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

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IHLRWM 2022

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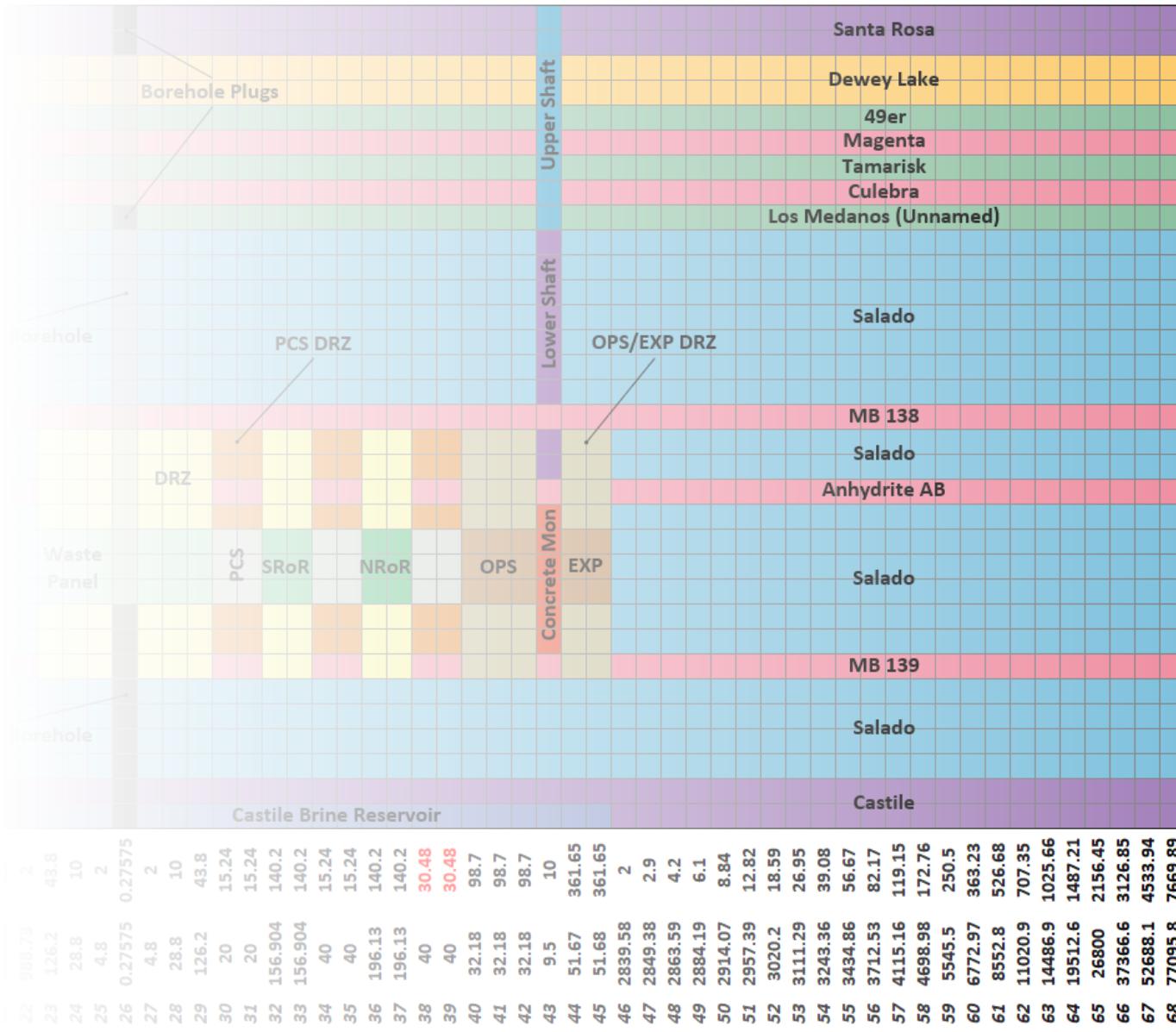
Disposal IV

