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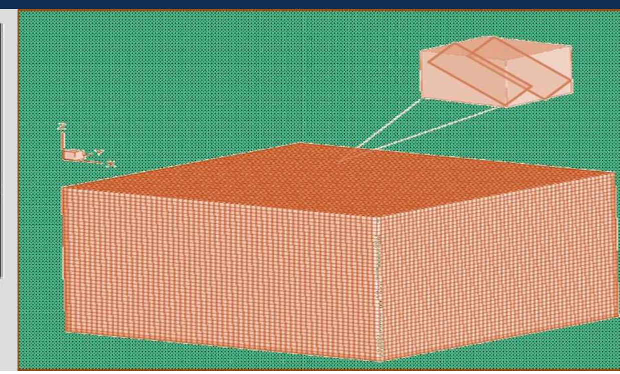

NUMERICAL MODELING OF FLOW AND TRANSPORT IN FRACTURED CRYSTALLINE ROCK

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Disposal Concept for Crystalline Repository

- Crystalline rocks are common in many stable continental regions
- Low permeability matrix rock and sparse fracture system
- Geochemically reducing conditions
- Rock characteristics favorable for repository construction

Fracture Characterization Methods

- A realistic representation of fractures in granite rock is needed
- Discrete Fracture Network and Equivalent Continuum Methods used
- The Fractured Continuum Model (FCM) used in this study
- FCM based on discrete fracture and effective continuum approaches (McKenna and Reeves, 2005, Kalinina et al. 2012, and Hadgu et al. 2016)

Flow and Transport Simulations

- Test case simulations of flow and transport in crystalline rock
- Relevant fracture data used
- Specified simulation domain and grid discretization
- FCM used to generate permeability and porosity of selected number of realizations
- Effective permeability and breakthrough curves evaluated
- PFLOTRAN (Lichtner et al., 2015)massively parallel subsurface flow and reactive transport code used in a high performance computing environment

Test Case Fracture Parameters

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Fracture statistics used for test case:

Fracture Set	Mean trend (degrees)	Mean plunge (degrees)	κ	α	R_u (m)	R_0 (m)	Number of fractures
North-South Vertical	90	0	22	2.5	500	15	2,100
East-West Vertical	0	0	22	2.7	500	15	2,000
West-East Horizontal	360	90	10	2.4	500	15	2,300

Fracture radius R follows a truncated power law distribution:

$$\mathbf{R} = R_0 \cdot \left[1 - \mathrm{u} + \mathrm{u} \cdot \left(\frac{R_0}{R_u}\right)^{\alpha}\right]^{-1/\alpha}$$

Fracture orientation ϴ follows Fisher distribution:

$$\mathbf{f}(\theta) = \frac{\kappa \cdot \sin\theta \cdot e^{\kappa \cdot \cos\theta}}{e^{\kappa} - e^{-\kappa}}$$

α = scaling factor, R_0 = radius lower limit, R_u = radius upper limit, κ= concentration parameter

