoint	3 days ago	✓
Piyosh Jaysaval	8f48ac7	Fixing derivati... piyosh/coupled-flow-ert	3 days ago	✓
Glenn Hammond	55dad4d	removed ... glenn/cleanup-inverse-adjoint	3 days ago	✓
Glenn Hammond	74c34f8	remove s... glenn/cleanup-inverse-adjoint	3 days ago	✓
Glenn Hammond	6ce0318	removed ... glenn/cleanup-inverse-adjoint	3 days ago	✓



WIPP Performance Assessment Requirements

WIPP PA Requirements Document for PFLOTRAN Version 3.0.1

Requirements Document
for PFLOTRAN Version 3.0.1

Darcy's law and liquid and gas equations of state. PFLOTRAN solves the discretized equations with a fully implicit Newton-Krylov iteration. Process models describing gas closure of the repository, and gas generation and brine iron, biodegradation of waste components, MgO hydrate radiolysis of water due to radioactive decay are fully coupled.

2.0 REQUIREMENTS

2.1 Functional Requirements

The functional requirements for simulating two-phase flow in PFLOTRAN 3.0.1 are listed below.

2.1.1 INPUT AND OUTPUT

- R.1 PFLOTRAN reads input parameters that define controls, and solution output format from a file.
- R.2 PFLOTRAN accepts material properties as parameters, intrinsic permeability, porosity. Also specified are the relative permeability for each material.
- R.3 PFLOTRAN outputs and reads back in a binary primary solution variables necessary to restart time-dependent source terms.
- R.4 PFLOTRAN writes output files of the primary gas saturation. Other user-specified outputs:
 - 1) liquid and gas fluxes across user-specified boundaries;
 - 2) liquid and gas fluxes across the boundaries;
 - 3) concentrations of reactants in rate-controlled gas and liquid source/sink terms;
 - 4) material properties: porosity, permeability;
 - 5) cell volume
- R.5 PFLOTRAN writes binary-format files containing variables at all grid cells in the model domain.

2.1.2 FINITE VOLUME GRID

- R.6 PFLOTRAN constructs a finite volume three-dimensional grid, cell interface areas, and locations of two inputs:

Requirements Document
for PFLOTRAN Version 3.0.1

ERM56 573098
June 2021

- 1) grid dimensions and spacing in three dimensions (a structured grid); or
- 2) x, y, and z coordinates of vertices and ordered lists of vertices associated with each cell in the grid (an implicit unstructured grid).

These input parameters may also specify whether regions of the model are dipping.

2.1.3 INITIAL AND BOUNDARY CONDITIONS

R.7 PFLOTRAN sets

- 1) PFLOTRAN input files; and
- 2) PFLOTRAN regions of the specified reference.

R.8 PFLOTRAN sets

- gas source/sink to domain. Reactant sulfate; and radio

R.9 PFLOTRAN imp

- boundary condition is specified over a

2.1.4 TWO-PHASE IMMISCIBLE FLOW

R.10 PFLOTRAN num

- of liquid and gas porous medium.

R.11 PFLOTRAN calc

- within each state linear models, an

R.12 PFLOTRAN calc

- function of liquid

R.13 PFLOTRAN calc

- of state for the sp

R.14 PFLOTRAN calc

2.1.5 PROCESS MODELING

R.15 PFLOTRAN sim

- by calculating po of the altered po

Requirements Document
for PFLOTRAN Version 3.0.1

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- R.16 PFLOTRAN simulates the evolution of porosity due to salt creep in user-specified excavated regions of the model domain (e.g., the waste emplacement regions) by interpolating between values in a look-up table describing porosity as a function of liquid pressure and time.

- R.17 PFLOTRAN simulates the Klinsberg effect, whereby the permeability of the porous medium to the gas phase is a function of both the intrinsic permeability of the medium and gas pressure.