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

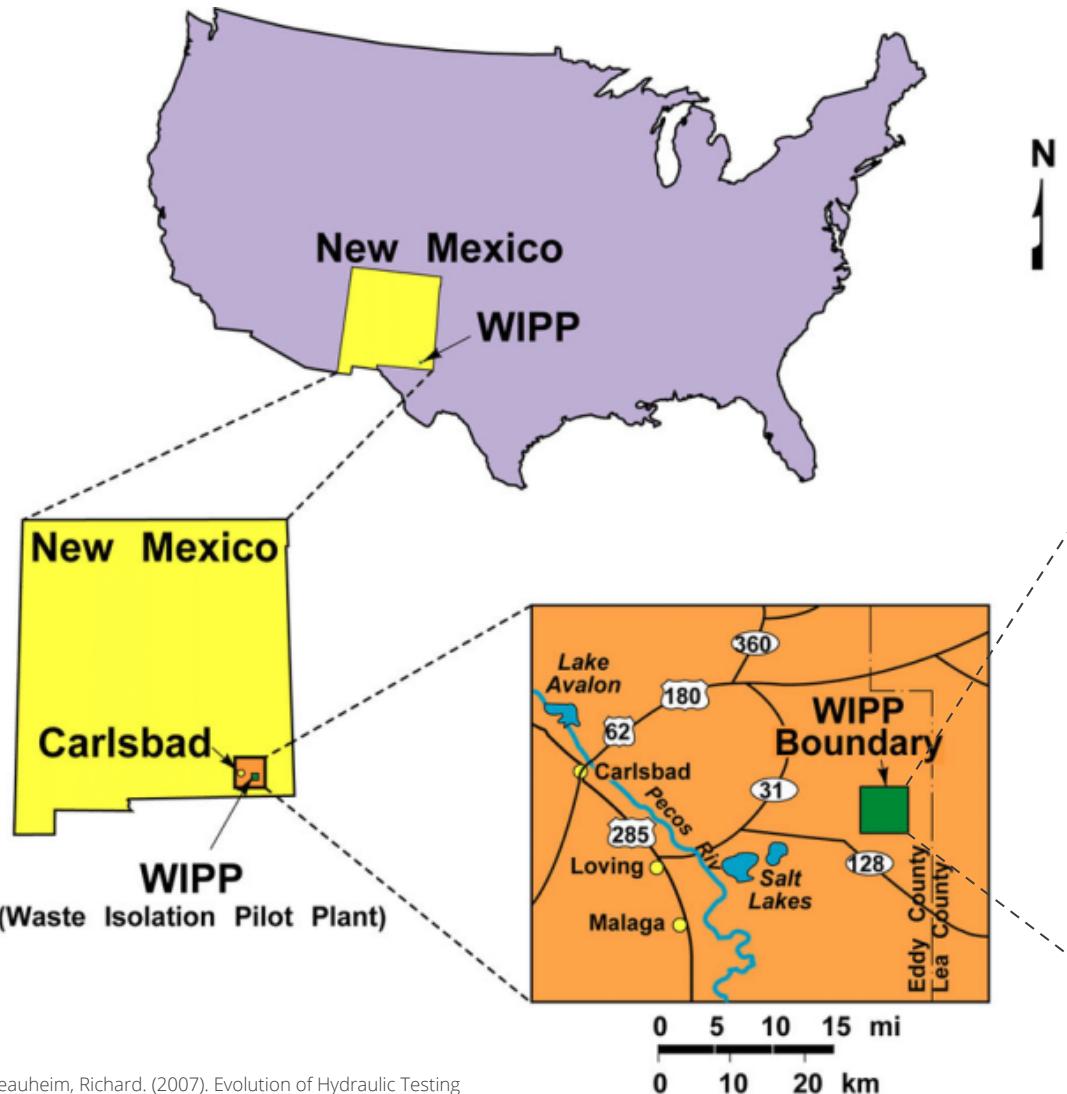


Presentation Topics

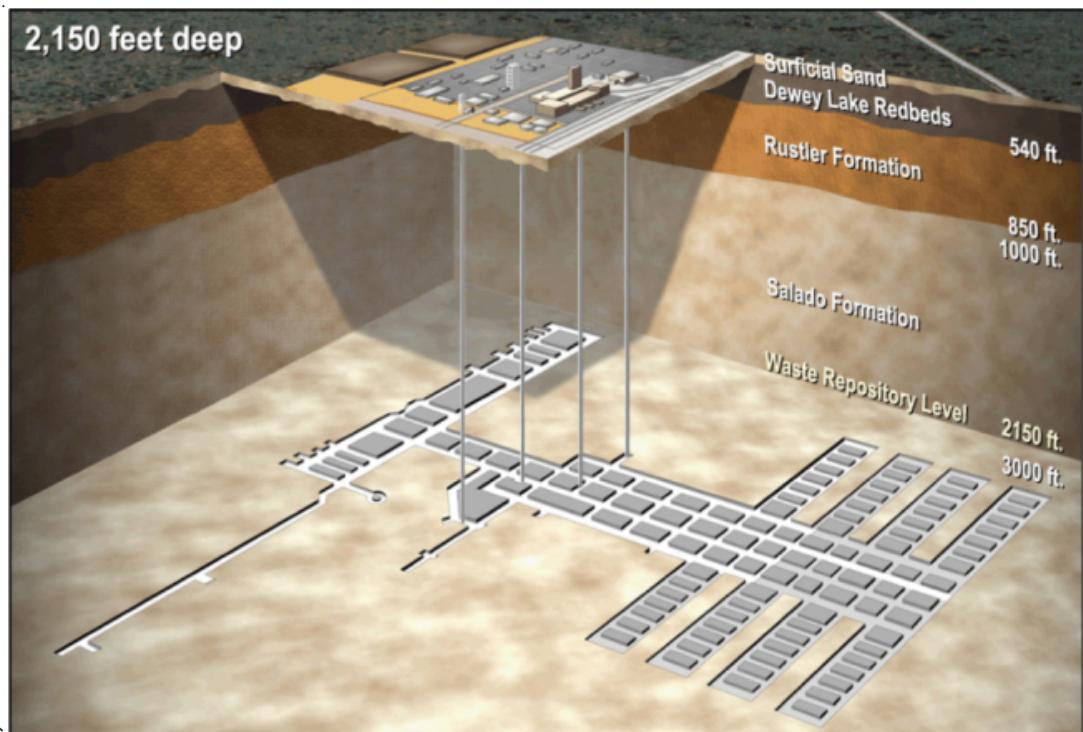
- Transport needs for WIPP performance assessment
- PFLOTRAN's Nuclear Waste Transport (NWT) Mode
 - Process model coupling
 - Governing equations
 - Solution technique



Waste Isolation Pilot Plant (WIPP)



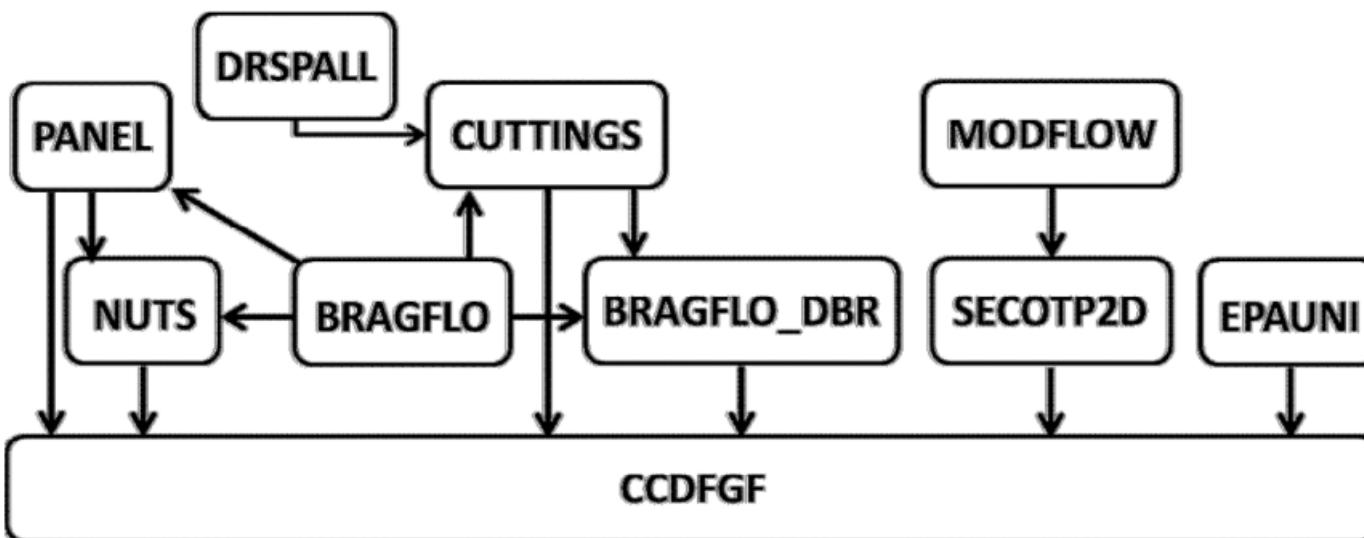
- The WIPP is the nation's only licensed deep geologic repository for defense-related transuranic waste
- Operated by U.S. Department of Energy (DOE)
- Long-term performance regulated by U.S. Environmental Protection Agency (EPA)



