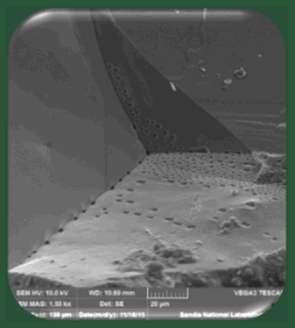
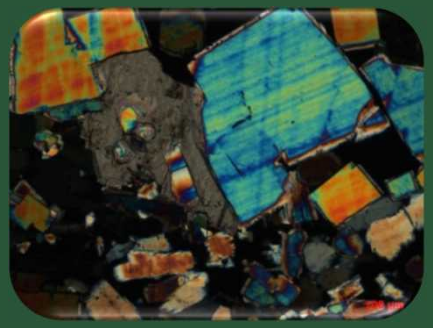

PFLOTRAN-RepoTREND Code Inter-comparison:
Inter-comparison Plan & First PFLOTRAN Results

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Code Inter-comparison Plan

- **What is a code inter-comparison?**
  - A comparison between two or more codes (software or programs) meant to *verify** or benchmark the codes
    - ensure mathematical equations are being solved correctly
  - Based on results of the *same** simulation
    - Same problem set-up or description, but implemented in each code independently

- PFLOTRAN (used and partially developed at Sandia National Laboratories, New Mexico, USA)
- RepoTREND (used and developed by GRS, Germany)
- *Do you want to join with your software?*

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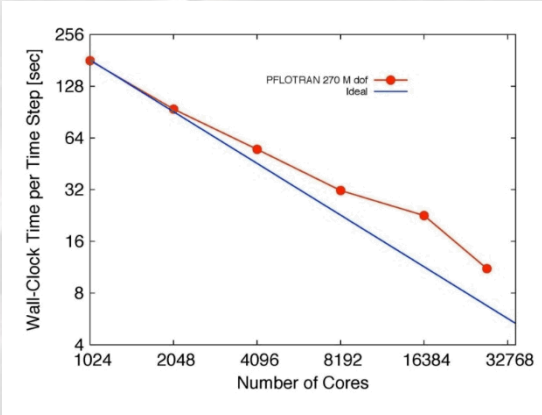
PFLOTRAN

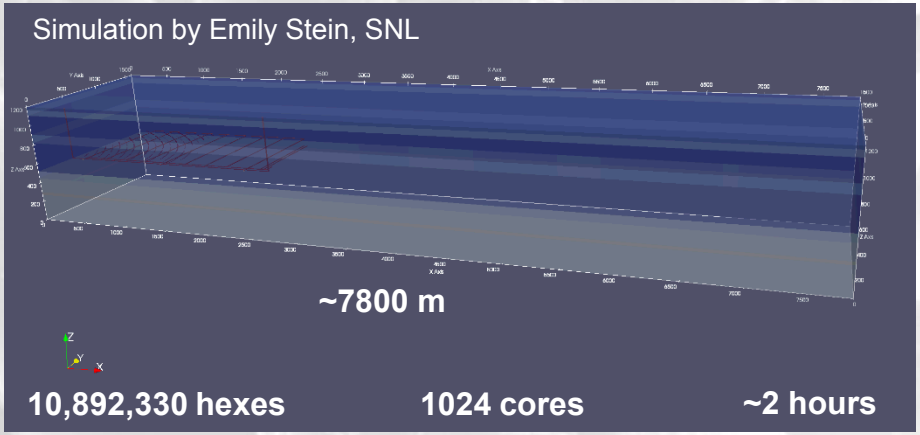
- Reactive multiphase flow and transport code for porous media
- Open source license (GNU LGPL 2.0)
- Object-oriented Fortran 2003/2008
  - Pointers to procedures
  - Classes (extendable derived types with member procedures)



- Founded upon well-known (supported) open source libraries
  - MPI, PETSc, HDF5, METIS/ParMETIS/CMAKE
- Demonstrated performance
  - Maximum # processes: 262,144 (Jaguar supercomputer)
  - Maximum problem size: 3.34 billion degrees of freedom
  - Scales well to over 10K cores