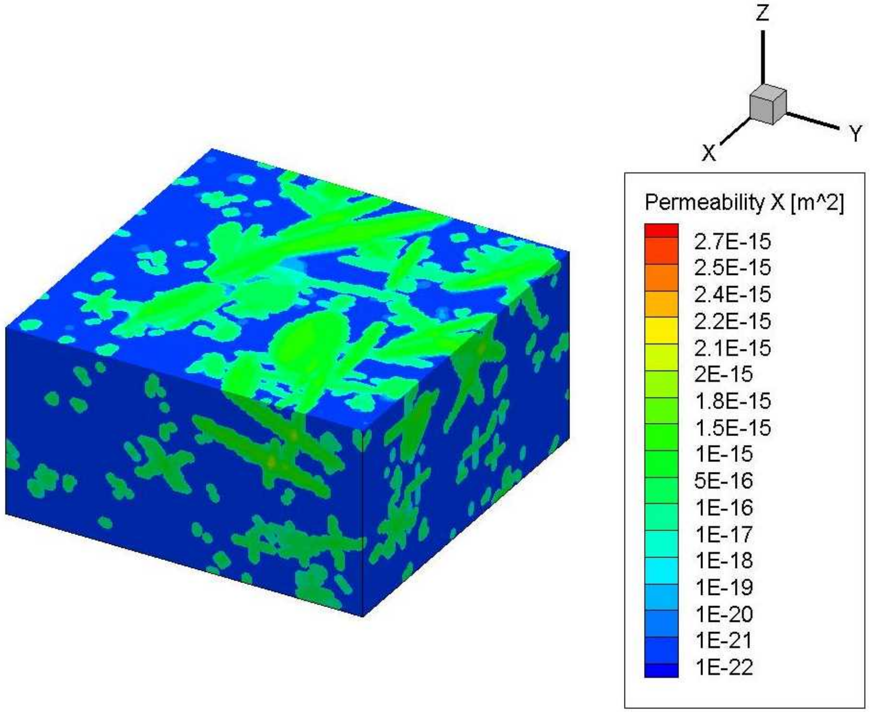
Simulation Model Setup

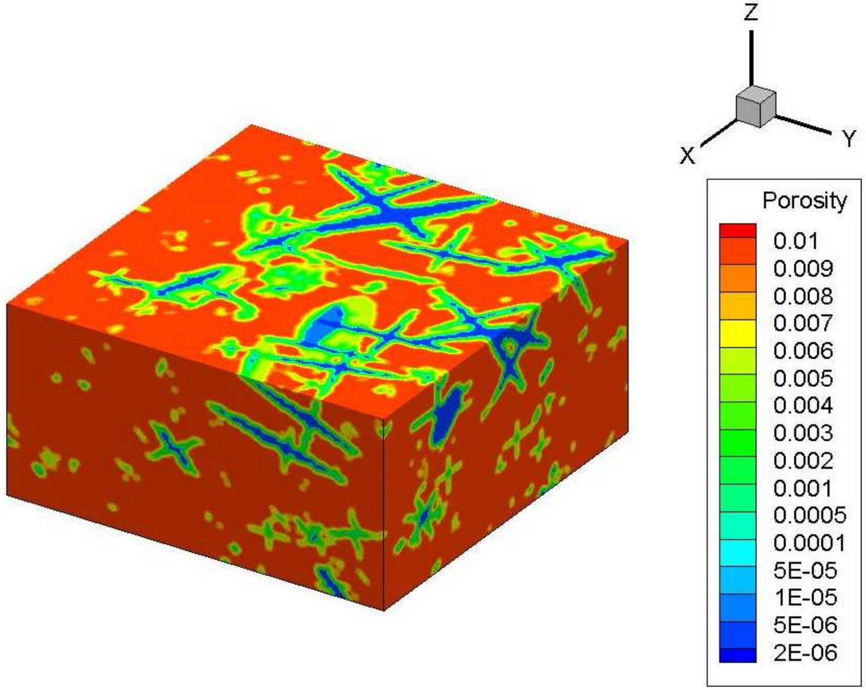
- Domain: 1000 m x 1000 m x 1000 m
  - Grid block size: 10 m x 10 m x 10 m
  - Number of grid blocks: 1,000,000
- Porosity: Anisotropic
- Permeability: Anisotropic
- Initial Conditions: Hydrostatic pressure
- Isothermal Conditions (T = 25 °C)
- Boundary Conditions:
  - Pressure at West Face: 1.001 MPa
  - Pressure at East Face: 1.0 MPa

Generation of Permeability and Porosity Fields

- Permeability and porosity fields generated using FCM with ELLIPSIM
- Specified fracture parameter distributions used in geostatistical representation of fractured domain
- Two sets of 25 realizations were selected
- Matrix rock permeability of 10^{-22} m^2 used to suppress matrix flow
- Matrix rock porosity of 0.01 used

