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

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IHLRWM 2022 Tues. November 15, 2022

Disposal IV

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

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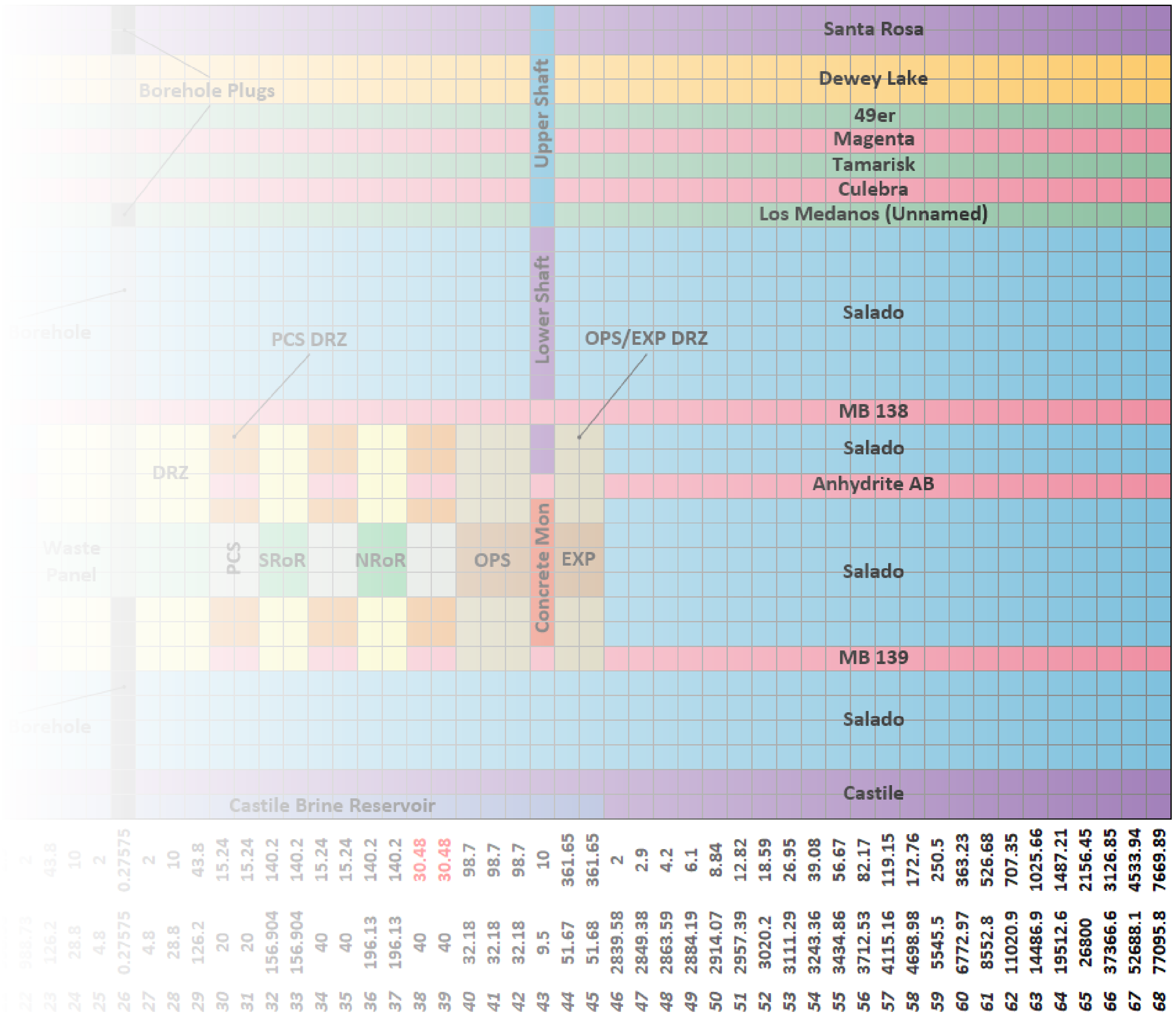
U.S. DEPARTMENT OF ENERGY