2.1.6 GAS AND LIQUID SOURCE/SINK TERMS

- R.18 PFLOTRAN simulates three primary gas-producing reactions:

- 1) anoxic corrosion of iron under:
 - (a) inundated and
 - (b) humid conditions;
- 2) microbial degradation of cellulose, plastics, and rubber under:
 - (a) inundated and
 - (b) humid conditions; and
- 3) radiolysis of brine from radionuclide alpha decay of:
 - (a) dissolved and sorbed radionuclides in solution and
 - (b) the remaining inventory of solid radionuclides that are in contact with brine.

These reactions produce a free gas phase (H_2) as a source term and consume brine as a sink term according to stoichiometric coefficients and rate constants specified as input to PFLOTRAN.

- R.19 PFLOTRAN simulates six additional rate-controlled chemical reactions:

- 1) sulfidation of iron hydroxide;
- 2) sulfidation of iron;
- 3) hydration of MgO under:
 - (a) inundated and
 - (b) humid conditions;
- 4) carbonation of MgO;
- 5) carbonation of $Mg(OH)_2$; and
- 6) conversion of hydromagnesite to magnesite.

Reactions 1, 2, 4, and 5 depend on the microbial degradation rate of cellulose, plastics, and rubber. Rate constants for reactions 3(a), 3(b), and 6 are specified as input to PFLOTRAN. Stoichiometric coefficients for each reaction are specified as input to PFLOTRAN.

Software quality assurance (QA) documents specify requirements for radionuclide transport calculations in WIPP PA.

As dictated by the CFR, per NQA-1,2,3.



WIPP Performance Assessment Requirements

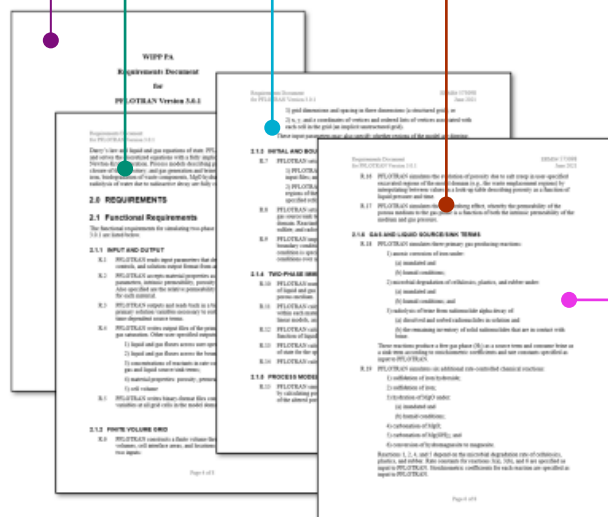
Advection of radioactive species in porous media without diffusion

Equilibrium chemistry with dissolution/precipitation based on solubility limits

Ability to handle completely dry conditions (no liquid)

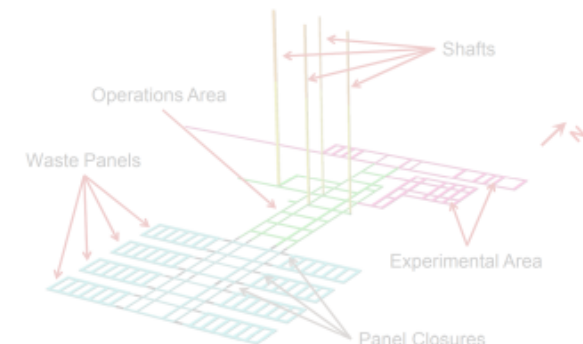
Must run on a 3D grid in parallel

A short selection of the requirements.



WIPP-specific:

Conserves mass across material changes, accommodates borehole intrusion events, can handle check pointing and re-starts, keeps track of species fluxes across arbitrary boundaries, etc. . .