Example Permeability and Porosity Fields





Permeability of a Realization **Porosity of a Realization**

Fluid Flow Simulation

- Steady state flow utilized
  - to estimate effective permeability for each realization
  - To generate flow field for transport simulation
- Darcy's law and east face flux used to calculate effective permeability

$$q = \frac{-k_{eff}\Delta P}{\mu L}$$

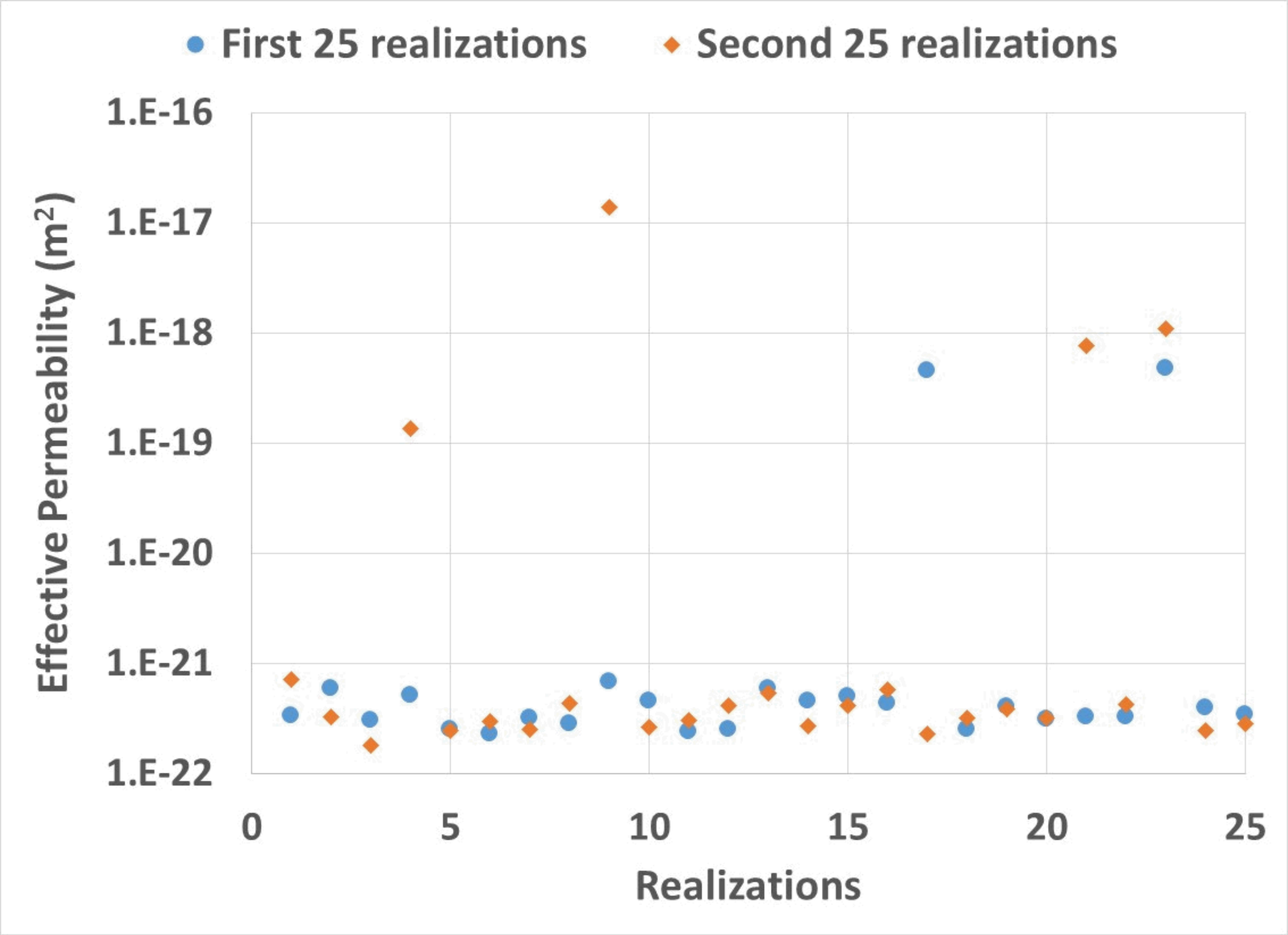
q = flux,

k_{eff} = effective permeability,

ΔP = pressure difference, μ = dynamic viscosity

L = distance between west and east faces

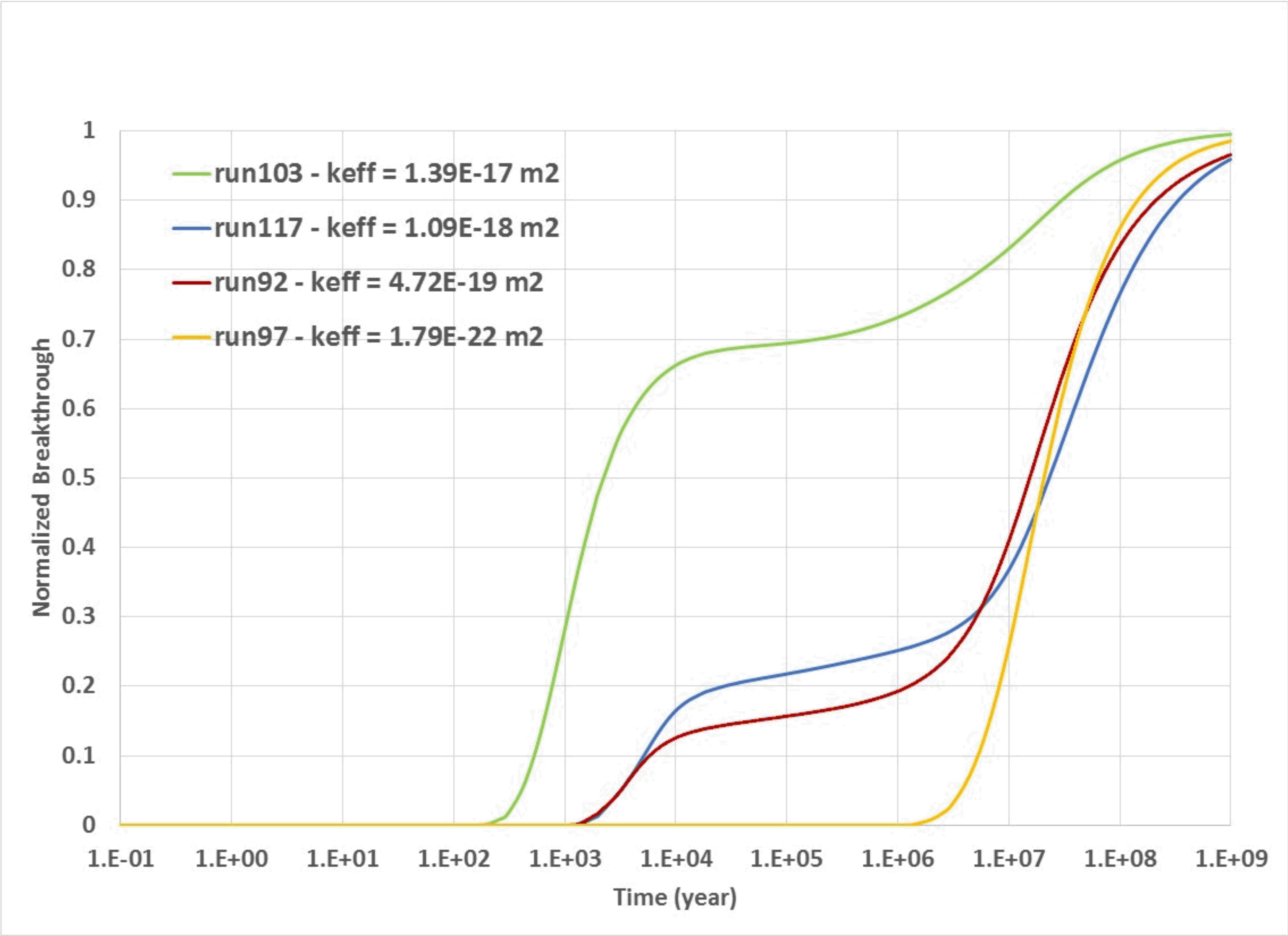
Effective Permeability Evaluation



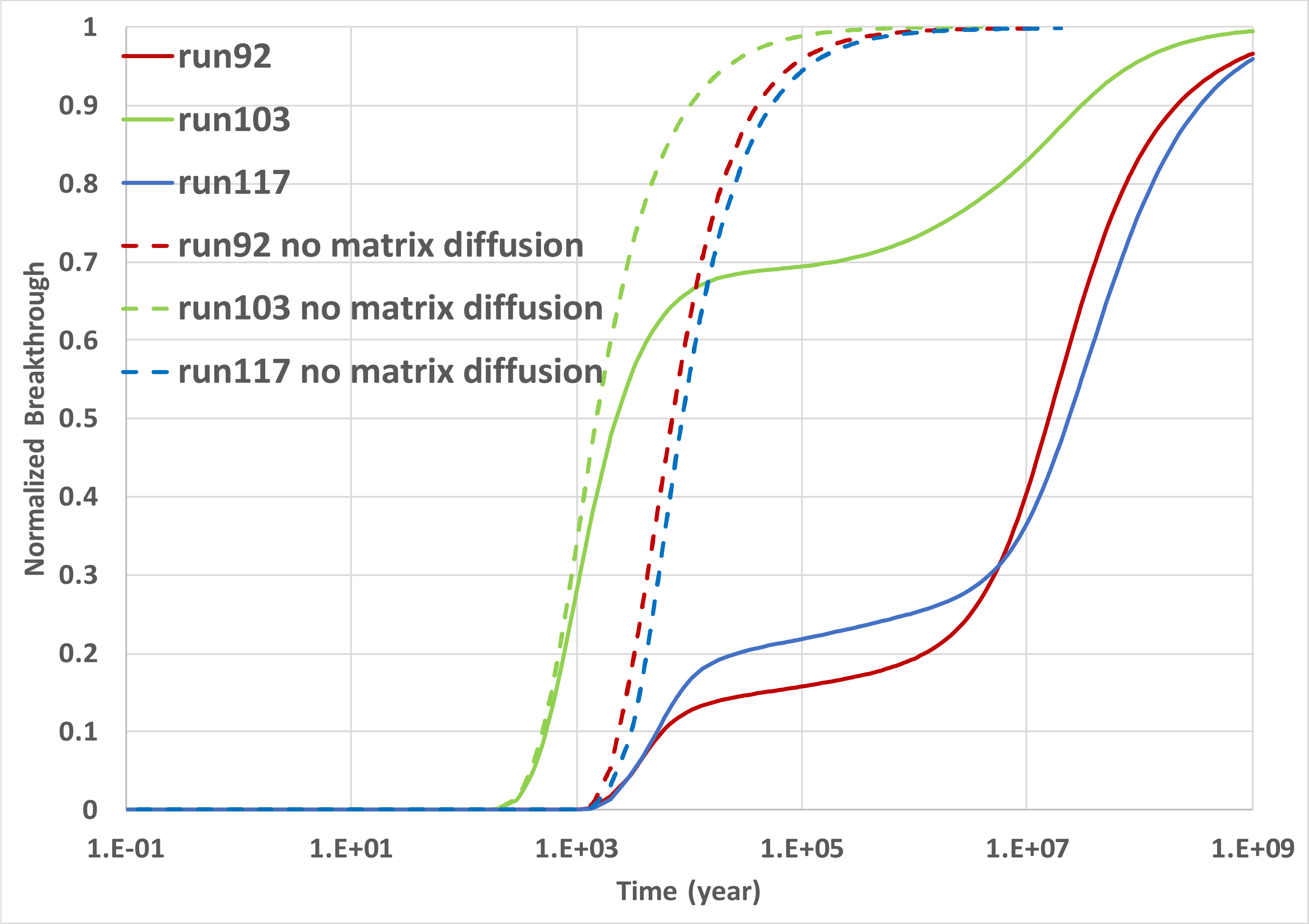
Transport Simulations: Tracer Breakthrough Curves Evaluation:

- PFLOTRAN numerical simulator used (advection-diffusion)
- Porosity and steady state flow fields for each realization utilized as input to transport simulations
- Transport of dissolved, nonreactive tracer through domain
- Tracer transport simulated with and without matrix diffusion
- Output used to calculate normalized breakthrough curve for each realization

