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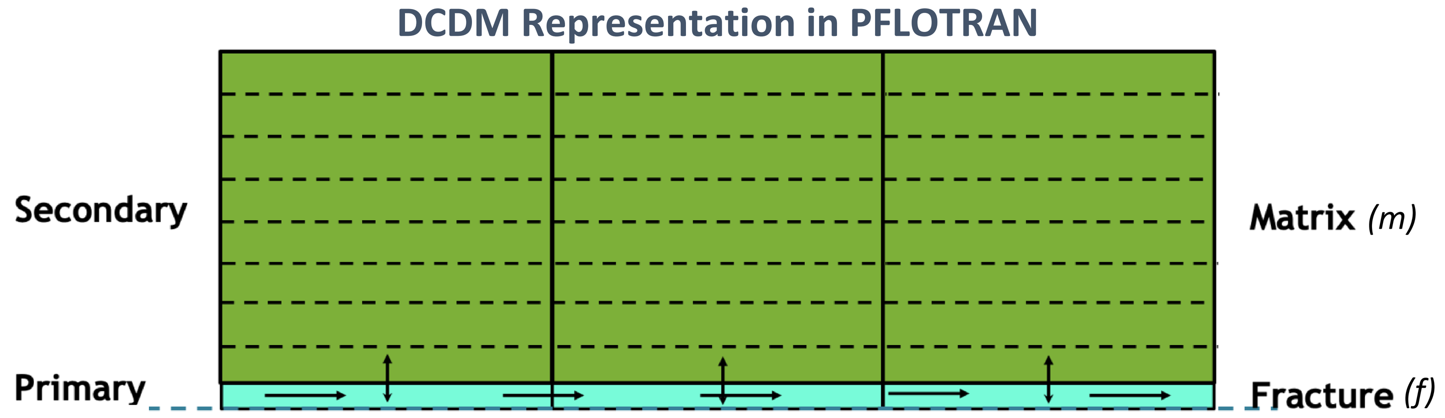
Rosie Leone[1], Glenn Hammond[2], Peter Lichtner[3], Michael Nole[1]
[1]Sandia National Laboratories, Albuquerque, NM
[2]Pacific Northwest National Laboratory, Richland, WA
[3]University of New Mexico, Albuquerque, NM

Multiple Continuum Approach to Modeling Radionuclide Transport in Fractured Networks

Introduction

Traditional discrete fracture models implementing matrix diffusion can be computationally expensive and only applicable to simplified transport problems. Upscaling to a continuum model can reduce computational burden, but models based on only a primary continuum neglect fracture-matrix interaction. PFLOTRAN, a subsurface flow and reactive transport code, simulates a secondary continuum (matrix) coupled to the primary continuum (fracture) modeled as a disconnected one-dimensional domain using a method known as the Dual Continuum Disconnected Matrix (DCDM) model. This work presents several benchmarks to compare PFLOTRAN's DCDM model to analytical solutions and a large-scale test problem in a one cubic km fractured domain modeling a conservative tracer with diffusion into the rock matrix. The tracer is compared using two different methods: first, with a Discrete Fracture Network (DFN) representation, and second, using the DCDM in PFLOTRAN where fractures were upscaled to an Equivalent Continuum Porous Medium (ECPM). We find that the DCDM representation of the upscaled fracture network produces results comparable to the DFN and analytical solutions where available, verifying this method. We then extend the DCDM model to be used in a fractured domain considering radionuclide isotope sorption, partitioning, decay, and ingrowth and find that radionuclide retardation is enhanced when considering these additional mechanisms.