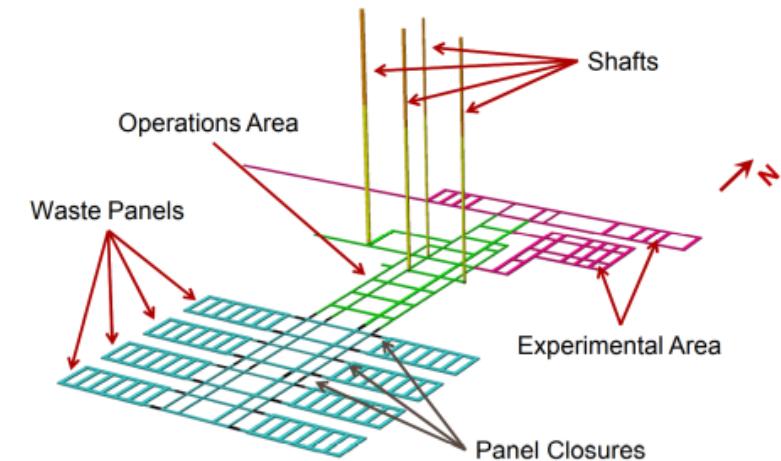
Beauheim, Richard. (2007). Evolution of Hydraulic Testing at the Waste Isolation Pilot Plant.

WIPP Performance Assessment

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



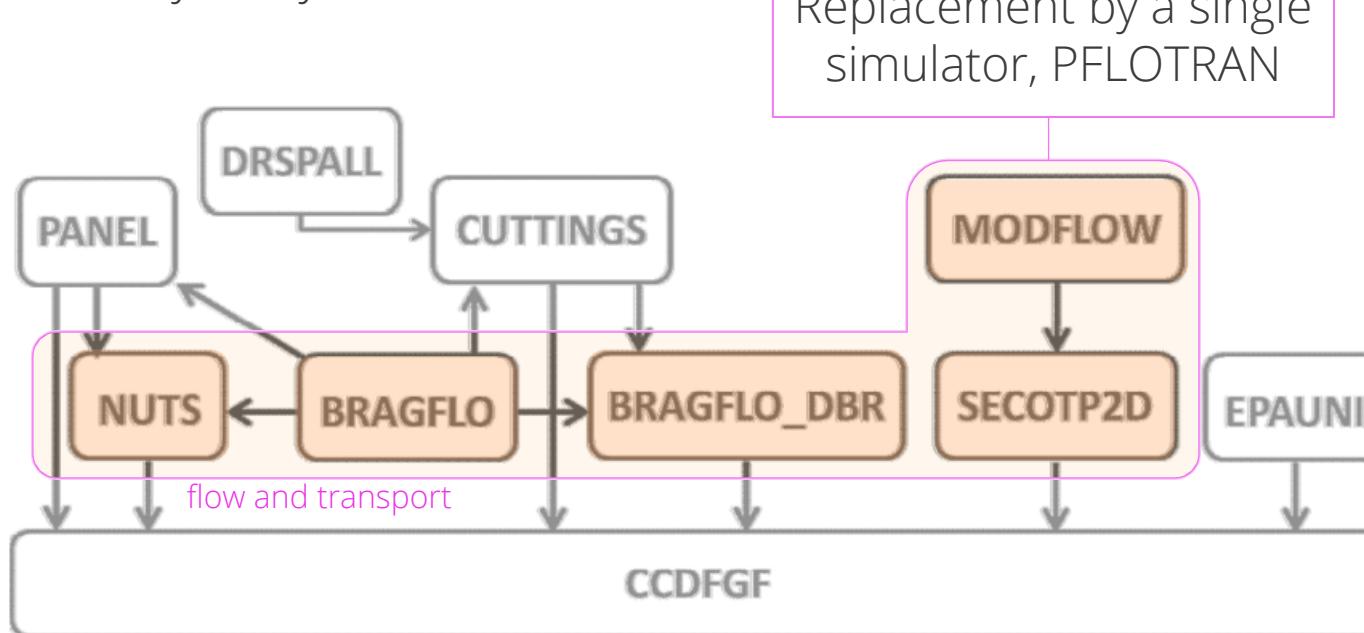
Long-term regulatory compliance is demonstrated via Performance Assessment (PA) undertaken by Sandia National Laboratories, Carlsbad.



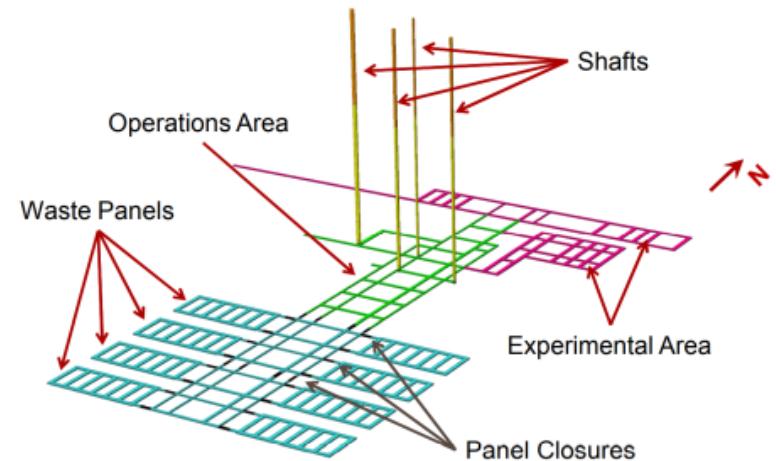
DOE is interested in reducing the number of principal codes to improve efficiencies for an asymmetric repository.