Tracer Breakthrough Curves

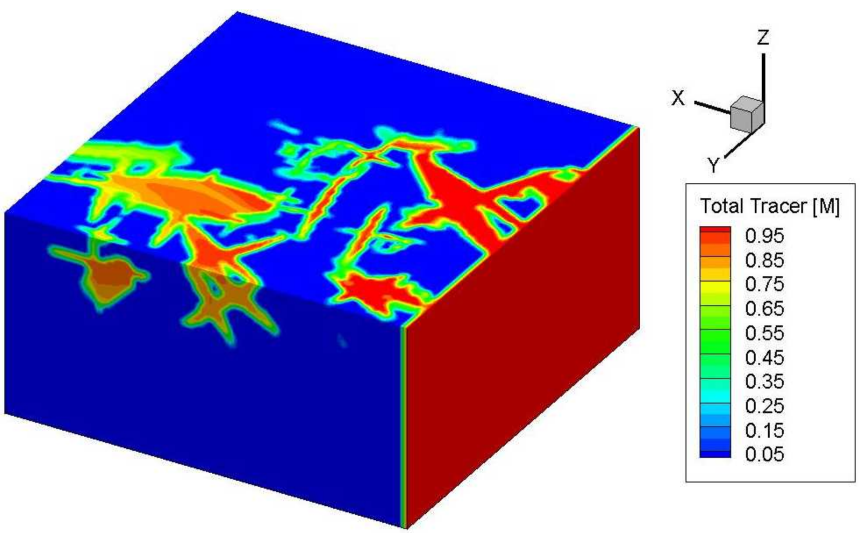


Tracer Breakthrough Curves: Effect of Matrix Diffusion

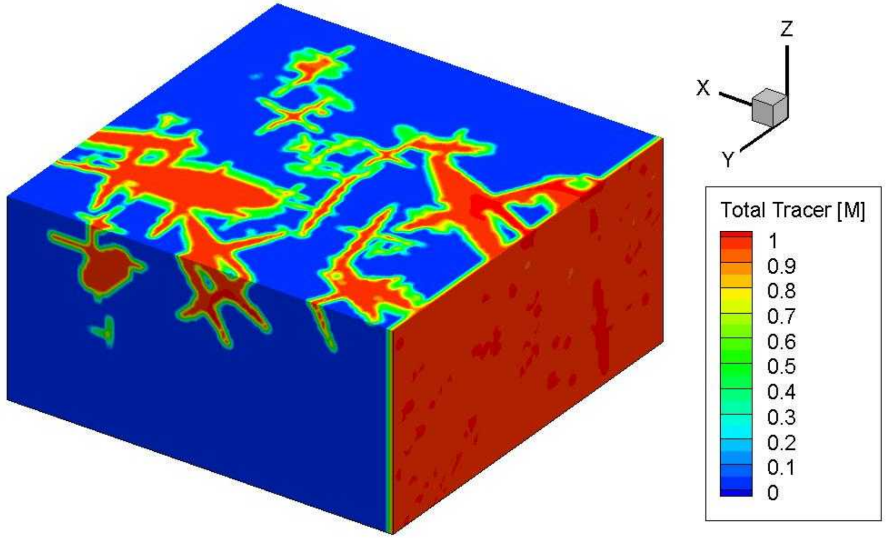


Tracer Distributions: No Matrix Diffusion

- Matrix Diffusion Excluded
- FCM Tracer Transport Results (after 1 x 10^3 and 1 x 10^5 years simulation time)