Modeling Approach



Transport in fracture occurs due to advection and diffusion
Transport in matrix occurs due to diffusion only

The primary continuum in the DCDM model in PFLOTRAN is solved via,

$$\frac{\partial}{\partial t}\left(\epsilon_f \varphi_f \Psi_j^f\right) + \nabla \cdot \Omega_j^f = -A_{fm}\Omega_j^{fm} - \epsilon_f \sum_k \nu_{jk}\Gamma_k^f - \epsilon_f \frac{\partial S_j^m}{\partial t}$$

ϵ_f is the fracture volume fraction, φ is porosity, Ψ_j is the total component concentration (includes aqueous complexes) of species *j*, Ω^f is total solute flux in the fracture, Ω^{fm} is total solute flux between the fracture and matrix, A_{fm} is the fracture-matrix interfacial area, ν is the stoichiometric coefficient, Γ is the mineral reaction, and *S* is the sorption isotherm. The secondary continuum is modeled as a one-dimensional domain where diffusive fluxes occur perpendicular to the fracture wall,

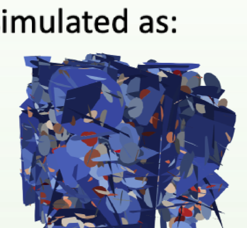
$$\frac{\partial}{\partial t}\left(\varphi_m \Psi_j^m\right) + \nabla_\xi \cdot \Omega_j^m = -\sum_k \nu_{jk}\Gamma_k^m - \frac{\partial S_j^m}{\partial t}$$

where the gradient operator ∇_ξ refers to the effective one-dimensional secondary continuum geometry. The equations for the primary and secondary continuum are solved separately and coupled together by the mass exchange flux assuming symmetry along the axis dividing them,

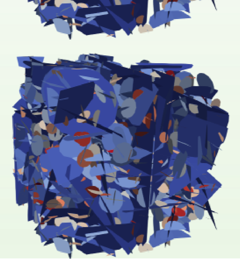
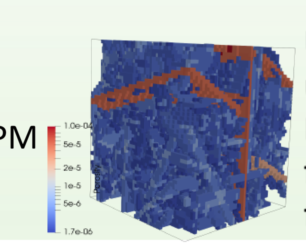
$$\Omega_j^{fm}(x,t) = \Omega_j^{m}(\xi_{fm}, x \mid t)$$

where *x* is a point in the fracture, *t* is time, and ξ_{fm} is the outer boundary of the matrix. Fractures were created and simulated as:

DFN:

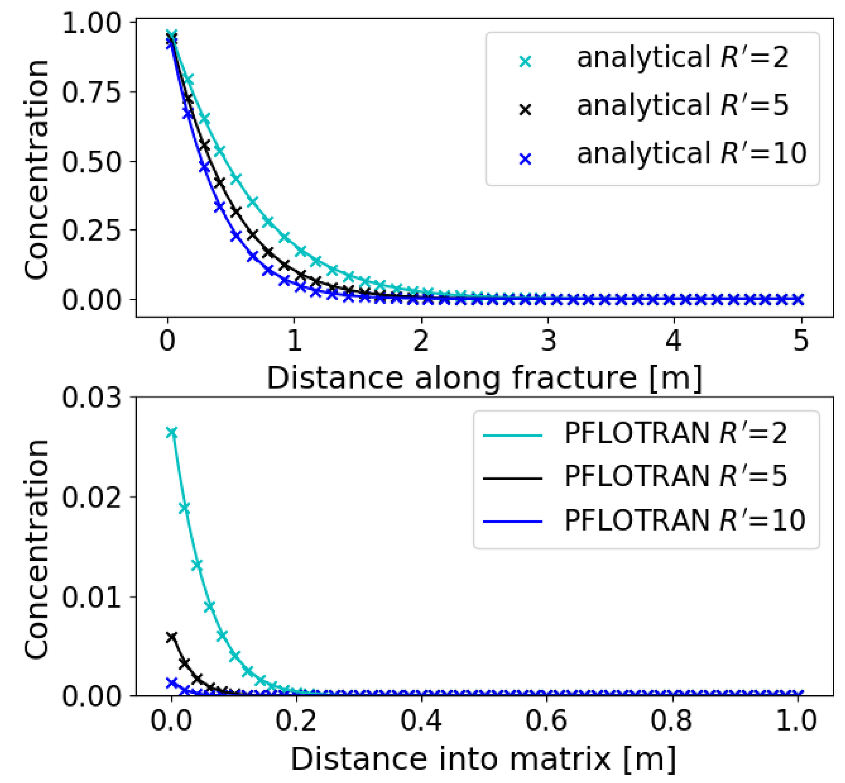
DFNWorks  → PFLOTRAN: Flow Solution → dfnTrans: Transport (particle tracking)