PFLOTRAN

- Nuclear waste disposal
  - Waste Isolation Pilot Plant (WIPP) in Carlsbad, NM
  - DOE Spent Fuel and Waste Science & Technology Program
  - SKB Forsmark Spent Fuel Nuclear Waste Repository (Sweden, Amphos^{21})
- Climate: coupled overland/groundwater flow; CLM
  - Next Generation Ecosystem Experiments (NGEE) Arctic
  - DOE Earth System Modeling (ESM) Program
- Biogeochemical transport modeling
- CO_2 sequestration
- Enhanced geothermal energy
- Radioisotope tracers
- Colloid-facilitated transport



PFLOTRAN-RepoTREND Comparison Table

Comparison Topics			PFLOTRAN	RepoTREND*
Repository Concepts		Near-field (EBS/CRZ)	3D/2D/1D	Coupled compartments (LOPOS)
		Far-field (Geosphere)	3D/2D/1D	1D (GeoTREND)
		Biosphere	Dose and water well/pumping under development	BioTREND
Process Physics	Flow	Single-phase	Yes	
		Multi-phase	Yes (air/water)	
		Miscible multi-phase	Yes	
		Permeability Tensor	Anisotropic, diagonal components only	
		Variable phase density	Yes	
		Variable phase viscosity	Yes	
		Soil compressibility	Yes	
	Reactive Transport	Advection	First-order upwinding	
		Diffusion	Yes	
		Mechan. dispersion	Yes	
		Sorption	Sorption onto solids and colloids with elemental material-specific Kd values	
		Dissolution and Precipitation	Yes	yes
		Geochemistry	Aqueous speciation, surface complexation, ion exchange	no
		Source/Sink ‚Sandbox'	Customizable source or sink with a user-defined reaction	
	Energy (Heat)	Conduction	Material-specific conductivity, specific heat	no
		Convection	Density-driven flow (density a function of temperature)	no
	Geomechanics		3D, finite element, elastic, no mesh deformation	

* ***RepoTREND has not fully filled in the table yet!***

PFLOTRAN-RepoTREND Comparison Table

Comparison Topics			PFLOTRAN	RepoTREND*
Radionuclides		Number of RNs	No limit except for practicality in computation time (~15)	
		Decay chain	Decay and ingrowth with implicit solution in solid and aqueous phases	
Waste package (source term)	Waste form	Number of RNs	No limit except for practicality in computation time (~15)	
		Decay Chain	Decay and ingrowth with explicit solution	
		Degradation/release mechanism	Slow dissolution or instantaneous release, custom dissolution rates or rates coupled to simulated T,pH,Q values.	
	Waste Package	Degradation	Waste package lifetime and performance terms, distributed breach times with rates coupled to simulated T values.	
Discretization	Grid/Meshing		Structured and unstructured	
	Serial/Parallel		Serial and parallel using domain decomposition via PETSc library	
	Solution method	Numerical Method	Finit volume, Newtons method using PETSc library package	
		Flow & Transport Coupling	Sequential	
		Transport & Reaction Coupling	Global implicit	
Radionuclides		Number of RNs	No limit except for practicality in computation time (~15)	
		Decay chain	Decay and ingrowth with implicit solution in solid and aqueous phases	

* ***RepoTREND has not fully filled in the table yet!***

PFLOTRAN-RepoTREND Comparison Table

Comparison Topics		PFLOTRAN	RepoTREND*
I/O and data exchange	Input	*.in file (ASCII file with structured keywords)	JSON file
	Output	HDF5 and Formatted ASCII (VTK, TECPLOT)	Formatted ASCII
	Data exchange	HDF5 and Formatted ASCII databases	
Documentation		Available at pflotran.org/documentation Documentation is version controlled in sync with the software version control.	
License		Open source GPL, bitbucket.org/pflotran/pflotran-dev	Private
Quality Assurance	Regression Tests	More than 200 tests that must be run before changes to the code become adopted.	
	Unit tests	Several tests that examine changes in output files when changes to code occur.	
	Verification Test Suite	More than 50 tests which calculate error against analytical solutions for fluid flow, energy, and mass transport. Automatic convergence testing is planned.	
	Version Control	Git with hosting on bitbucket.org	