WIPP Performance Assessment

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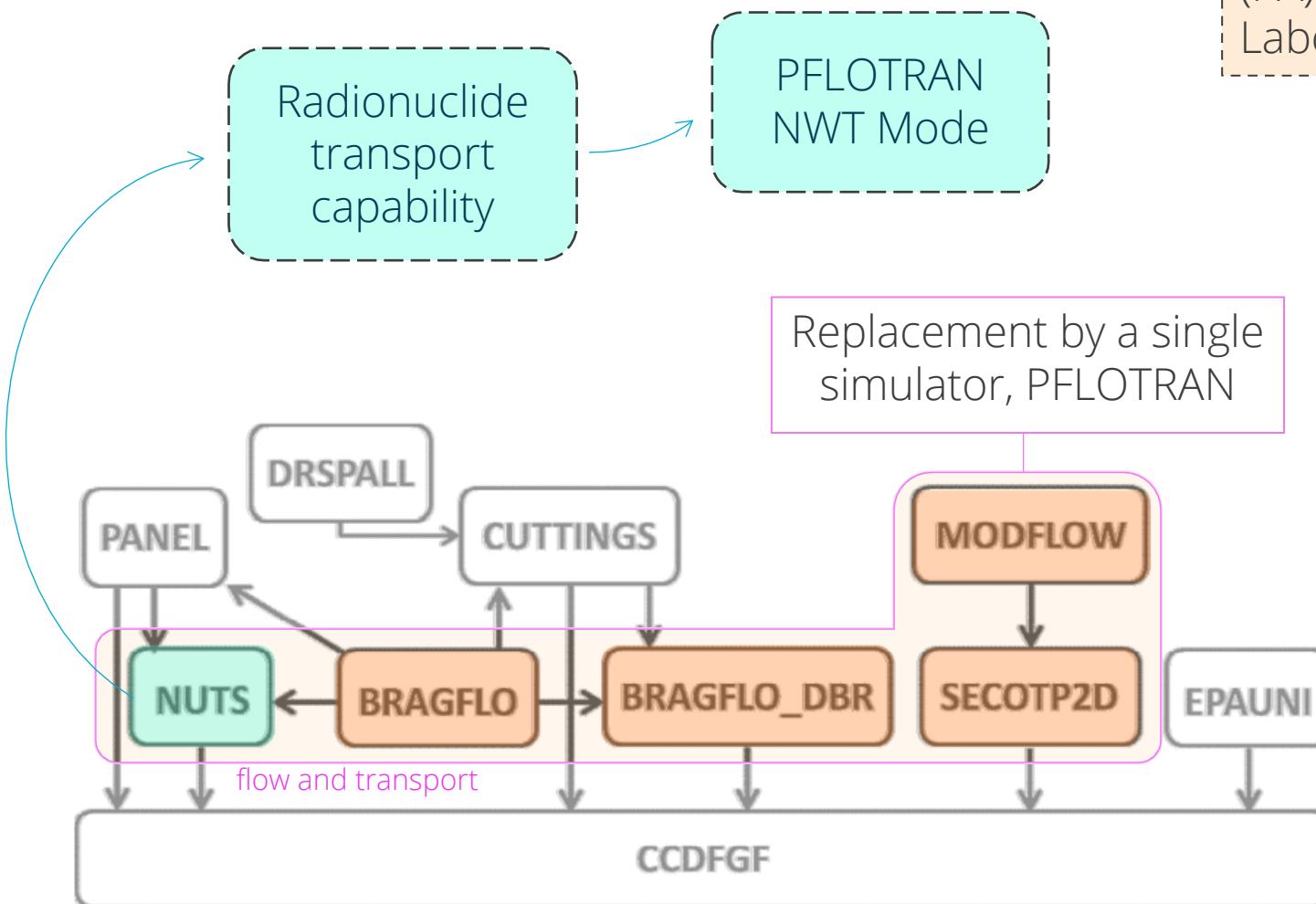


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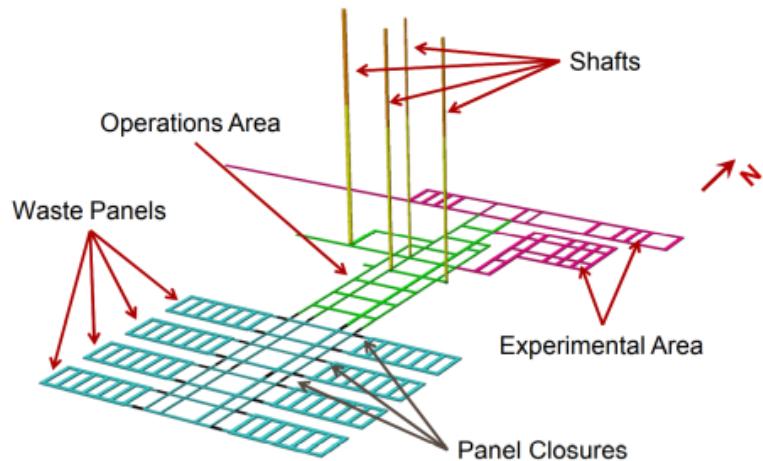


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WIPP Performance Assessment



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

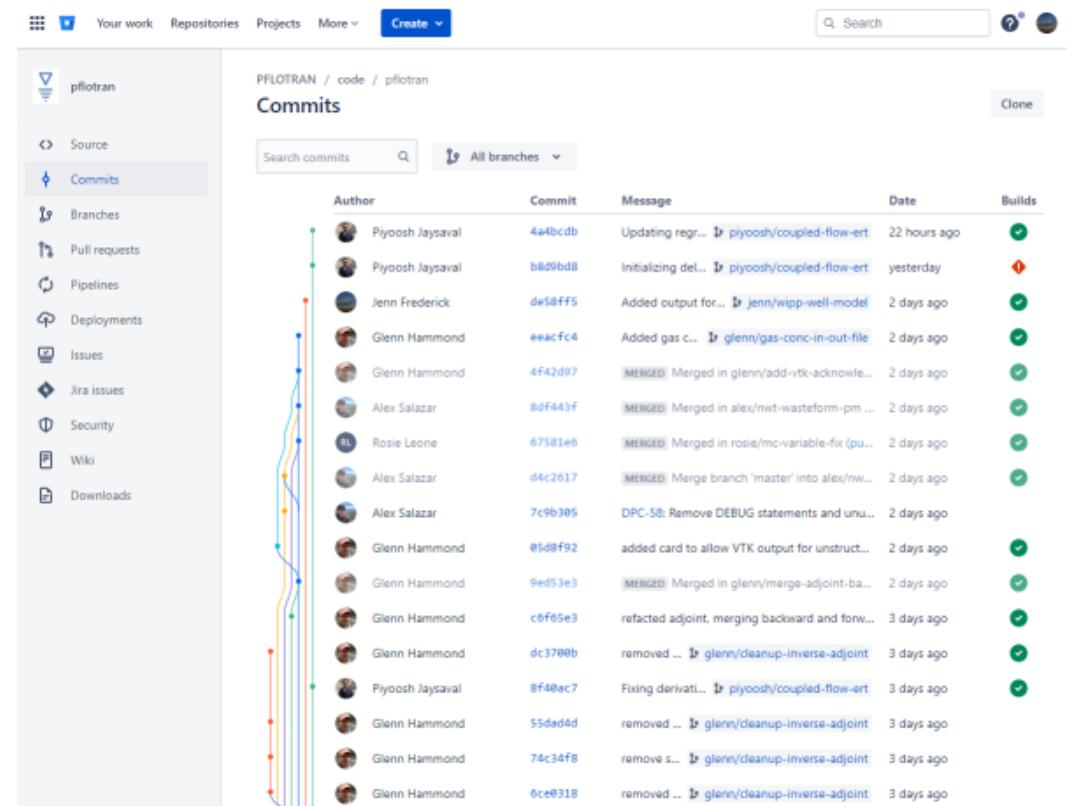


DOE is interested in reducing the number of principal codes to improve efficiencies for an asymmetric repository.