DCDM:

DFNWorks  → ECPM  Upscaled porosities used as input to DCDM model for fracture volume fraction (ϵ_f) → PFLOTRAN: Flow + Transport

Benchmarks

Single Fracture Analytical Solution – Tang et al., 1981

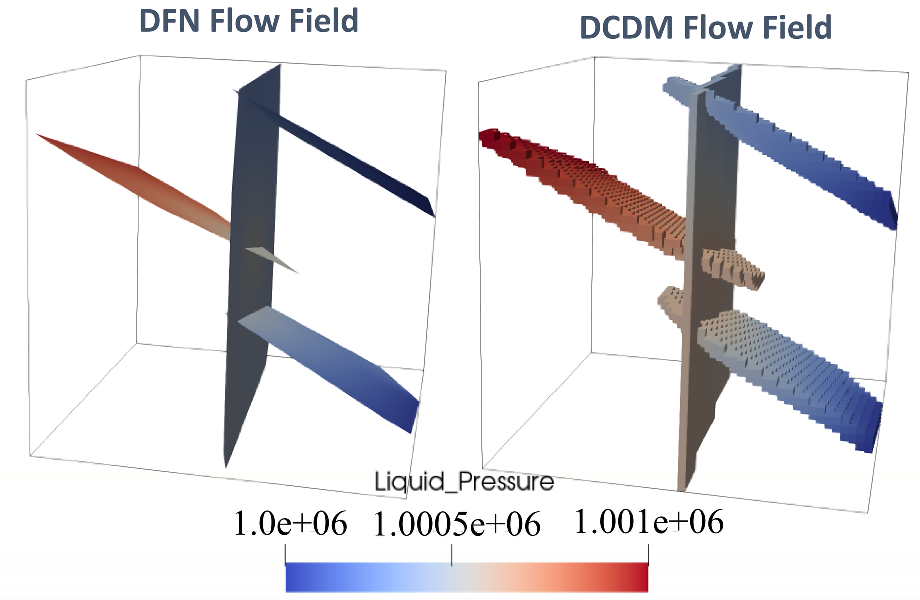


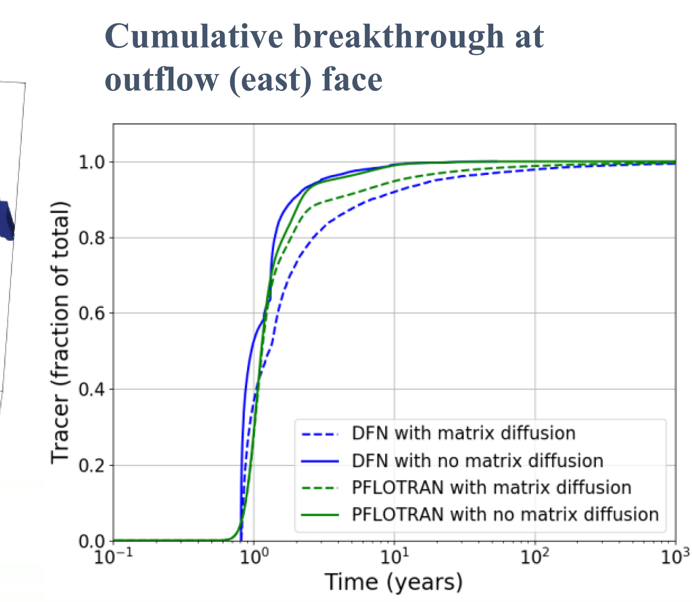
Parameter	Value
Fracture width	10^{-4} m
Dispersivity	0.5 m
Half-life	12.35 y
Matrix retardation factor (R')	2,5,10
Matrix porosity	0.01
Inlet concentration	1.0 M
Linear velocity	0.01 m/d

Four-Fracture DFN

Transport of a conservative tracer is simulated through four deterministic fractures in a one km cubic domain with diffusion into the rock matrix. Constant pressure boundary conditions were applied on the west and east faces. An initial pulse of tracer was inserted uniformly along the fractures on the west face. The tracer exits the domain through the fractures on the east face. All other faces were assigned no flow boundary conditions. Diffusion into the matrix occurs along the fractures.