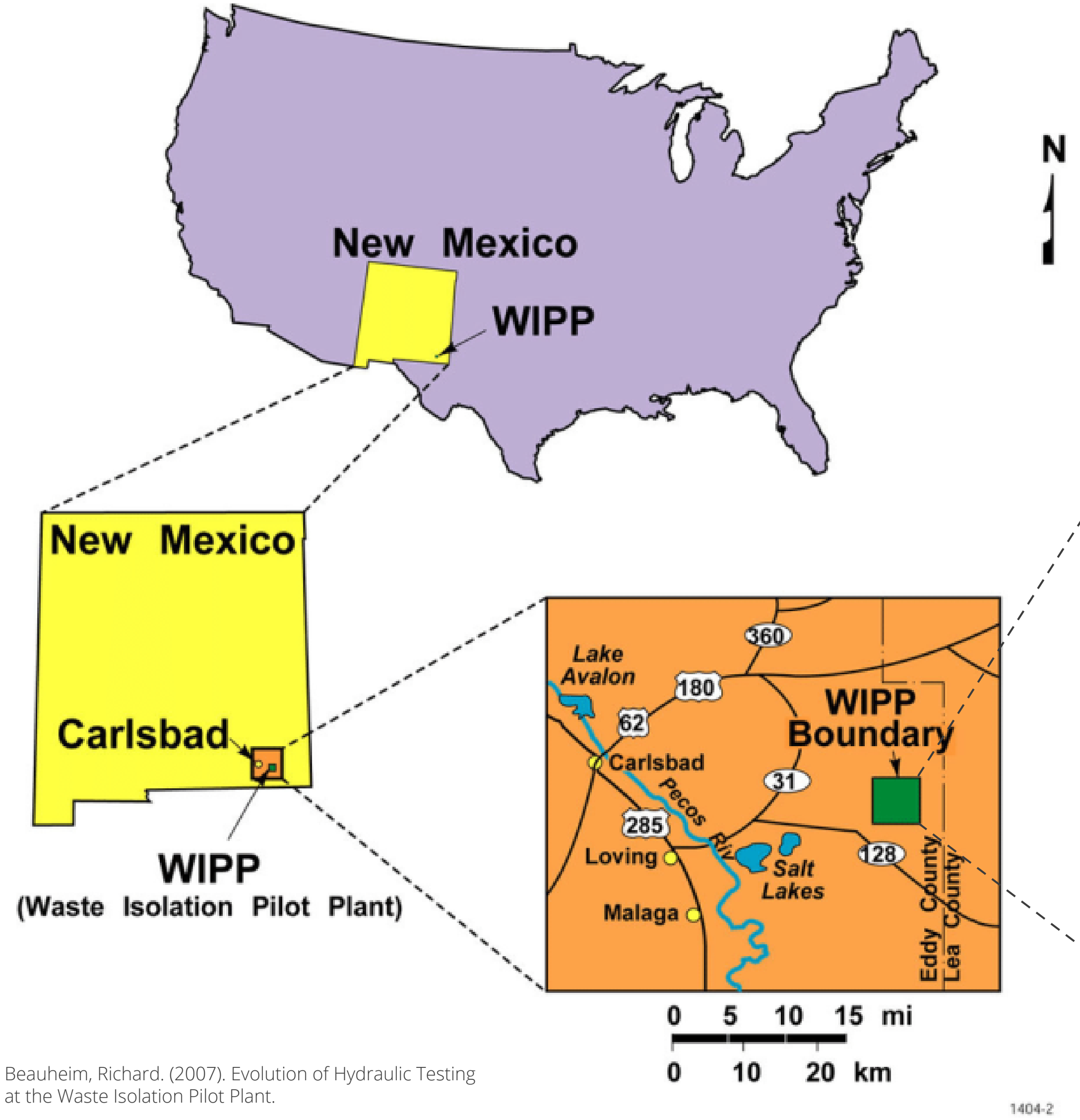
NNSA

Presentation Topics

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

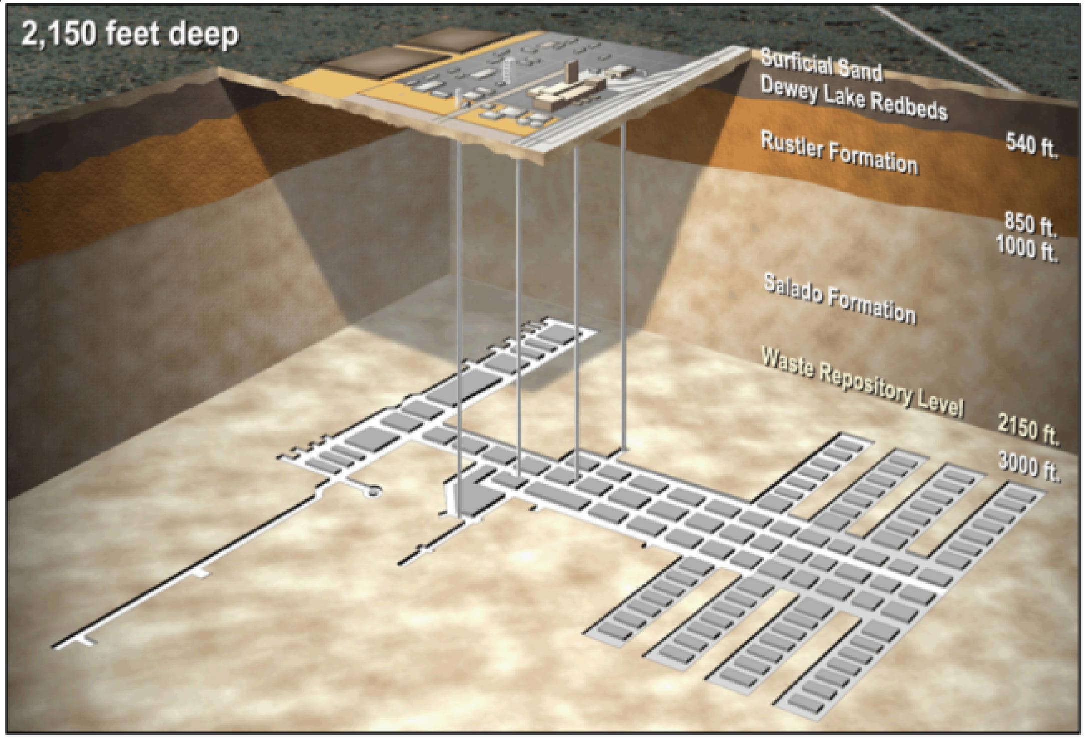


Waste Isolation Pilot Plant (WIPP)



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

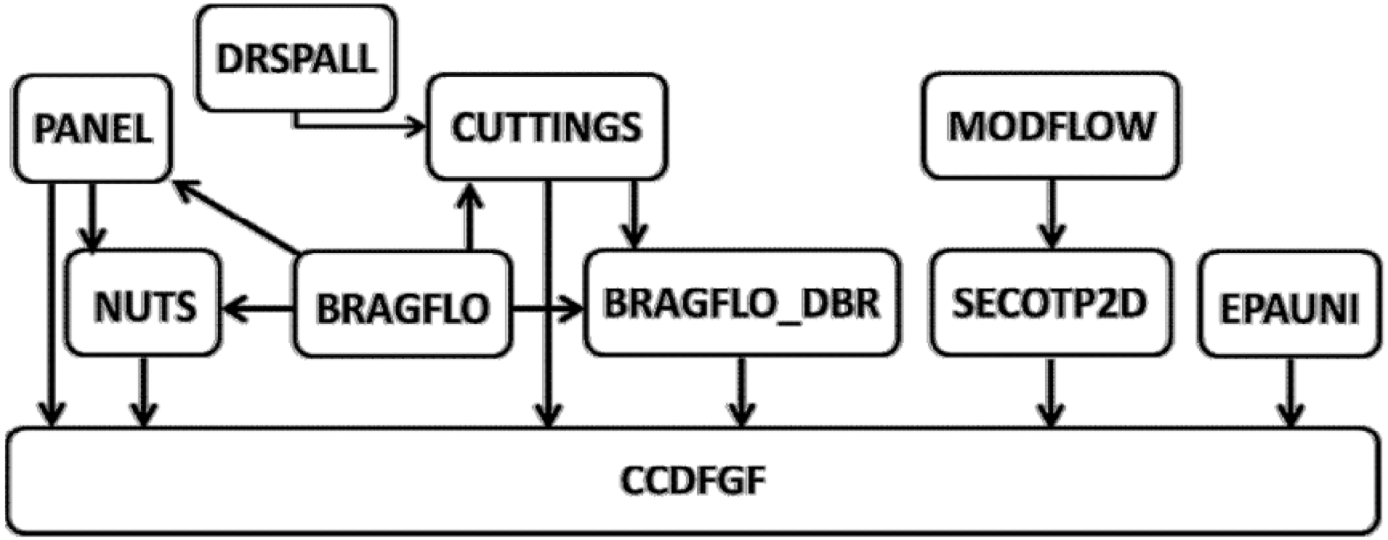
- The WIPP is the nation's only licensed deep geologic repository for defense-related transuranic waste
- Operated by U.S. Department of Energy (DOE)
- Long-term performance regulated by U.S. Environmental Protection Agency (EPA)