PFLOTTRAN

- 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 interface for the PFLOTTRAN repository. The left sidebar has a 'Source' tab selected, showing options like 'Commits', 'Branches', 'Pull requests', 'Pipelines', 'Deployments', 'Issues', 'Jira issues', 'Security', 'Wiki', and 'Downloads'. The main area is titled 'Commits' for the 'pflotran' repository. It includes a search bar and a dropdown for 'All branches'. The commit list is as follows:

Author	Commit	Message	Date	Builds
Piyush Jaysaval	4ae4cd8	Updating regu...	22 hours ago	Green
Piyush Jaysaval	b8d9bd8	Initializing del...	yesterday	Red
Jenn Frederick	de58ff5	Added output for...	2 days ago	Green
Glenn Hammond	eeacfc4	Added gas c...	2 days ago	Green
Glenn Hammond	4f42d97	MERGED: Merged in glenn/add-vtk-acknowle...	2 days ago	Green
Alex Salazar	86f443f	MERGED: Merged in alex/nwt-wastefrom-pm ...	2 days ago	Green
Rosie Leone	67581e6	MERGED: Merged in rosie/mc-variable-fix (pu...	2 days ago	Green
Alex Salazar	d4c2617	MERGED: Merge branch 'master' into alex/nw...	2 days ago	Green
Alex Salazar	7cb3085	DPC-58: Remove DEBUG statements and unu...	2 days ago	Green
Glenn Hammond	05d8f92	added card to allow VTK output for unstruct...	2 days ago	Green
Glenn Hammond	9ed53e3	MERGED: Merged in glenn/merge-adjoint-ba...	2 days ago	Green
Glenn Hammond	c6f65e3	refactored adjoint, merging backward and forw...	3 days ago	Green
Glenn Hammond	dc3700b	removed ...	3 days ago	Green
Piyush Jaysaval	8f48ac7	Fixing derivat...	3 days ago	Green
Glenn Hammond	55dad4d	removed ...	3 days ago	Green
Glenn Hammond	74c34f8	remove s...	3 days ago	Green
Glenn Hammond	6ce0318	removed ...	3 days ago	Green



WIPP Performance Assessment Requirements

WIPP PA
Requirements Document
for
PFLOTTRAN Version 3.0.1

Requirements Document
for PFLOTTRAN Version 3.0.1

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

2.0 REQUIREMENTS

2.1 Functional Requirements

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

2.1.1 INPUT AND OUTPUT

R.1 PFLOTTRAN reads input parameters that define controls, and solution output format from a

R.2 PFLOTTRAN accepts material properties as parameters, intrinsic permeability, porosity. Also specified are the relative permeability for each material.

R.3 PFLOTTRAN outputs and reads back in a binary solution variables necessary to rest time-dependent source terms.

R.4 PFLOTTRAN writes output files of the primary saturation. Other user-specified outputs

- liquid and gas fluxes across user-specified
- liquid and gas fluxes across the boundary
- concentrations of reactants in rate-controlled gas and liquid source/sink terms,
- material properties: porosity, permeability
- cell volume

R.5 PFLOTTRAN writes binary-format files containing variables at all grid cells in the model domain

2.1.2 FINITE VOLUME GRID

R.6 PFLOTTRAN constructs a finite volume three-dimensional volumes, cell interface areas, and locations two inputs:

Requirements Document
for PFLOTTRAN Version 3.0.1

ERMIS# 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 PFLOTTRAN sets

- PFLOTTRAN input files; and
- PFLOTTRAN regions of the specified reference

R.8 PFLOTTRAN sets gas source/sink to domain. Reactant, sulfide, and radioactive

R.9 PFLOTTRAN imports boundary conditions specification over a

2.1.4 TWO-PHASE IMMOBILIZATION

R.10 PFLOTTRAN num of liquid and gas porous medium.

R.11 PFLOTTRAN calc within each state linear models, an

R.12 PFLOTTRAN calc function of liquid

R.13 PFLOTTRAN calc of state for the species

R.14 PFLOTTRAN calc

2.1.5 GAS AND LIQUID SOURCE/SINK TERMS

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

- anoxic corrosion of iron under:
 - inundated and
 - humid conditions;
- microbial degradation of celluloses, plastics, and rubber under:
 - inundated and
 - humid conditions; and
- radionuclide of brine from radionuclide alpha decay of:
 - dissolved and sorbed radionuclides in solution and
 - 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 PFLOTTRAN.

2.1.6 PROCESS MODELS

R.15 PFLOTTRAN simulates six additional rate-controlled chemical reactions:

- sulfidation of iron hydroxide;
- sulfidation of iron;
- hydration of MgO under:
 - inundated and
 - humid conditions;
- carbonation of MgO;
- carbonation of Mg(OH)₂; and
- conversion of hydromagnesite to magnesite.

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

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

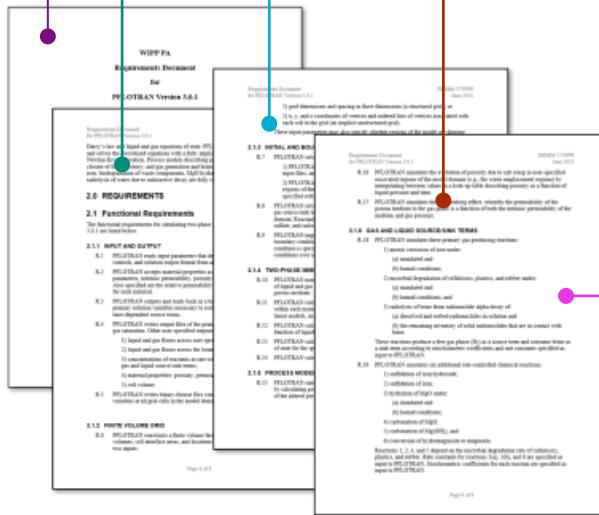
As dictated by the CFR, per NQA-1,2,3.