PFLOTRAN Nuclear Waste Transport (NWT) Mode

Governing equation formulated in terms of total mass, M .

$$M_j^\alpha = M_j^A + M_j^P$$
$$\frac{\partial}{\partial t} \sum_\alpha (M_j^\alpha) + \nabla \cdot \sum_\alpha (\mathbf{u}^\alpha M_j^\alpha) = \sum_\alpha (\dot{Q}_j^\alpha) + \sum_\alpha (\dot{R}_j^\alpha)$$

total mass

aqueous

precipitated

sources/sink

fluid velocity

decay/ingrowth

α phase (aqueous, precipitated)

j species (radionuclide, tracer, etc.)



PFLOTRAN Nuclear Waste Transport (NWT) Mode

Governing equation formulated in terms of total mass, M .

total mass

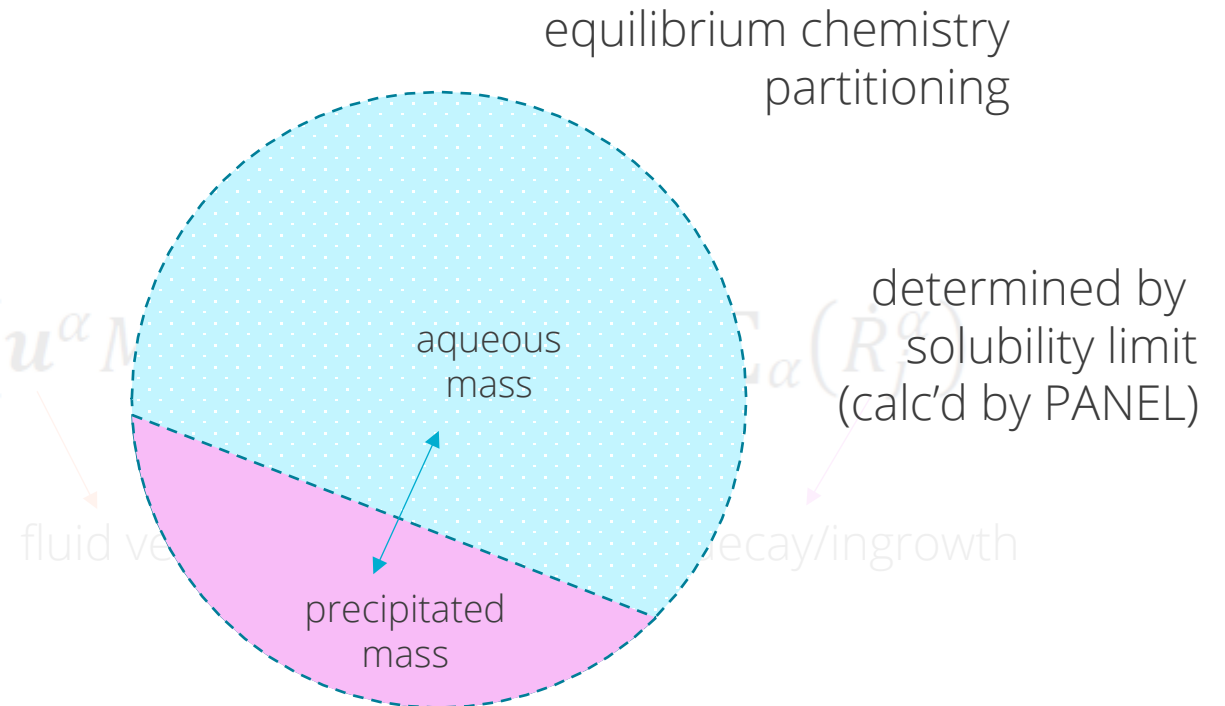
$$M_j^\alpha = M_j^A + M_j^P$$

aqueous precipitated

$$\frac{\partial}{\partial t} \sum_\alpha (M_j^\alpha) + \nabla \cdot \sum_\alpha (\mathbf{u}^\alpha M_j^\alpha)$$

α phase (aqueous, precipitated)

j species (radionuclide, tracer, etc.)