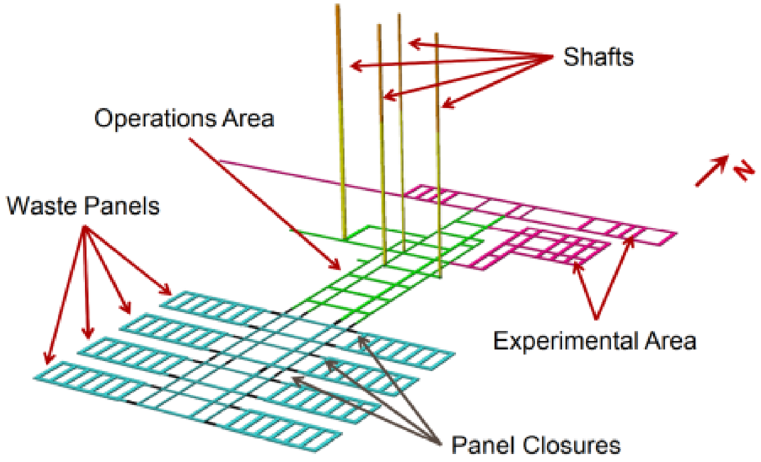


WIPP Performance Assessment

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

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





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

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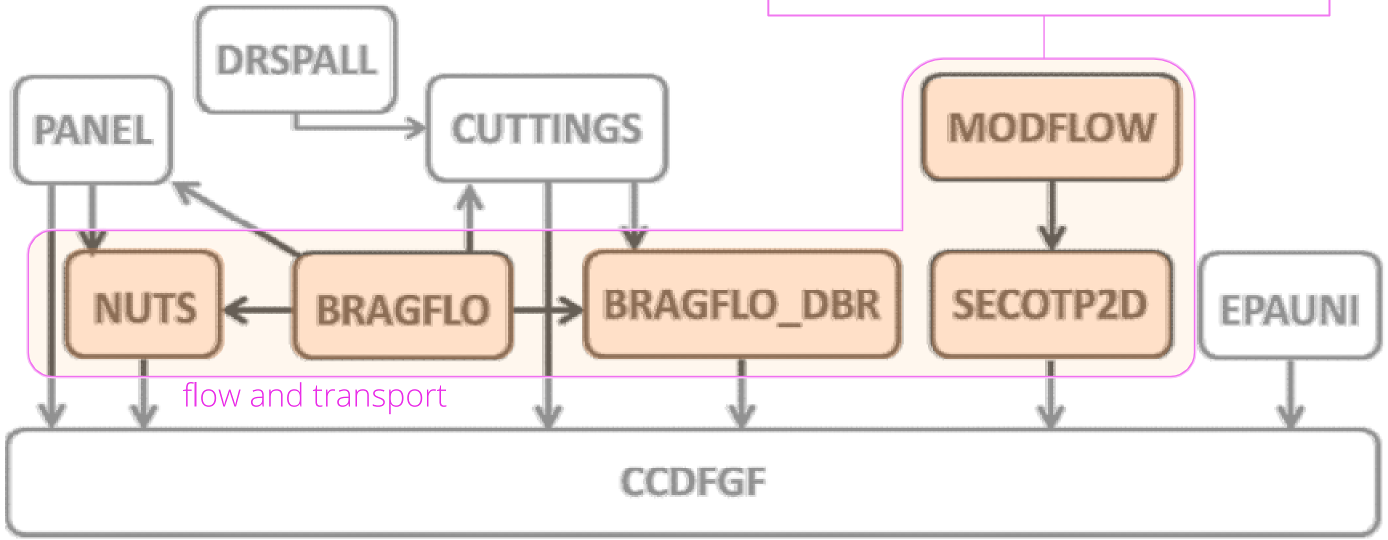
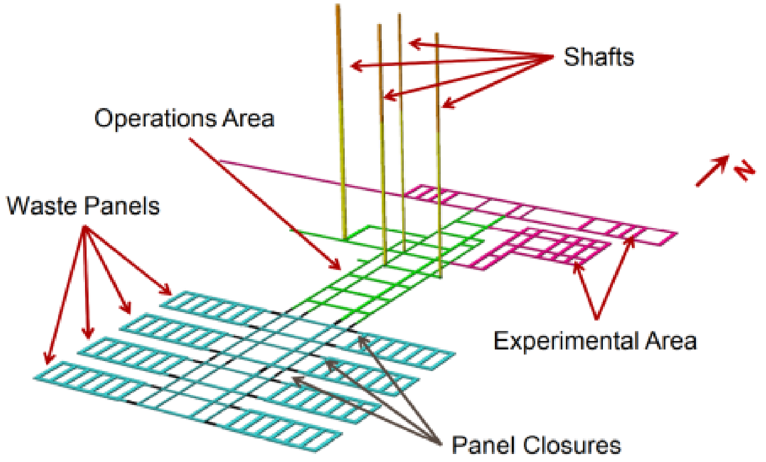
- PA computations include 10 principal codes and many utility codes.