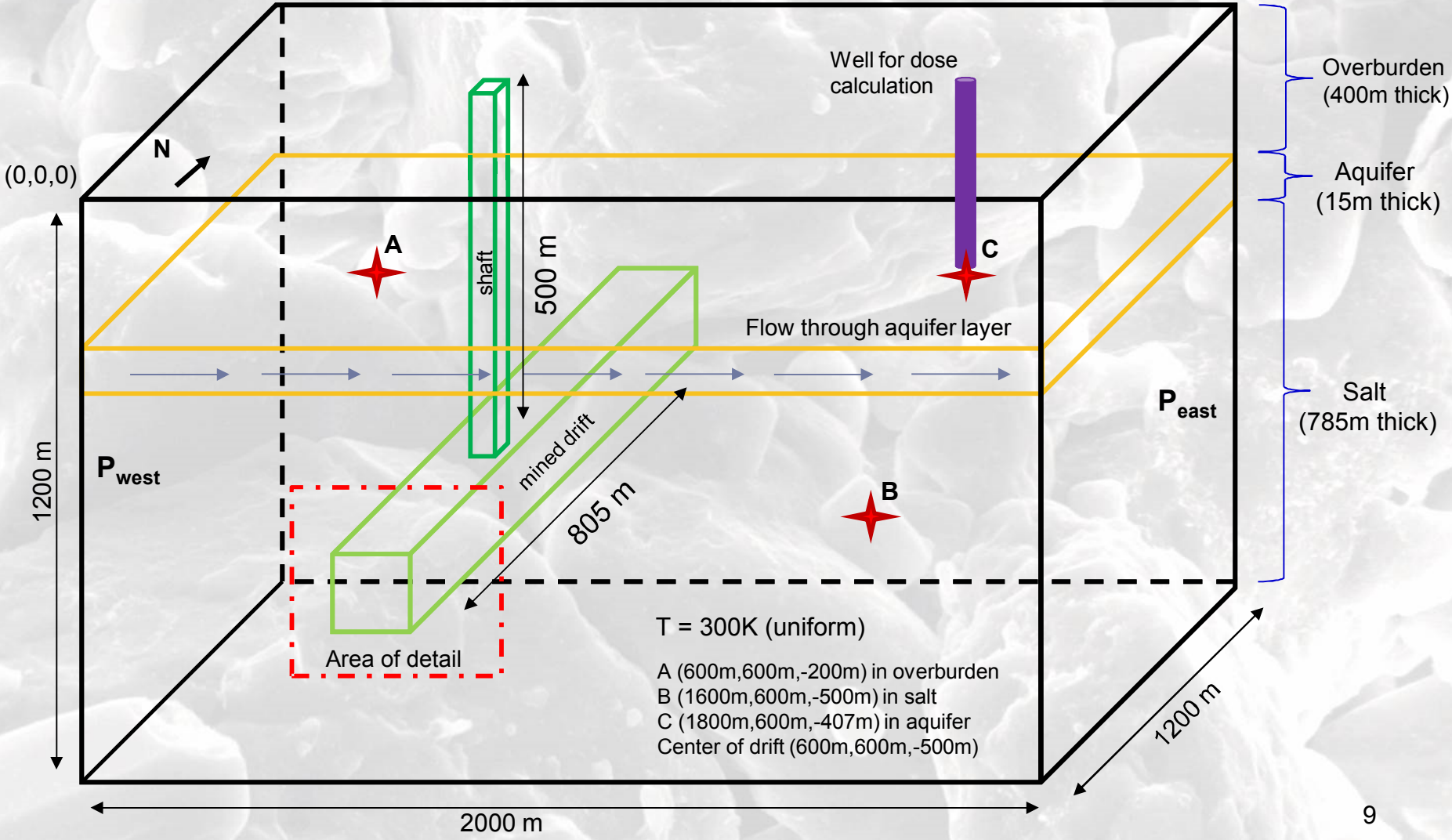
* ***RepoTREND has not fully filled in the table yet!***