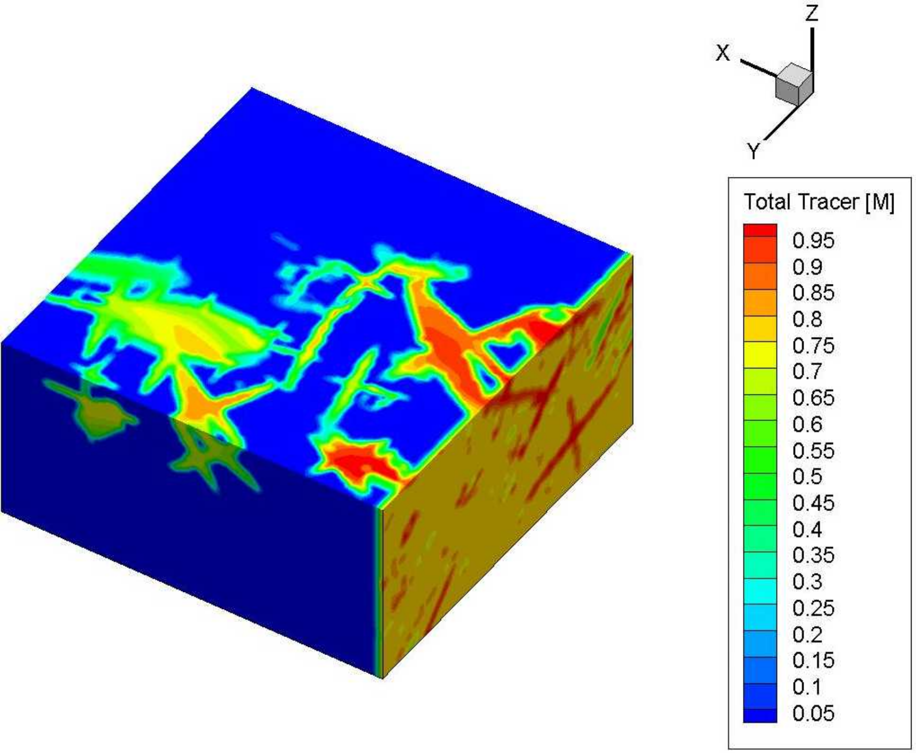
Tracer distributions after 10^3 years



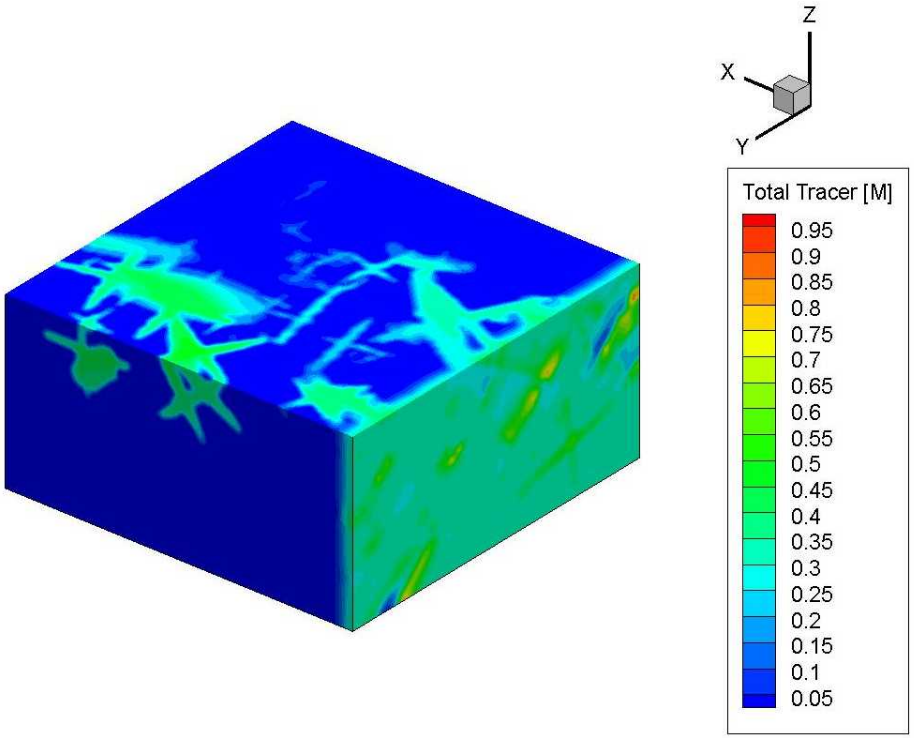
Tracer distributions after 10^5 years

Tracer Distributions: With Matrix Diffusion

- Matrix Diffusion included
- FCM Tracer Transport Results (after 1 x 10^3 and 1 x 10^5 years simulation time)