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 .

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

total mass M_j^{α} = aqueous M_j^A + precipitated M_j^P

sources/sink \dot{Q}_j^{α}

decay/ingrowth \dot{R}_j^{α}

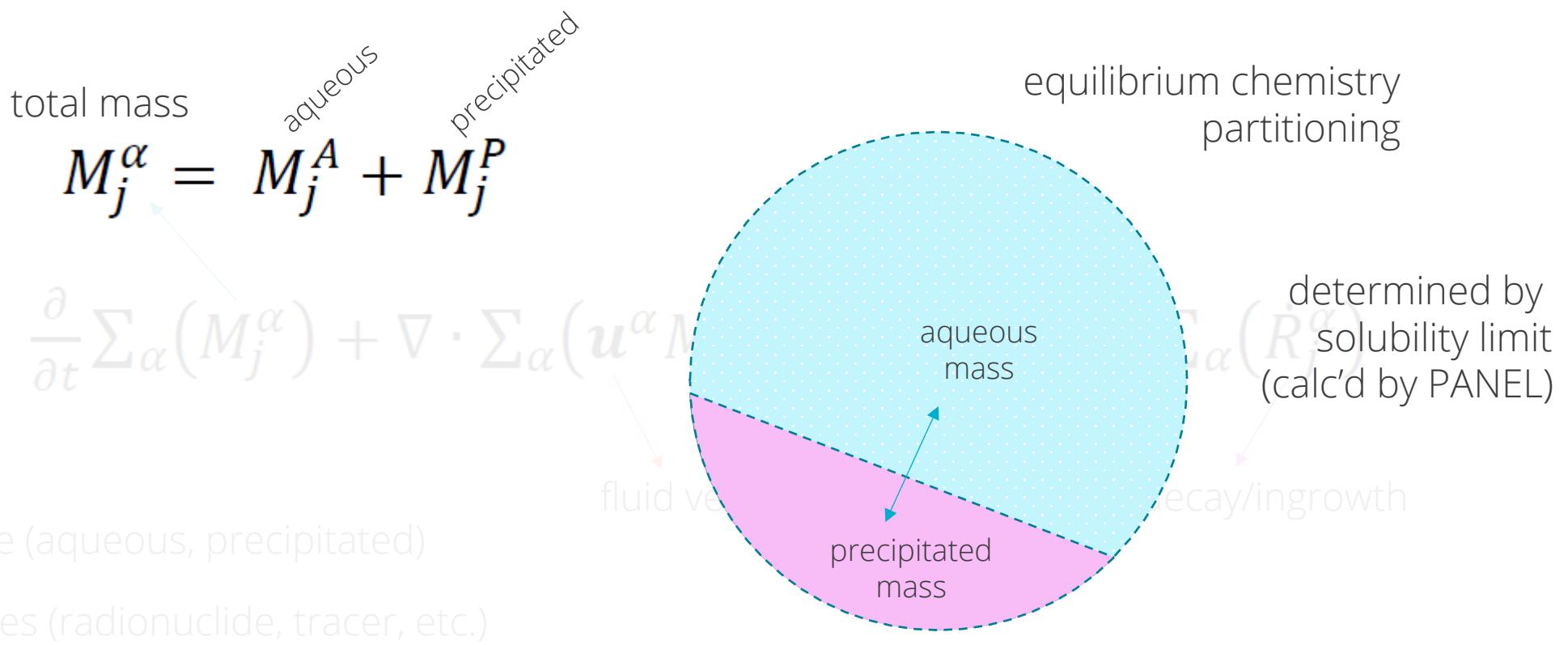
fluid velocity \mathbf{u}^{α}

α phase (aqueous, precipitated)

j species (radionuclide, tracer, etc.)

PFLOTRAN Nuclear Waste Transport (NWT) Mode

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PFLOTRAN Nuclear Waste Transport (NWT) Mode

Governing equation formulated in terms of total mass, M .

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

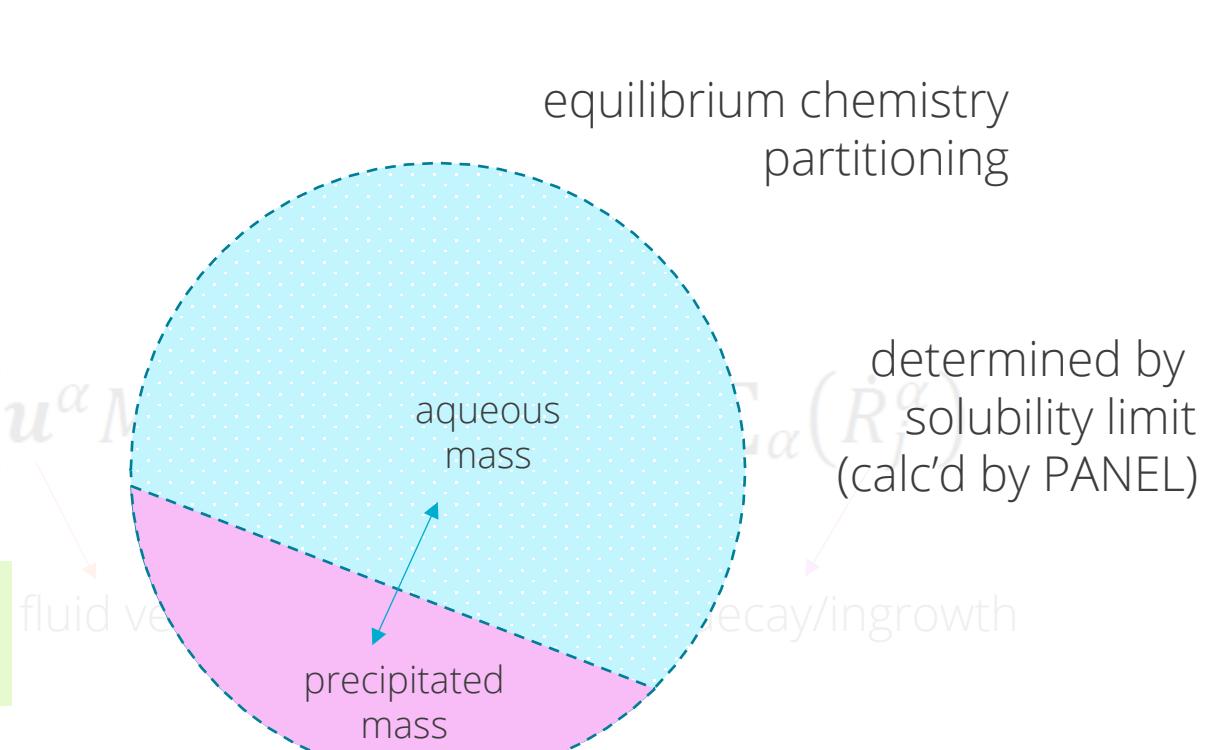
total mass aqueous precipitated

 α

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

 j

species (radionuclide, tracer, etc.)