PFLOTRAN Nuclear Waste Transport (NWT) Mode

Governing equation formulated in terms of total mass, M .

$$\overset{\text{total mass}}{M_j^\alpha} = \overset{\text{aqueous}}{M_j^A} + \overset{\text{precipitated}}{M_j^P}$$

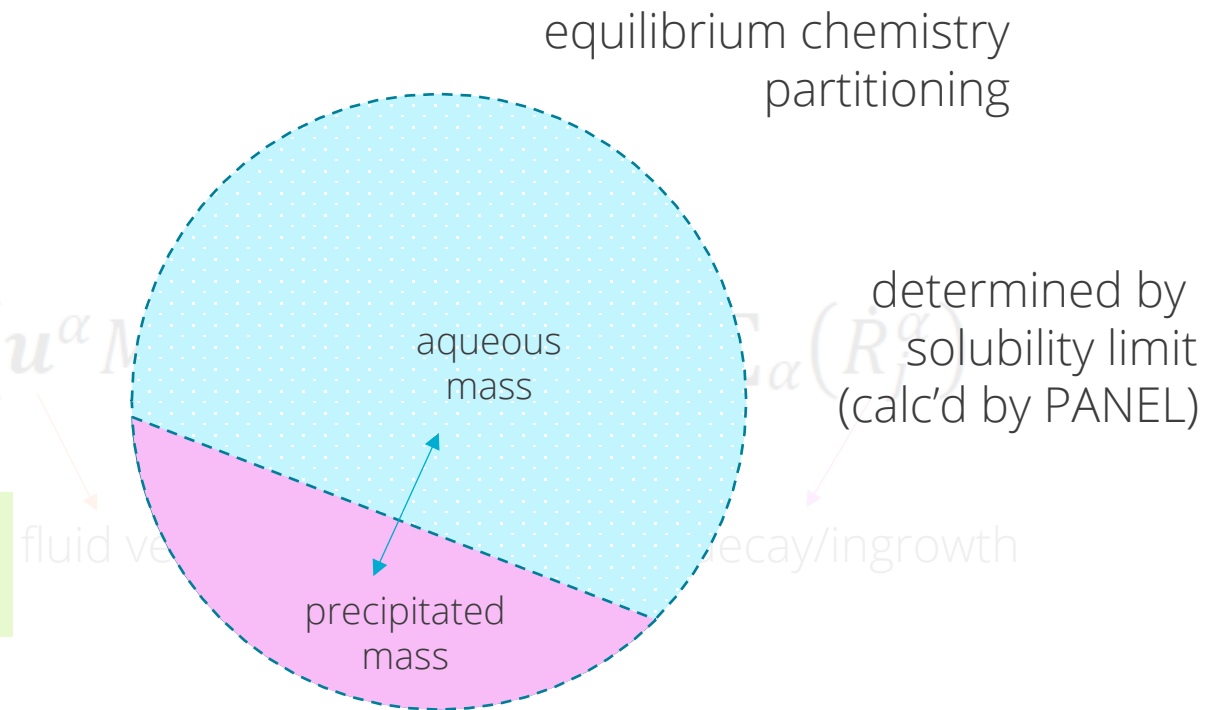
$$\frac{\partial}{\partial t} \sum_\alpha (M_j^\alpha) + \nabla \cdot \sum_\alpha (\mathbf{u}^\alpha M_j^\alpha)$$

The total mass is always defined, even when the grid cell goes completely dry!

α

j

species (radionuclide, tracer, etc.)





PFLOTRAN Nuclear Waste Transport (NWT) Mode

Governing equation formulated in terms of total mass, M .

$$M_j^\alpha = M_j^A + M_j^P$$
$$\frac{\partial}{\partial t} \sum_\alpha (M_j^\alpha) + \nabla \cdot \sum_\alpha (\mathbf{u}^\alpha M_j^\alpha) = \sum_\alpha (\dot{Q}_j^\alpha) + \sum_\alpha (\dot{R}_j^\alpha)$$

total mass

aqueous

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α phase (aqueous, precipitated)

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PFLOTRAN Nuclear Waste Transport (NWT) Mode

Governing equation formulated in terms of total mass, M .