Replacement by a single simulator, PFLOTRAN





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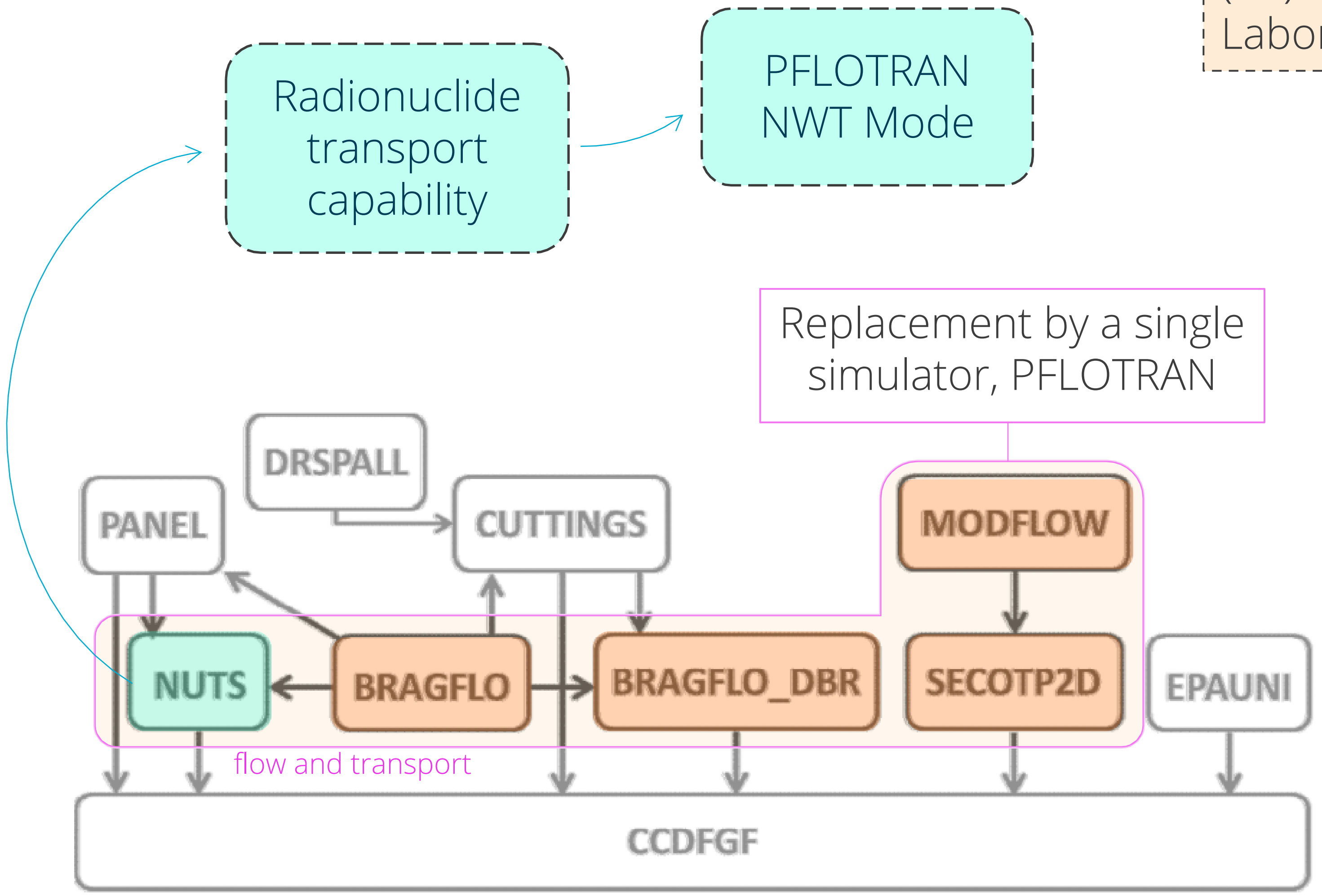
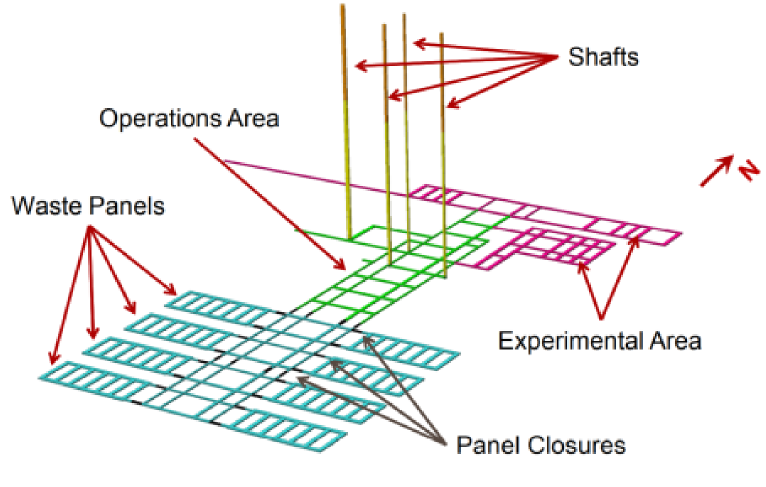