Code Inter-comparison Plan

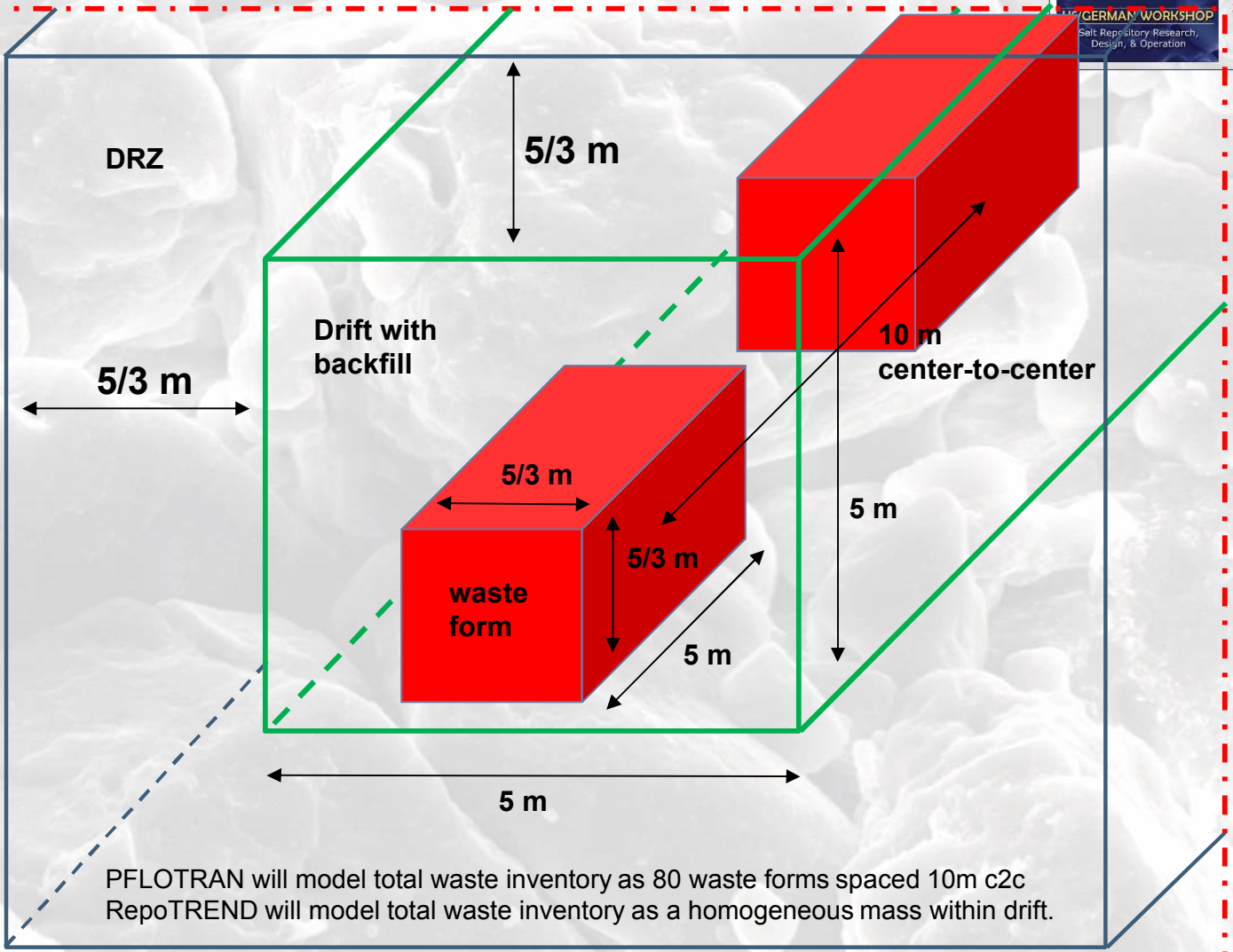
- **The PFLOTRAN-RepoTREND inter-comparison plan consists of:**
  - *single grid cell simulation*
  - A "batch" waste form simulation to compare the source term
    - spent nuclear fuel waste form that breaches instantly
    - RN inventory: ^{241}Am -> ^{237}Np -> ^{233}U -> ^{229}Th and ^{129}I
    - comparison metric: evolution of RN release [mol-RN/m^3/yr]
  - A 'full' simulation of a generic salt repository
    - a single mined drift within a salt body undergoing creep closure
    - a single vertical shaft that connects the drift to an aquifer above
    - uses same waste form inventory as tested in the batch simulation
    - transport can occur via advection and diffusion
    - comparison metric: break-through curves of each RN at specified points in aquifer and salt body, and dose calculation at a water well in aquifer