PFLOTRAN Nuclear Waste Transport (NWT) Mode

Governing equation formulated in terms of total mass, M .

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

total mass M_j^{α} = aqueous M_j^A + precipitated M_j^P

sources/sink \dot{Q}_j^{α}

decay/ingrowth \dot{R}_j^{α}

fluid velocity \mathbf{u}^{α}

α phase (aqueous, precipitated)

j species (radionuclide, tracer, etc.)

PFLOTRAN Nuclear Waste Transport (NWT) Mode

Governing equation formulated in terms of total mass, M .

Bateman equation

total mass

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

sources/sink

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

λ radioactive decay constant

parent

fluid velocity

α phase (aqueous, precipitated)

decay/ingrowth

j species (radionuclide, tracer, etc.)



PFLOTRAN Nuclear Waste Transport (NWT) Mode

Governing equations are solved using Newton-Krylov iteration.

residual of non-linear system

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



$f_i(x_1, x_2, \dots, x_n) =$ linear system of equations, $Ax=b$

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

$$\sum_{j=1}^n \left(\frac{\frac{\partial R_i(M_j^{\alpha,t+1})}{\partial M_j^\alpha}}{\frac{\partial R_i(M_j^{\alpha,t+1})}{\partial M_j^\alpha}} \right)^k (\delta M_j^{\alpha,t+1}) = -R(M_j^{\alpha,t+1})^k$$

PFLOTRAN Nuclear Waste Transport (NWT) Mode

Governing equations are solved using Newton-Krylov iteration.

Convergence is declared
based on infinity norms of:

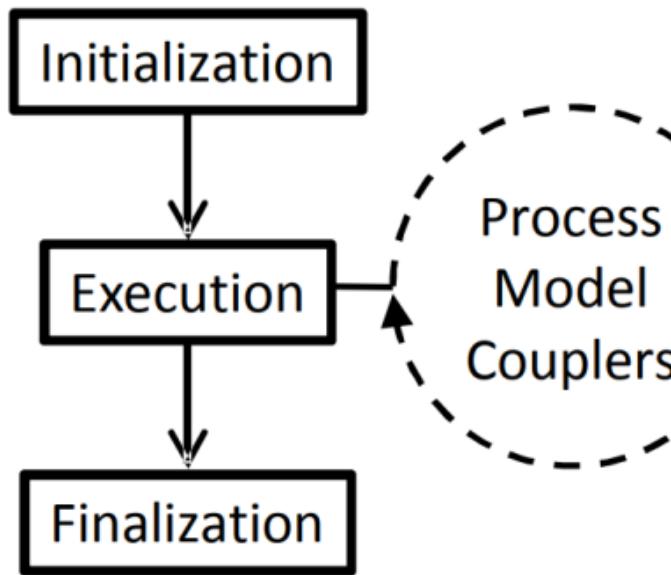
- $\frac{R(M_j^{\alpha,t+1})}{(\Sigma_\alpha(M_j^{\alpha,t})\forall)}$ scaled residual
- $R(M_j^{\alpha,t+1})$ absolute residual
- $\delta M_j^{\alpha,t+1}/M_j^{\alpha,t}$ relative solution update

Tolerances can be
assigned to each
species.

$$\sum_{j=1}^n \left(\frac{\frac{\partial R_i(M_j^{\alpha,t+1})}{\partial M_j^\alpha}}{k} (\delta M_j^{\alpha,t+1}) = -R(M_j^{\alpha,t+1})^k \right)$$

PFLOTRAN Nuclear Waste Transport (NWT) Mode

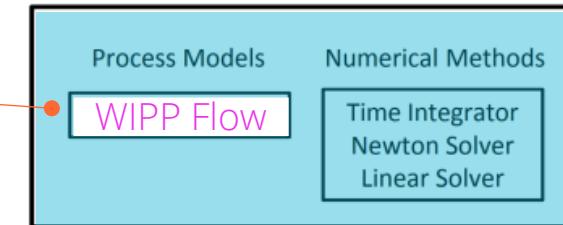
PFLOTRAN



Flow & transport are sequentially coupled.

replaces
BRAGFLO

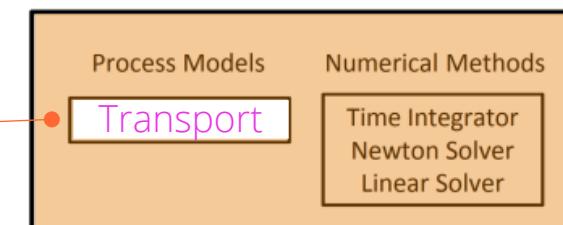
Process Model Coupler



Peer
(sync-point)

Child
(catch-up)

Process Model Coupler

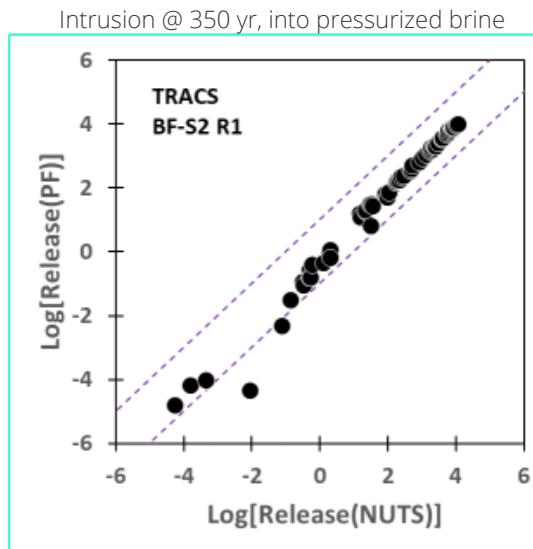


Peer
(sync-point)