Bateman equation

$$\dot{R}_j^\alpha = \frac{\partial M_j^\alpha}{\partial t} = -\lambda_j M_j^\alpha + \lambda_p M_p^\alpha$$

sources/sink

parent

$$\frac{\partial}{\partial t} \sum_\alpha (M_j^\alpha) + \nabla \cdot \sum_\alpha (\mathbf{u}^\alpha M_j^\alpha) = \sum_\alpha (\dot{Q}_j^\alpha) + \sum_\alpha (\dot{R}_j^\alpha)$$

λ radioactive decay constant

α phase (aqueous, precipitated)

j species (radionuclide, tracer, etc.)

fluid velocity

decay/ingrowth



PFLOTRAN Nuclear Waste Transport (NWT) Mode

Governing equations are solved using Newton-Krylov iteration.

residual of non-linear system

$$R(M_j^{\alpha, t+1}) = 0$$



linear system of equations, $Ax=b$

$$f_i(x_1, x_2, \dots, x_n) = f_i(x_1^k, x_2^k, \dots, x_n^k) + \sum_{j=1}^n (x_j^{k+1} - x_j^k) \frac{\partial f_i(x_1^k, x_2^k, \dots, x_n^k)}{\partial x_j} = 0$$

$$\sum_{j=1}^n \left(\overbrace{\frac{\partial R_i(M_j^{\alpha, t+1})^k}{\partial M_j^{\alpha}}}_{\text{Jacobian}} \underbrace{(\delta M_j^{\alpha, t+1})}_{\text{solution update}} = - \overbrace{R(M_j^{\alpha, t+1})^k}_{\text{residual}} \right)$$



PFLOTRAN Nuclear Waste Transport (NWT) Mode

Governing equations are solved using Newton-Krylov iteration.

Convergence is declared
based on infinity norms of:

$\frac{R(M_j^{\alpha,t+1})}{(\sum_{\alpha} (M_j^{\alpha,t})^{\forall})}$ scaled residual

$R(M_j^{\alpha,t+1})$ absolute residual

$\delta M_j^{\alpha,t+1} / M_j^{\alpha,t}$ relative solution update

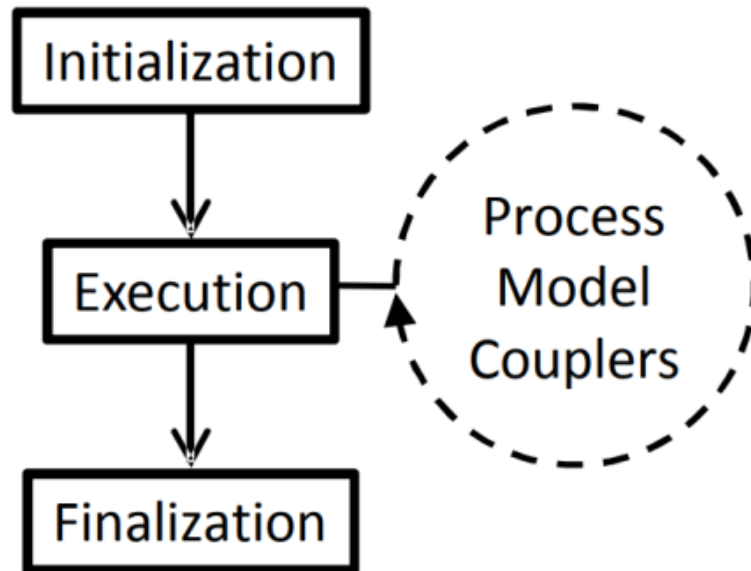
Tolerances can be
assigned to each
species.