“Full” Salt Repository Simulation

Observation points A, B, and C



“Full” Salt Repository Simulation



PFLOTRAN will model total waste inventory as 80 waste forms spaced 10m c2c
RepoTREND will model total waste inventory as a homogeneous mass within drift.

Material Properties

MATERIAL	PERMEABILITY [M^2]	EFFECTIVE POROSITY [-]	TORTUOSITY [-]	GRAIN DENSITY [KG/M^3]
Salt	3.1e-23	0.018	0.01	2710
DRZ	1.1e-16 @ t=0yr 1.0e-19 @ t=200yr	0.013	0.23	2170
Overburden	1e-17	0.20	0.20	2700
Aquifer	1e-12	0.15	0.15	2820
Drift Backfill	?	?	?	2170
Shaft Backfill	1e-18	0.10	?	2170
Waste Form (SNF)	1e-17	0.50	1	5000

* Calculate effective diffusion coefficient: $D_e = (\text{porosity})(\text{tortuosity})(2.3\times10^{-9})\ m^2/s$

Waste Inventory

RNs considered as waste

	129I	241Am	237Np	233U	229Th
Kd value [mL/g]	0	62.5	5.5	0.6	550
Decay rate [1/s]	1.29e-15	5.08e-11	1.03e-14	1.38e-13	2.78e-12
Element solubility limit [mol/L]	unlimited	6e-6	1e-9	4e-10	4e-7
Mass fraction in waste form* [g/g]	2.17e-4	1.01e-3	9.72e-4	3.01e-8	1.03e-11
Total inventory (g)	1.3e5	6.07e5	5.85e5	1.81e1	6.19e-3

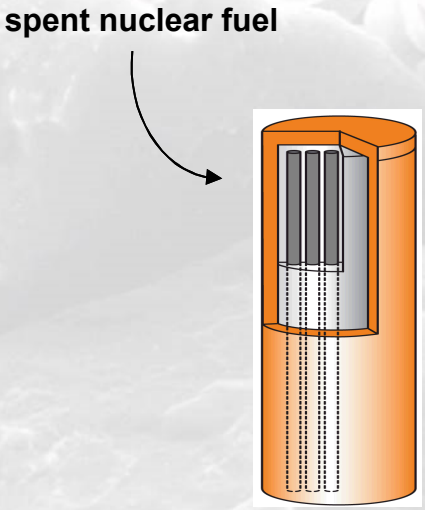
extra RNs for more accurate solubility calculation

	243Am	234U	236U	238U	230Th
Kd value [mL/g]	62.5	0.6	0.6	0.6	550
Decay rate [1/s]	2.98e-12	8.90e-14	9.20e-16	4.87e-18	2.75e-13
Element solubility limit [mol/L]	6e-6	4e-10	4e-10	4e-10	4e-7
Mass fraction in waste form* [g/g]	1.87e-4	3.55e-4	4.35e-4	6.32e-1	7.22e-8
Total inventory (g)	1.125e5	2.135e5	2.616e5	3.8e8	4.342e1

* PFLOTRAN requires a mass fraction, but RepoTREND should use the next row, total inventory.
* These mass fractions are based on 12-PWR 100 y OoR waste.