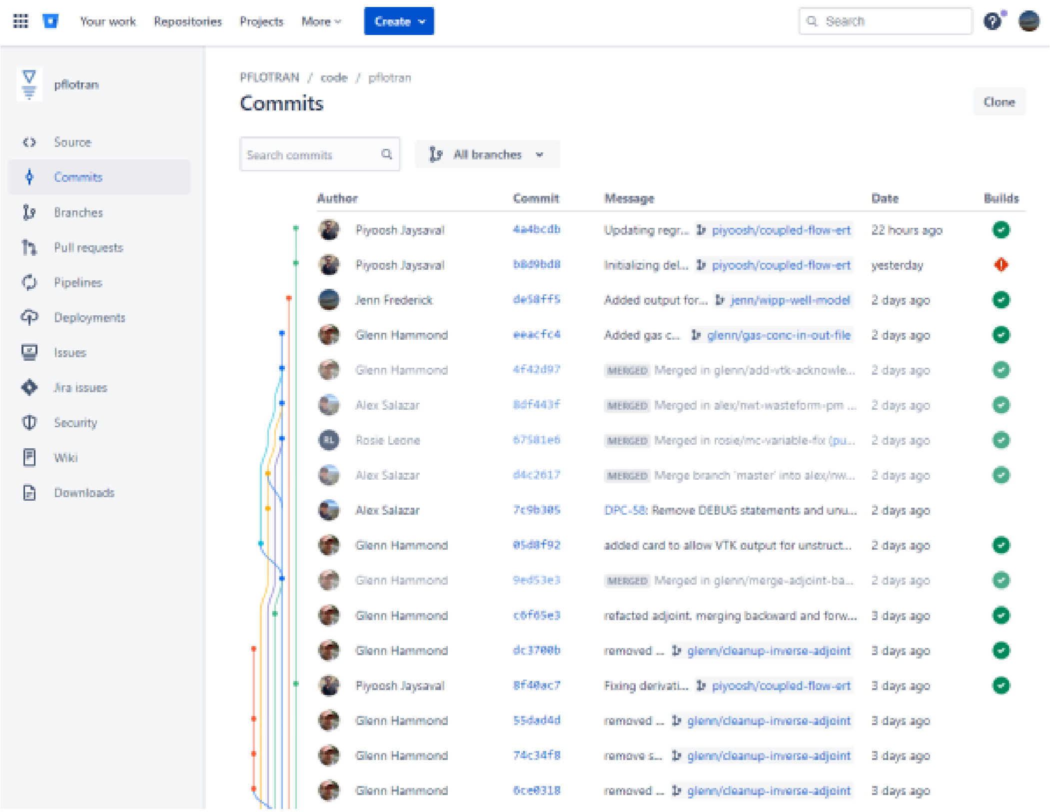


DOE is interested in reducing the number of principal codes to improve efficiencies for an asymmetric repository.

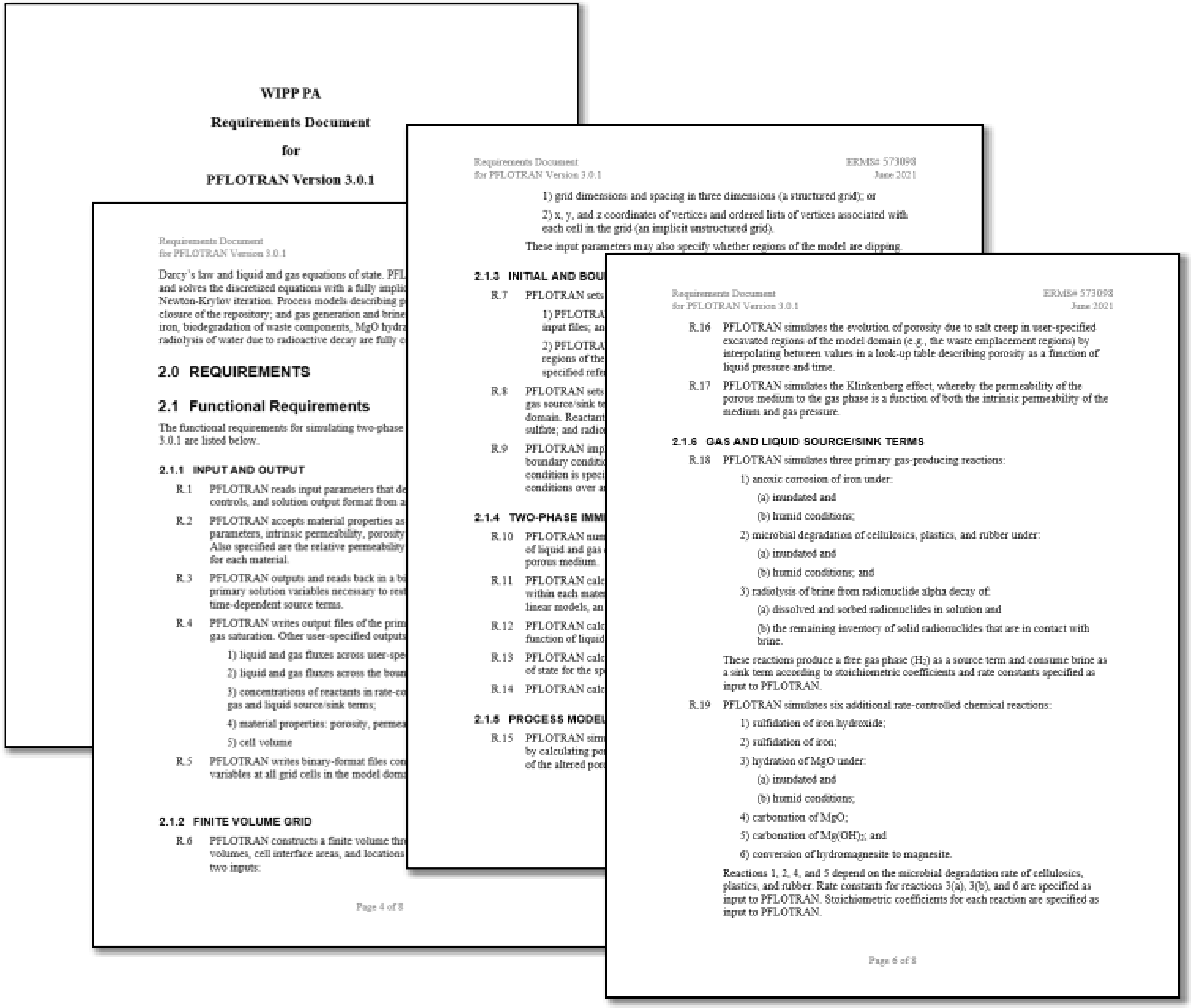
PFLOTRAN

- Petascale reactive multiphase flow and transport simulator
- Open source license (GNU LPGL-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)



WIPP Performance Assessment Requirements



WIPP PA
Requirements Document
for
PFLOTRAN Version 3.0.1

Requirements Document
for PFLOTRAN Version 3.0.1

2.0 REQUIREMENTS

2.1 Functional Requirements

2.1.1 INPUT AND OUTPUT

2.1.2 FINITE VOLUME GRID

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Requirements Document
for PFLOTRAN Version 3.0.1
ERMS# 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.