$$\sum_{j=1}^n \left(\overbrace{\frac{\partial R_i(M_j^{\alpha,t+1})^k}{\partial M_j^{\alpha}}}_{\text{Jacobian}} \overbrace{(\delta M_j^{\alpha,t+1})}_{\text{solution update}} = - \overbrace{R(M_j^{\alpha,t+1})^k}_{\text{residual}} \right)$$



PFLOTRAN Nuclear Waste Transport (NWT) Mode

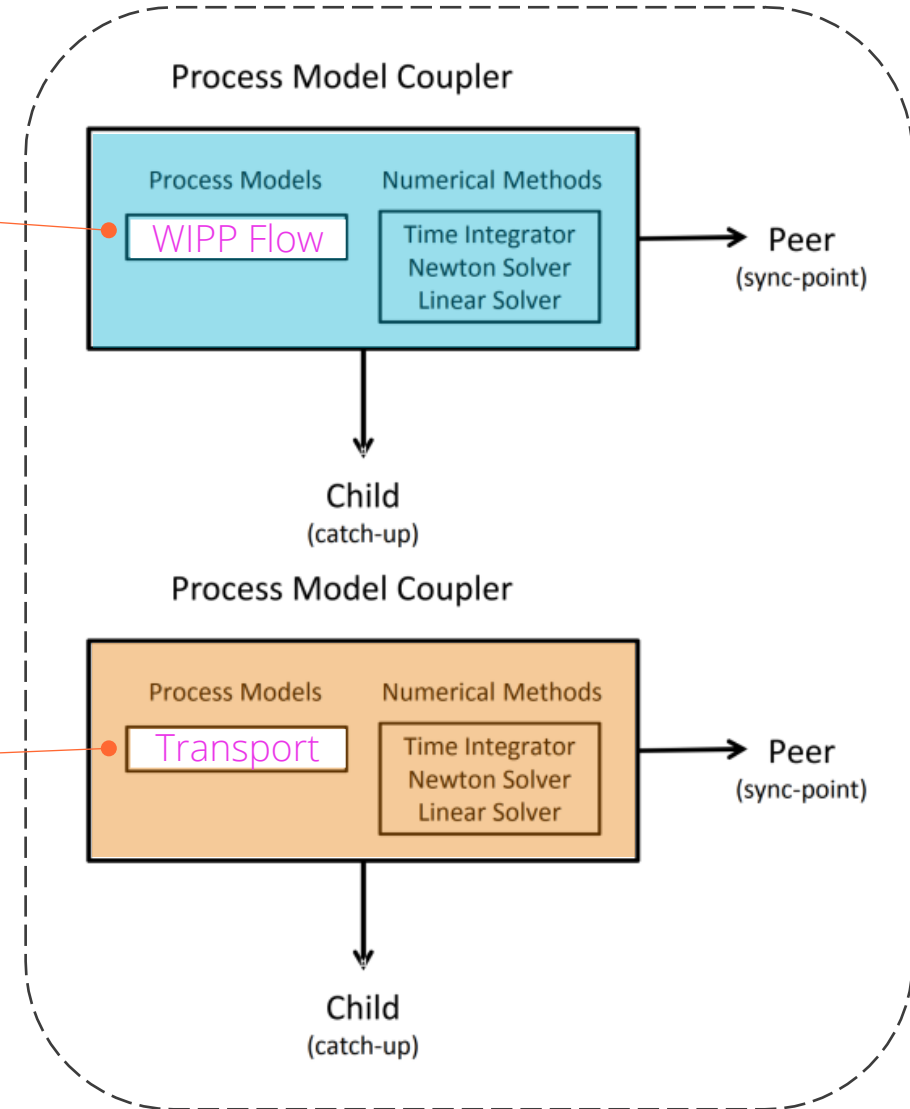
PFLOTRAN



Flow & transport are sequentially coupled.