Batch Simulation: First PFLOTRAN Results

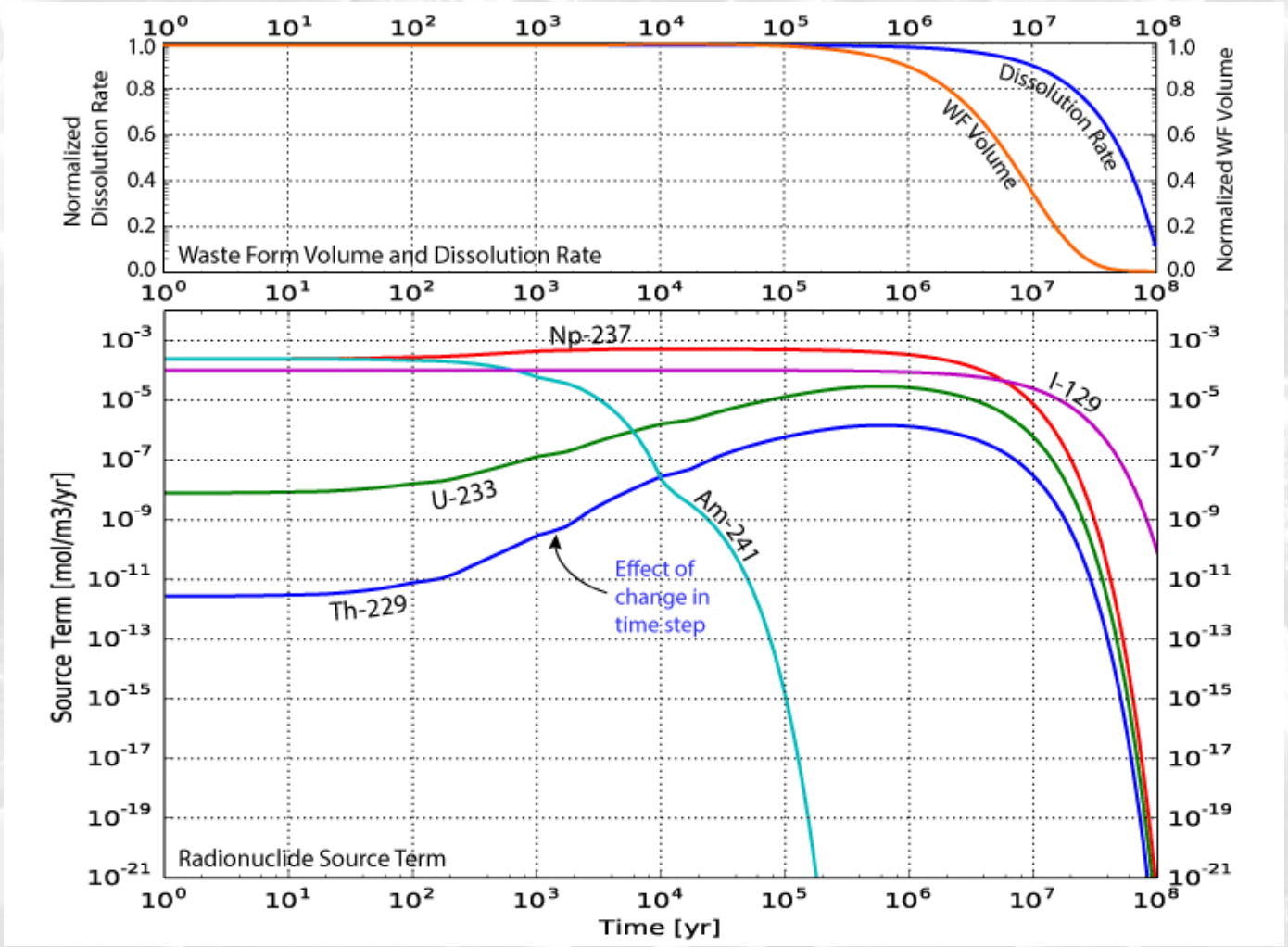
- First PFLOTRAN results for the batch simulation
  - designed to compare the source term calculation from dissolving spent nuclear fuel waste forms