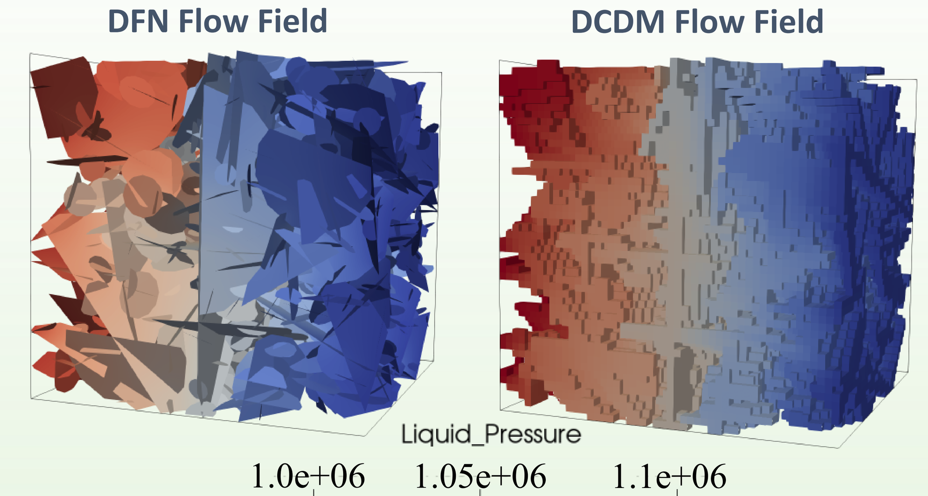
Parameter	Value
Matrix porosity	0.005
Matrix permeability	10^{-18} m^2
Matrix effective diffusion coefficient	1.6×10^{-10} m^2/s