replaces
BRAGFLO

replaces
NUTS

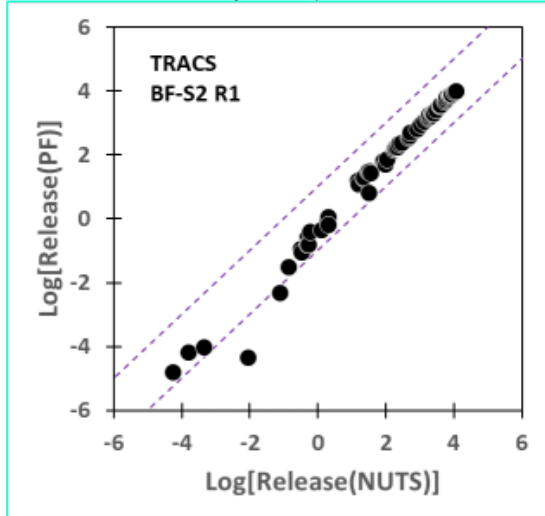




Initial Results: Comparison of NUTS & PFLOTRAN-NWT Mode

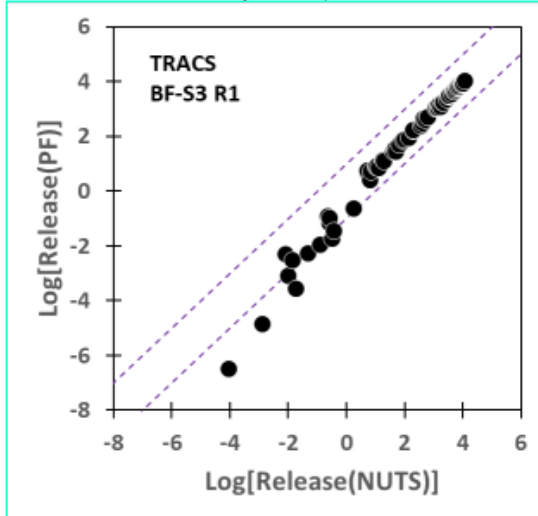
Screened-in* vector tracer simulations for S2, S3, S4, S5 scenarios

Intrusion @ 350 yr, into pressurized brine



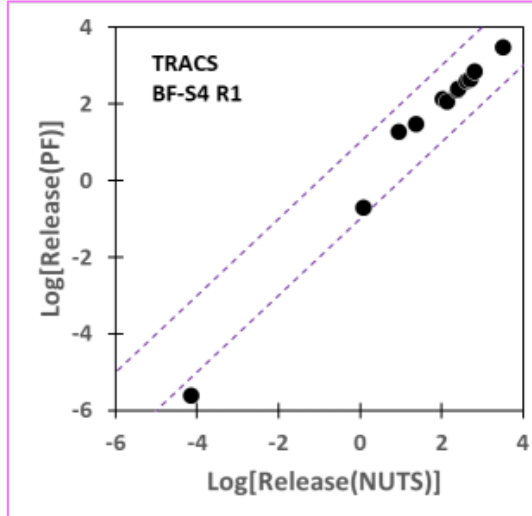
Mean Releases:
PF: 1.715E+03 kg
NUTS: 1.934E+03 kg

Intrusion @ 1000 yr, into pressurized brine



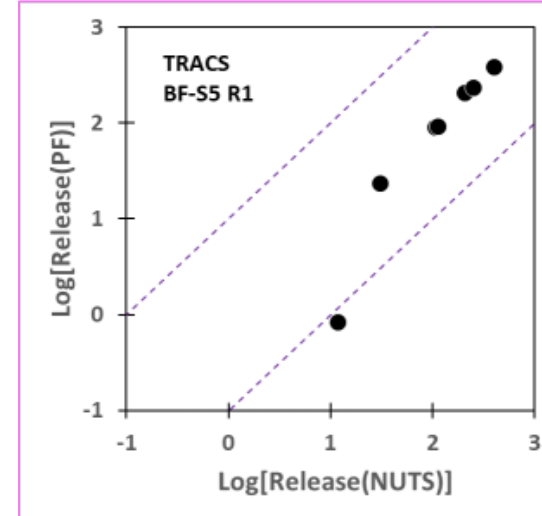
Mean Releases:
PF: 1.817E+03 kg
NUTS: 2.036E+03 kg