- RN inventory: (shown previously)
  - ^{241}Am -> ^{237}Np -> ^{233}U -> ^{229}Th and ^{129}I
  - based on 12-PWR 100 y OoR waste
- 80 waste forms make up total inventory
- Breach time is t = 0 yrs
- Fractional dissolution rate is $1x10^{-7}$ 1/yr

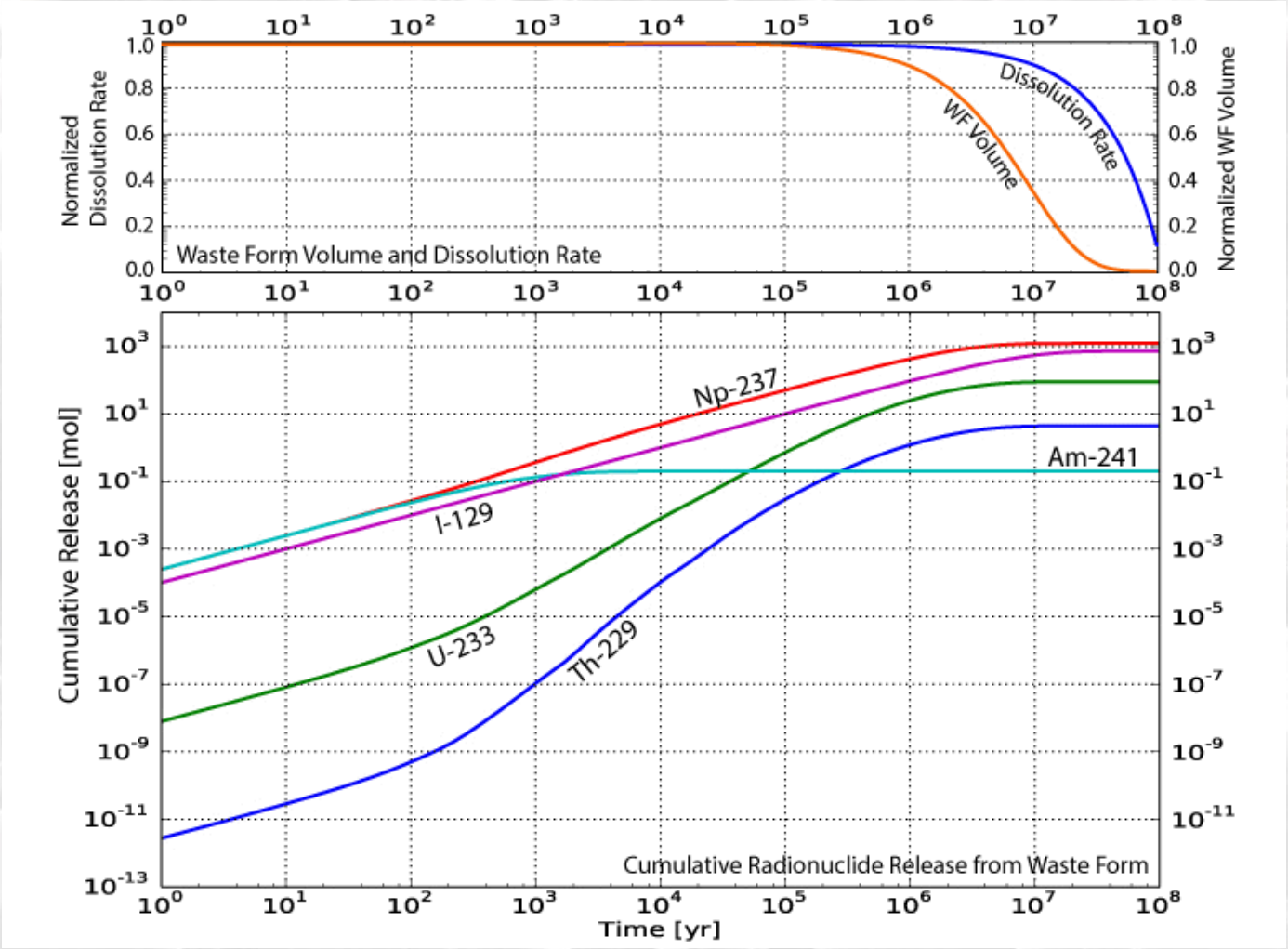
Batch Simulation: PFLOTRAN First Results