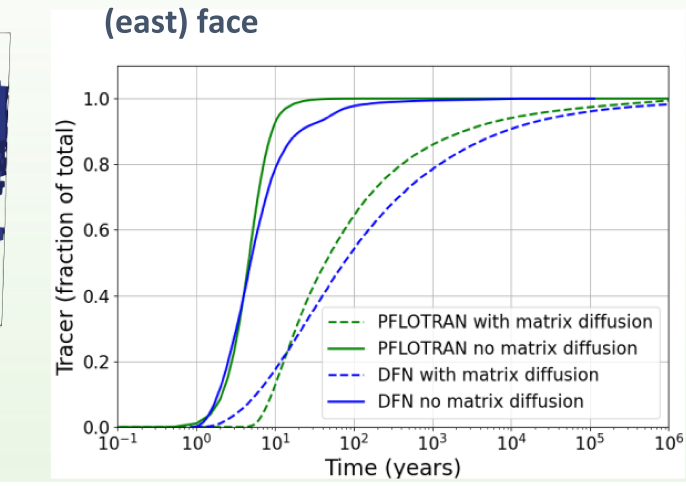




Four-Fracture DFN Plus Stochastic Fractures

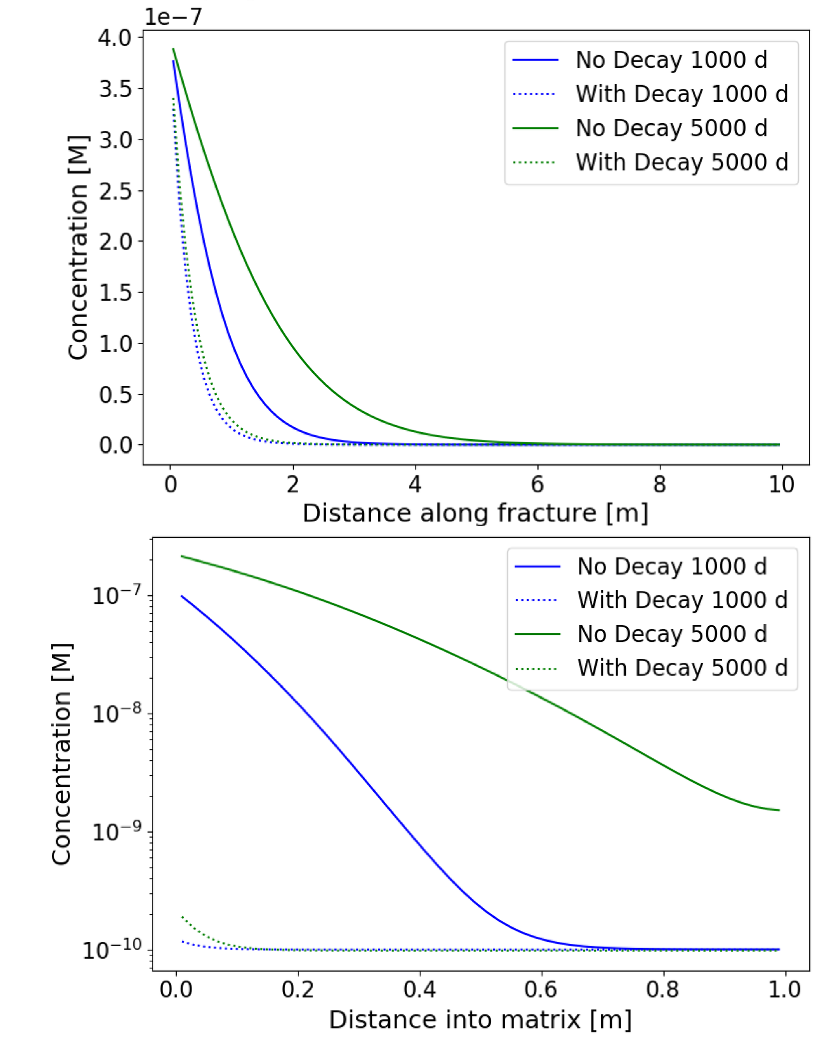
The four-fracture benchmark case was expanded on by adding stochastic fractures in the domain. Pressure and effective diffusion coefficient were altered to reduce breakthrough time.





Used Fuel Disposition Decay Model

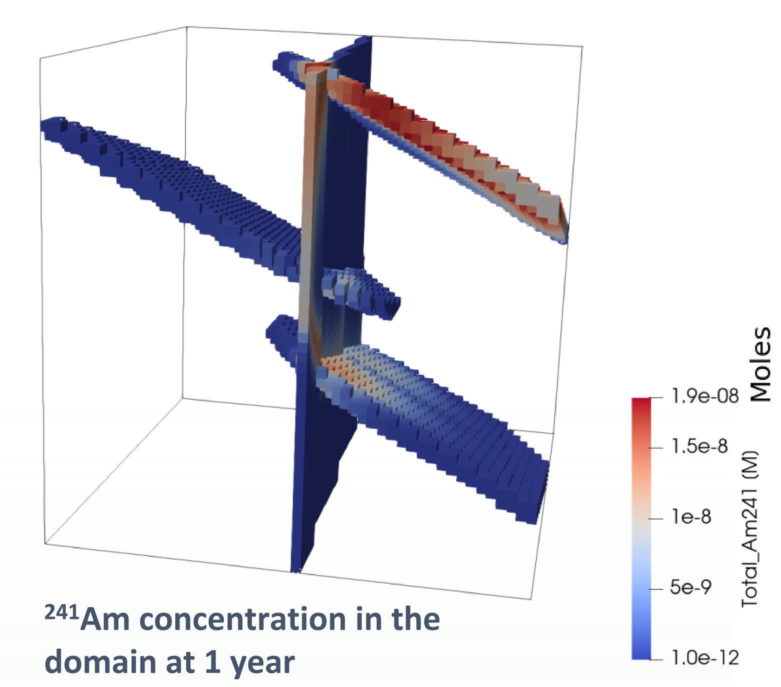
The Used Fuel Disposition (UFD) Decay Model in PFLOTRAN models radionuclide isotope decay, ingrowth, and phase partitioning and was created as part of the Geologic Disposal Safety Assessment (GDSA) Framework. The total mass of each isotope decays according to the Bateman Equations. The UFD decay model was applied to the single fracture problem considering the isotope ^{241}Am decaying to ^{237}Np versus a non-decaying tracer with diffusion into the rock matrix via the DCDM model.