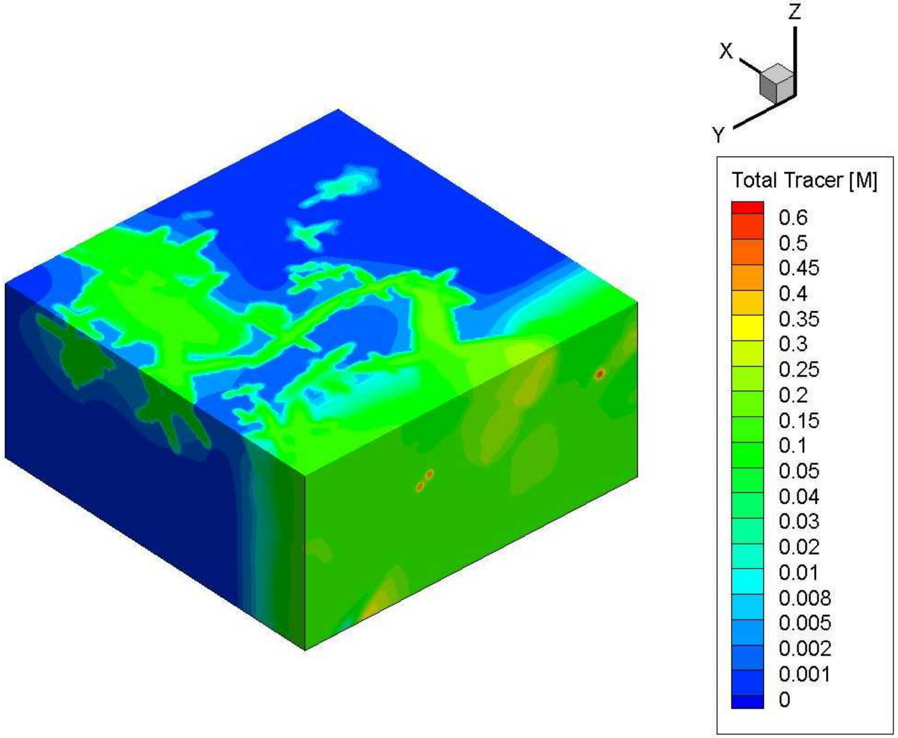
Tracer distributions after 10^3 years



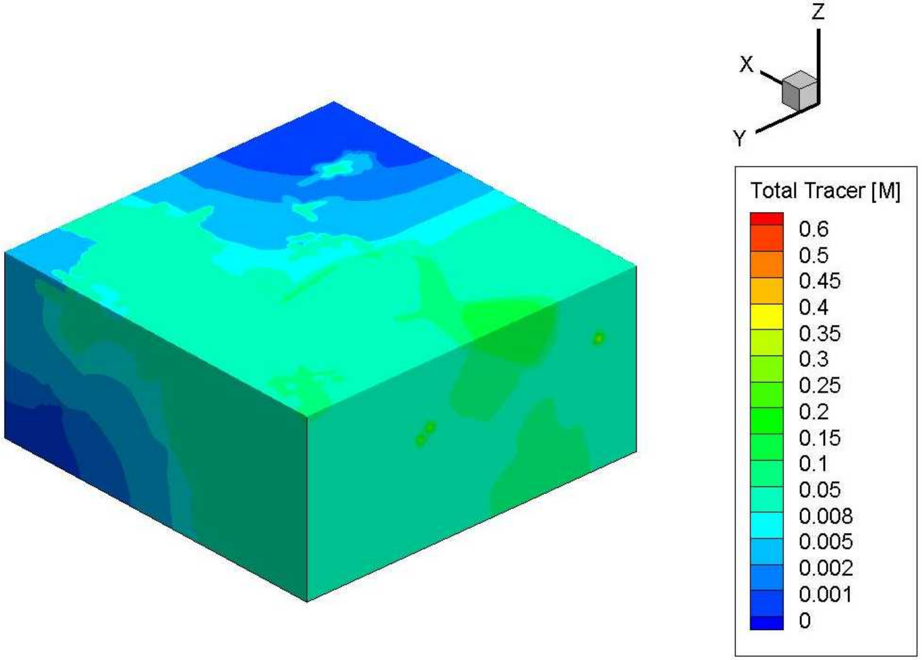
Tracer distributions after 10^4 years

Tracer Distributions: With Matrix Diffusion, Contd.

- Matrix Diffusion included
- FCM Tracer Transport Results (after 1 x 10^5 and 1 x 10^6 years simulation time)



Tracer distributions after 10^5 years



Tracer distributions after 10^6 years

Conclusions

- Flow and Transport simulations conducted using the FCM with applications to a generic nuclear waste repository in crystalline rock
- Advection in matrix rock excluded using low permeability
- Transport simulations conducted with and without matrix diffusion
- Inclusion of advection and diffusion through small fractures and matrix are important
- FCM can be applied to large domains with large number of fractures
- Further testing of FCM to be based on measured field data

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