Radionuclide Source Term

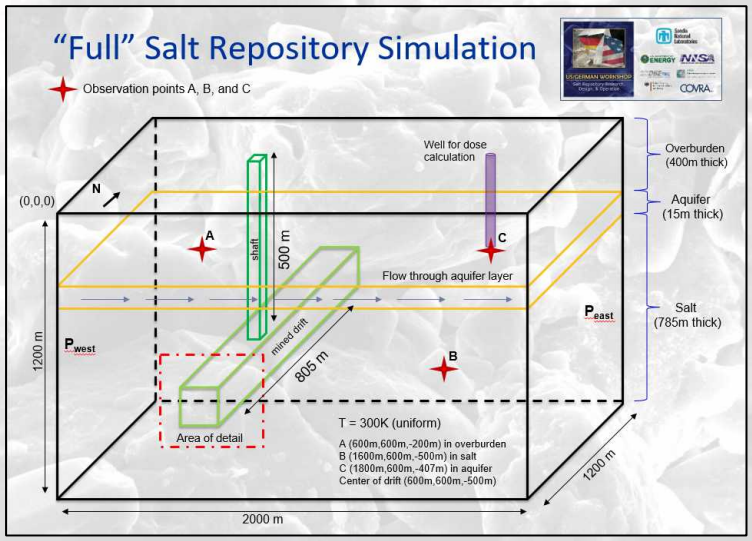


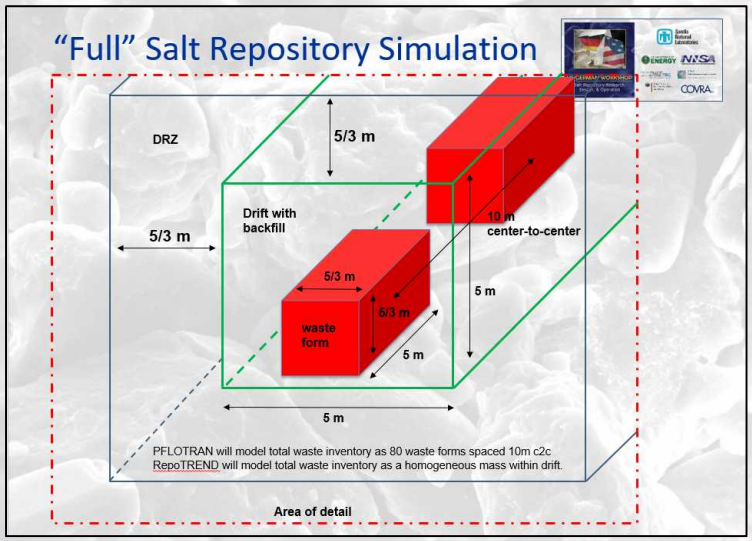
Batch Simulation: PFLOTRAN First Results

Cumulative Radionuclide Release



Next Steps for PFLOTRAN





- Next, we will set up the "full" repository simulation in PFLOTRAN