Intrusion @ 350 yr, misses pressurized brine



Mean Releases:
PF: 4.376E+02 kg
NUTS: 4.627E+02 kg

Intrusion @ 1000 yr, misses pressurized brine



Mean Releases:
PF: 1.477E+02 kg
NUTS: 1.608E+02 kg

Preliminary Conclusions:

- Larger relative differences are observed for vectors with small releases ($\log(\text{release}) < 0$).
- PFLOTRAN-NWT consistently calculates lower releases than NUTS (~ 10% less).
- Mean releases are comparable between two simulators.

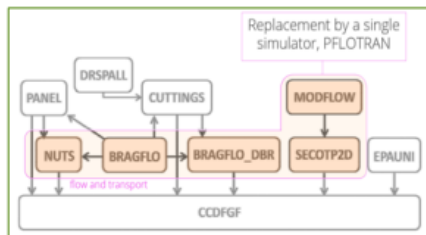
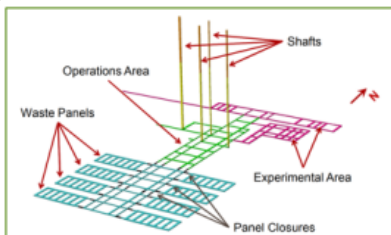
* Vectors with release quantities above threshold cumulative amount ($1.0\text{e-}7$ kg).

Fundamental Scenario	Specific Scenario	Time of Drilling Intrusion(s)
E0: no drilling intrusions.	S1-BF	N/A
E1: single intrusion through an excavated area of the repository that penetrates pressurized brine in the Castle.	S2-BF	350 years
	S3-BF	1,000 years
E2: single intrusion through an excavated area of the repository that does not penetrate pressurized brine in the Castle.	S4-BF	350 years
	S5-BF	1,000 years
E2E1: two intrusions into the same waste panel, the first being an E2 intrusion and the second being an E1 intrusion.	S6-BF	1,000 years for E2 intrusion 2,000 years for E1 intrusion

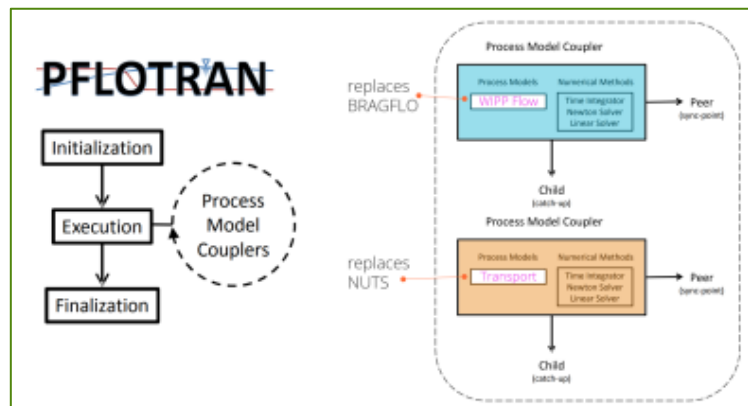
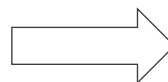


CONCLUSIONS

A Next-Generation Transport Simulator for the Waste Isolation Pilot Plant (WIPP) Performance Assessment



DOE is interested in a tool to handle a more asymmetric layout with a modern 3-D code.



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$$M_j^\alpha = M_j^A + M_j^P$$
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α phase (aqueous, precipitated)
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sources/sink
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