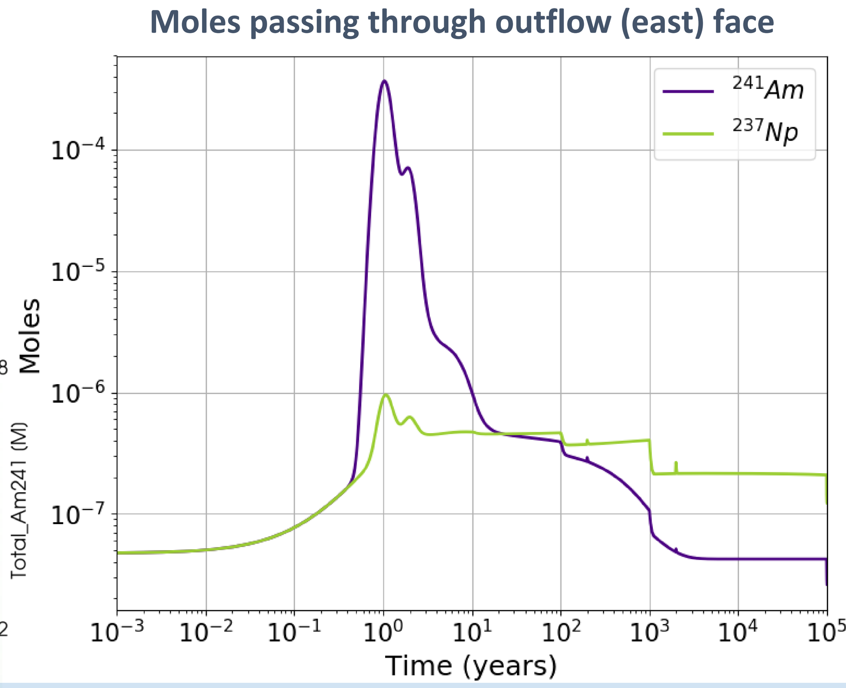
Parameter	Value
Inlet ^{241}Am	4×10^{-7} mol/kg
Inlet ^{237}Np	1×10^{-12} mol/kg
^{241}Am solubility	4×10^{-7} mol/L
^{237}Np solubility	4×10^{-9} mol/L
^{241}Am matrix K_d	0.04 m^3/kg
^{237}Np matrix K_d	0.2 m^3/kg
^{241}Am decay rate	5.08×10^{-11} 1/s
^{237}Np decay rate	1.03×10^{-14} 1/s

Values from Mariner et al., 2011

An increase in radionuclide retardation is seen when considering decay. The problem was then applied to the 4-fractures with an inlet pulse of ^{241}Am decaying to ^{237}Np.



^{241}Am concentration in the domain at 1 year



Conclusions

- The DCDM model in PFLOTRAN allows for representation of fracture-matrix interactions in large scaled fractured rock, and has recently been updated to model advanced radionuclide transport via the UFD Decay process model.
- We present verification of the DCDM model against single-fracture analytical solutions and a DFN particle tracking example in several multi-fracture domains.
- This analysis demonstrates the ability of PFLOTRAN's DCDM model to be used as part of a full-scale performance assessment of a deep geological repository in fractured crystalline rock.

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Stein, E. R., J. M. Frederick, G. E. Hammond, K. L. Kuhlmann, P. E. Mariner, and S. D. Sevougian. April 9-13, 2017. *Modeling Coupled Reactive Flow Processes in Fractured Crystalline Rock*. Paper presented at the International High-Level Radioactive Waste Management Conference, Charlotte, NC.
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