Requirements Document
for PFLOTRAN Version 3.0.1
ERMS# 573098
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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 Klinkenberg 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 cellulosics, 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 cellulosics, 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.

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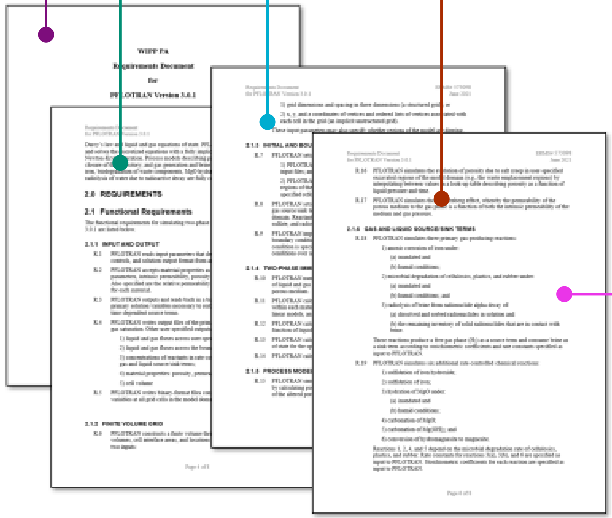
Software quality assurance (QA) documents specify requirements for radionuclide transport calculations in WIPP PA.

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, $\boldsymbol{M}$.

total mass (aqueous) (precipitated)

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

sources/sink

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

fluid velocity

decay/ingrowth

α phase (aqueous, precipitated)

j species (radionuclide, tracer, etc.)

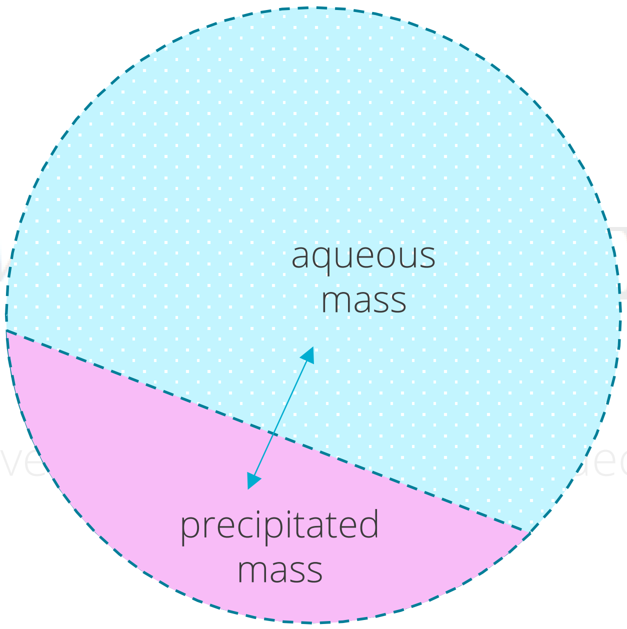
PFLOTRAN Nuclear Waste Transport (NWT) Mode

Governing equation formulated in terms of total mass, $\boldsymbol{M}$.

total mass — aqueous — precipitated

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

equilibrium chemistry partitioning



determined by solubility limit (calc'd by PANEL)

α phase (aqueous, precipitated)

j species (radionuclide, tracer, etc.)

PFLOTRAN Nuclear Waste Transport (NWT) Mode

Governing equation formulated in terms of total mass, $\boldsymbol{M}$.

total mass, aqueous, precipitated

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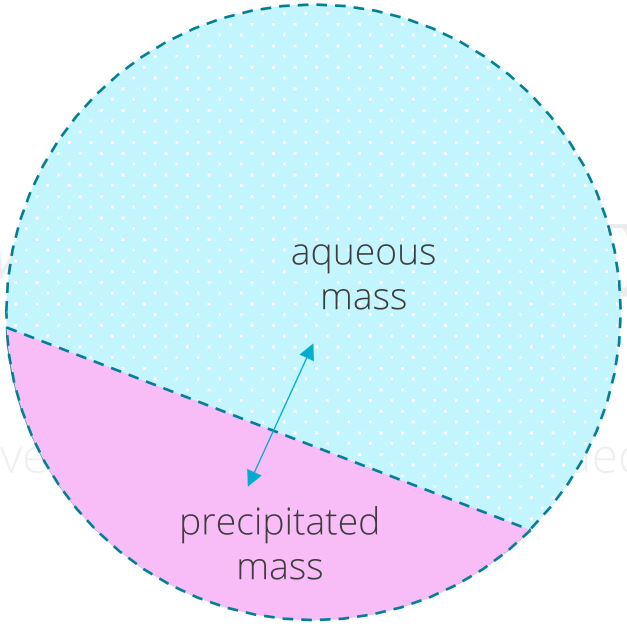


determined by solubility limit (calc'd by PANEL)

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, $\boldsymbol{M}$.

total mass, aqueous, precipitated

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

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

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, $\boldsymbol{M}$.

Bateman equation

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

parent

total mass

precipitated

sources/sink

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

fluid velocity

decay/ingrowth

λ radioactive decay constant

α phase (aqueous, precipitated)

j species (radionuclide, tracer, etc.)

PFLOTRAN Nuclear Waste Transport (NWT) Mode

Governing equations are solved using Newton-Krylov iteration.

residual of non-linear system

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

linear system of equations, Ax=b

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

Jacobian

solution update

residual

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

PFLOTRAN Nuclear Waste Transport (NWT) Mode

Governing equations are solved using Newton-Krylov iteration.