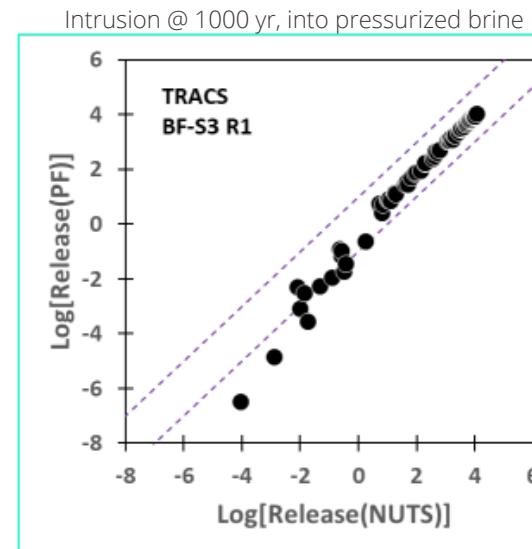
Child
(catch-up)

Initial Results: Comparison of NUTS & PFLOTRAN-NWT Mode

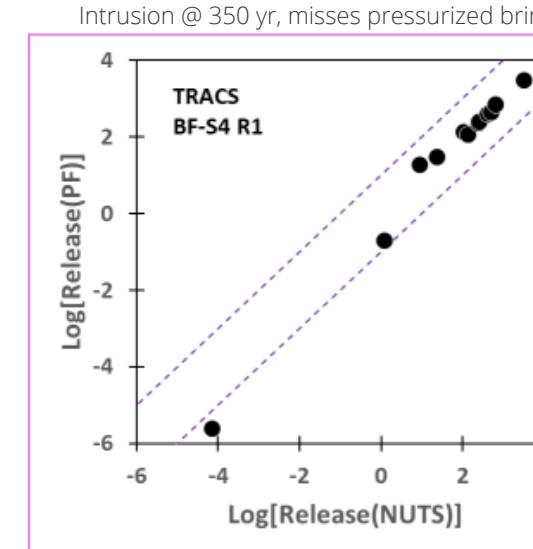
Screened-in* vector tracer simulations for S2, S3, S4, S5 scenarios



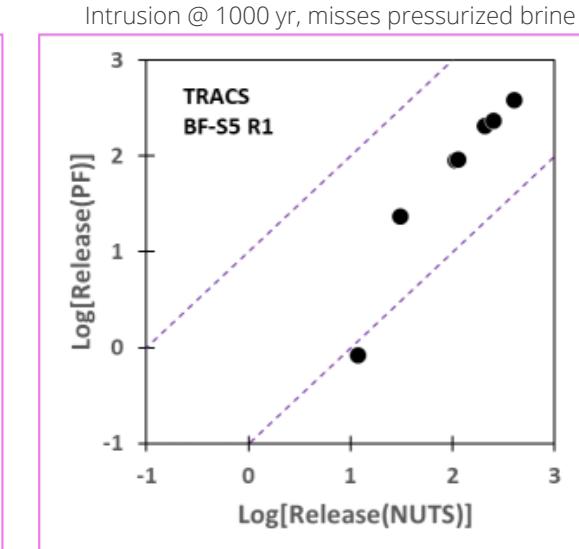
Mean Releases:
PF: 1.715E+03 kg
NUTS: 1.934E+03 kg



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



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



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

Preliminary Conclusions:

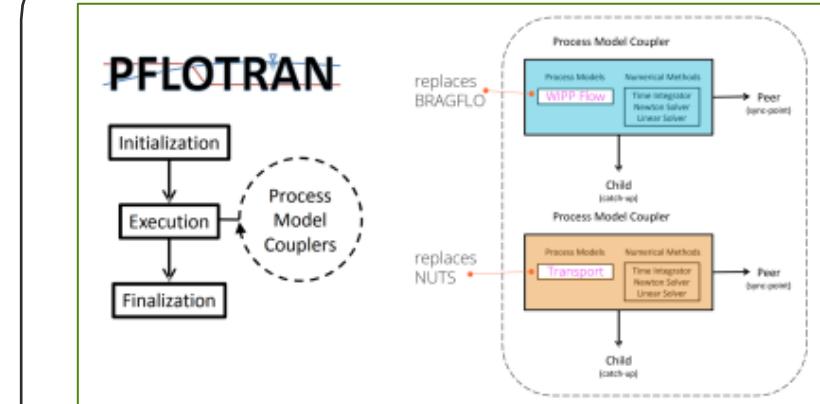
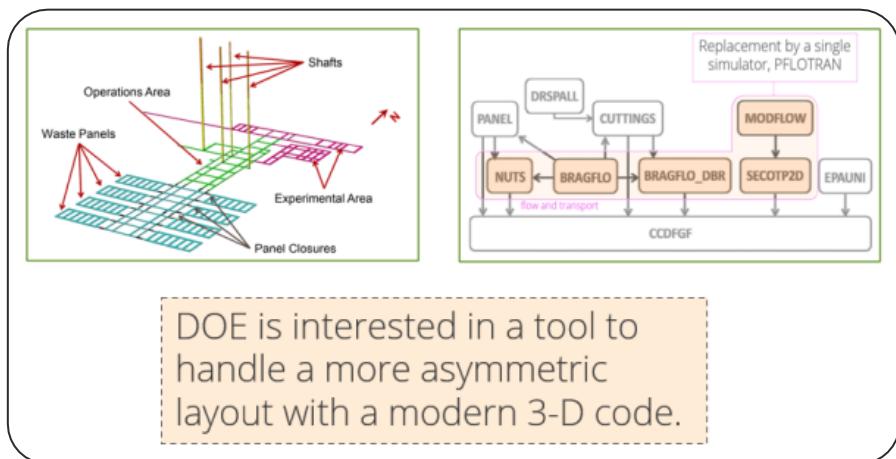
- Larger relative differences are observed for vectors with small releases ($\log(\text{release}) < 0$).
- PFLOTRAN-NWT consistently calculates lower releases than NUTS (~ 10% less).
- Mean releases are comparable between two simulators.

* Vectors with release quantities above threshold cumulative amount (1.0e-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
E3: single intrusion through an excavated area of the repository that does not penetrate pressurized brine in the Castle	S3-BF	1,000 years
E2: two intrusions into the same waste panel, the first being an E2 intrusion and the second being an E1 intrusion	S4-BF	350 years
E2E1: two intrusions into the same waste panel, the first being an E2 intrusion and the second being an E1 intrusion	S5-BF	1,000 years
E6: two intrusions into the same waste panel, the first being an E6 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



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α phase (aqueous, precipitated)
 j species (radionuclide, tracer, etc.)

total mass
 aqueous
 precipitated
 sources/sink
 fluid velocity
 decay/ingrowth