Convergence is declared based on infinity norms of:

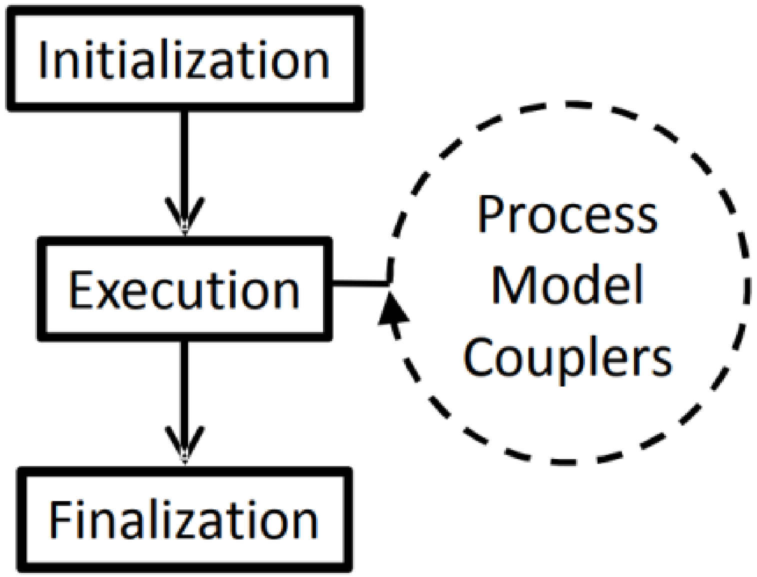
- $\frac{R\left(M_j^{\alpha,t+1}\right)}{\left(\Sigma_\alpha\left(M_j^{\alpha,t}\right)\forall\right)}$ scaled residual
- $R\left(M_j^{\alpha,t+1}\right)$ absolute residual
- $\delta M_j^{\alpha,t+1}/M_j^{\alpha,t}$ relative solution update

Tolerances can be assigned to each species.

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

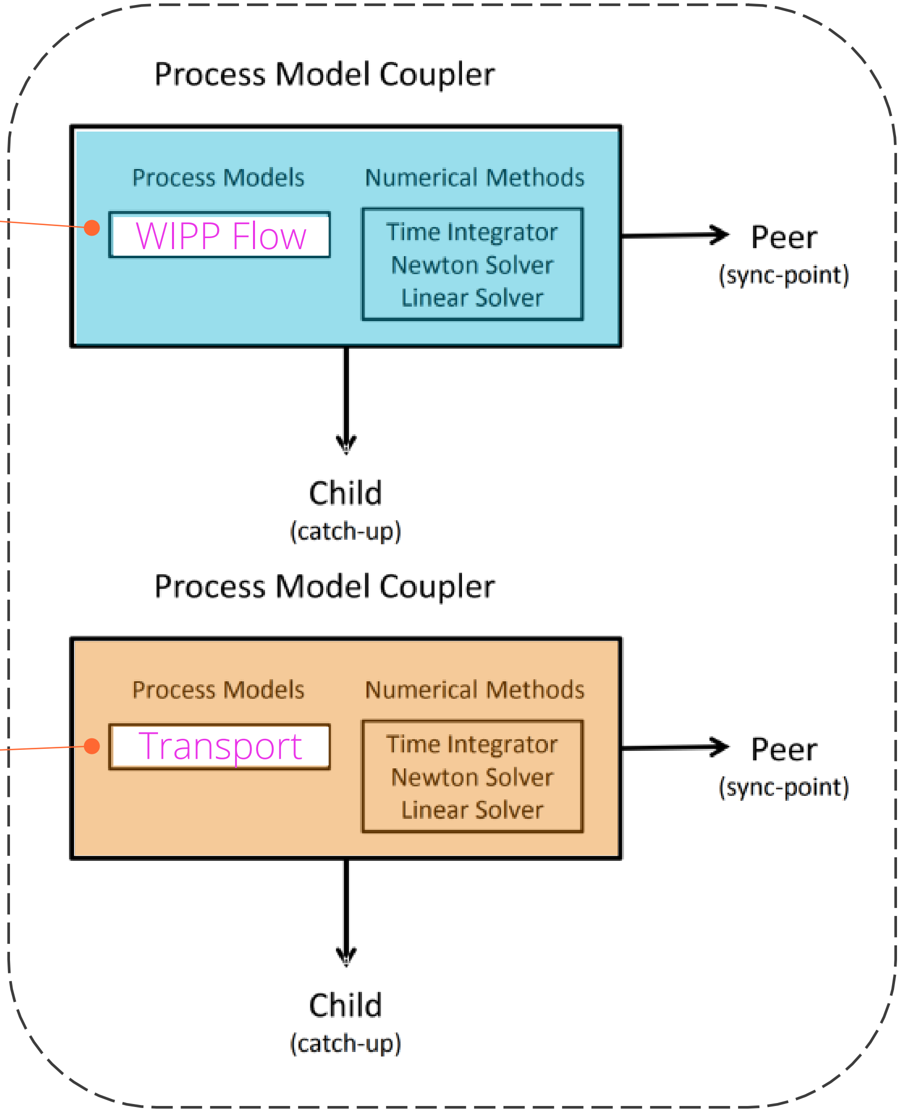
PFLOTRAN Nuclear Waste Transport (NWT) Mode

PFLOTRAN



replaces BRAGFLO

replaces NUTS

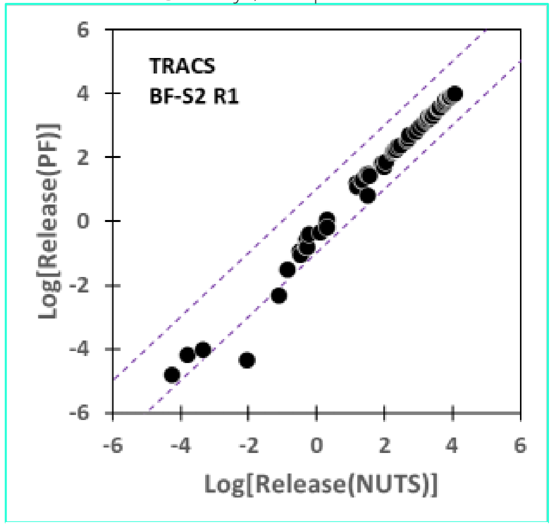


Flow & transport are sequentially coupled.

Initial Results: Comparison of NUTS & PFLOTRAN-NWT Mode

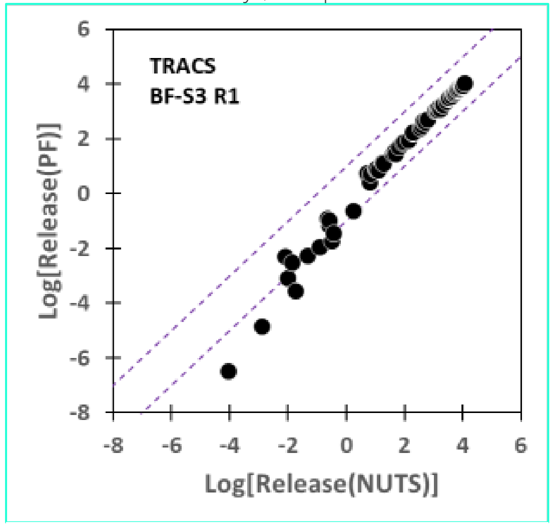
Screened-in* vector tracer simulations for S2, S3, S4, S5 scenarios

Intrusion @ 350 yr, into pressurized brine



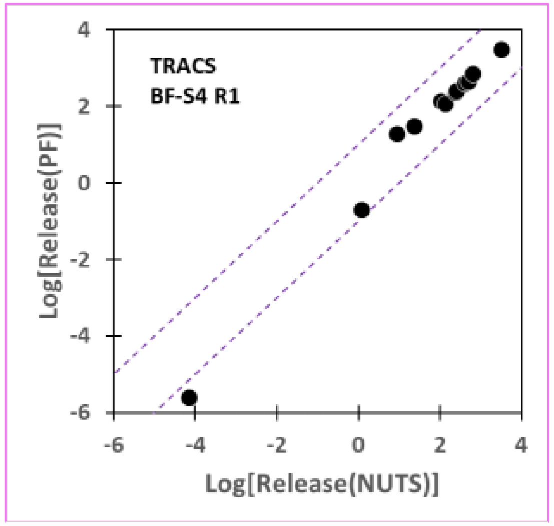
Mean Releases:
PF: 1.715E+03 kg
NUTS: 1.934E+03 kg

Intrusion @ 1000 yr, into pressurized brine



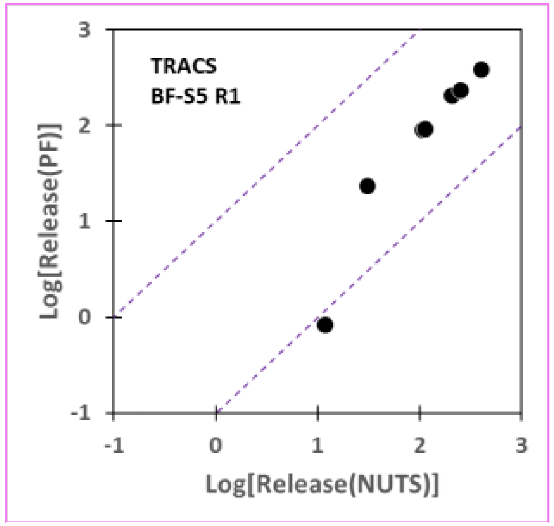
Mean Releases:
PF: 1.817E+03 kg
NUTS: 2.036E+03 kg

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:

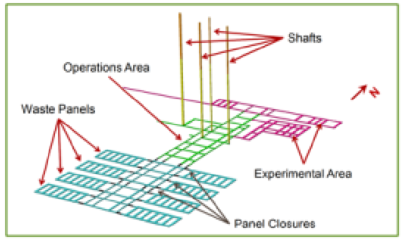
- Larger relative differences are observed for vectors with small releases (log(release) < 0).
- PFLOTRAN-NWT consistently calculates lower releases than NUTS (~ 10% less).
- Mean releases are comparable between two simulators.

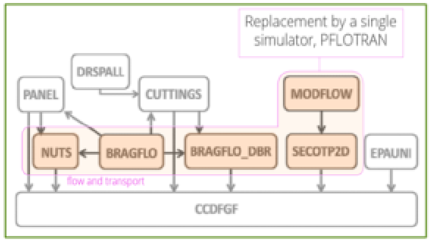
Fundamental Scenario	Specific Scenario	Time of Drilling Intrusion(s)
E0: no drilling intrusions.	S1-BF	N/A
E1: single intrusion through an excavated area of the repository that penetrates pressurized brine in the Castile	S2-BF	350 years
	S3-BF	1,000 years
E2: single intrusion through an excavated area of the repository that does not penetrate pressurized brine in the Castile.	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

* Vectors with release quantities above threshold cumulative amount (1.0e-7 kg).

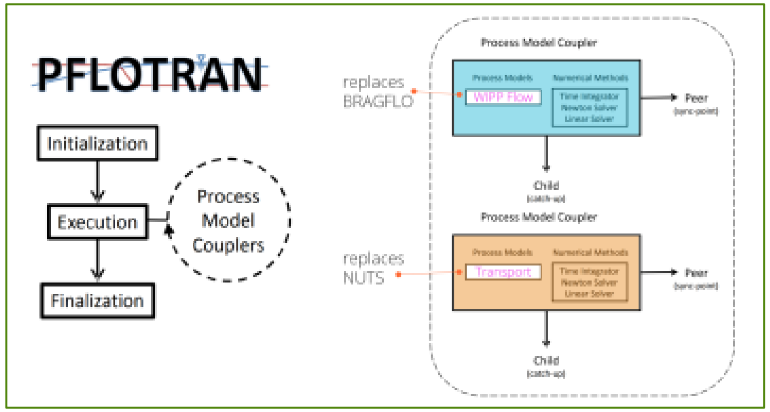
CONCLUSIONS

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.



Governing equation formulated in terms of total mass, M.

total mass, aqueous, precipitated

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

sources/sink

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

fluid velocity, decay/ingrowth

α phase (aqueous, precipitated)

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