Simulation of Radionuclide Transport in Fractured Porous Media

Seminar presentation

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Outline

Introduction
- Final disposal of HLW
- Deep geological disposal

Radionuclide Transport
- Solution transport in fractured porous media

Fractured porous media
- Numerical simulation
- Hybrid domain

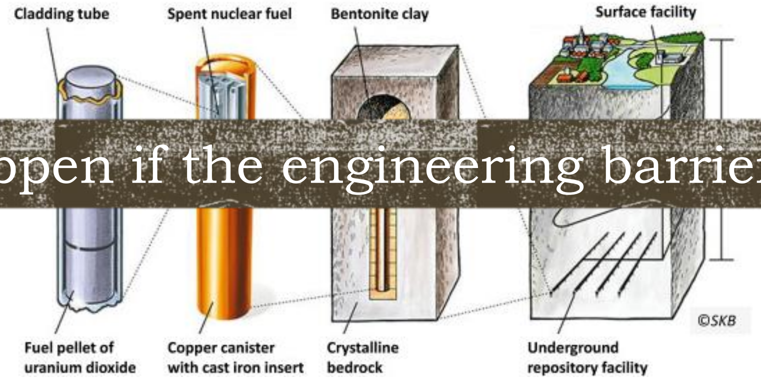
Conclusion

Introduction

- Final disposal of high-level radioactive waste (HLW)
- Deep geological disposal
  - Deposit in stable geological formations
  - Isolate waste from the scope of human activities (and biosphere)
  - Over time, the radionuclides decay to a level that does not affect human beings (Apted and Ahn, 2017).
- KBS-3 disposal concept (Swedish Nuclear Fuel Supply Company, 1983)
  - multi-barrier system = engineering barrier + natural barrier

Natural barrier system:
Host rock
(e,g., crystalline rock, clay)

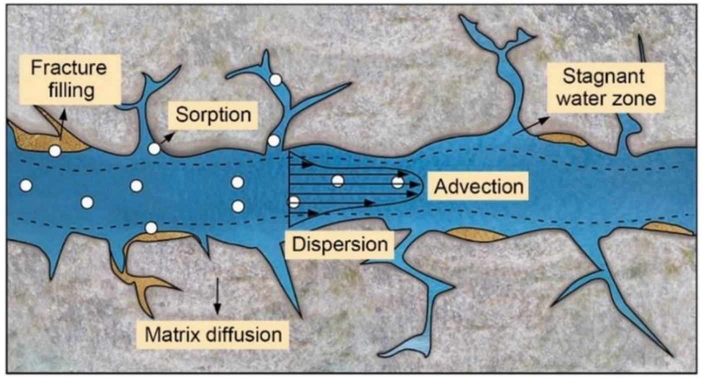
Engineering barrie
Canister
Buffer
Backfill



(SKB, 2006)

What will happen if the engineering barrier system fail?

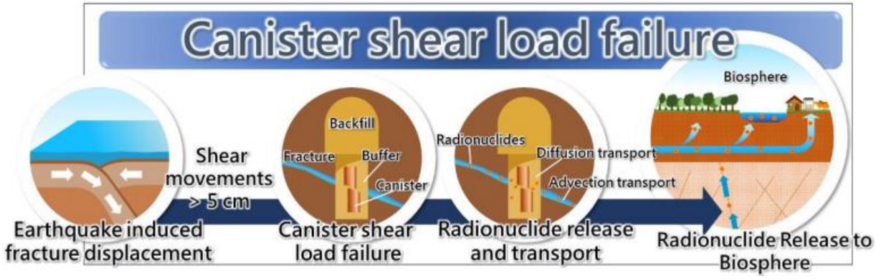
Radionuclide Transport



(Zhang et al., 2022)

- Radionuclide transport is one kind of solution transport. (with chemical reaction)
- **Fractures** provide major conduits (or barriers) for fluid flows in many types of media. (Berre et al., 2019)
- In solid rock (e.g., crystalline rock), the hydraulic properties of the fracture and surrounding porous medium (matrix) may be huge difference, which made the simulations challenging.
- **Fractured porous media** (fracture–matrix system)

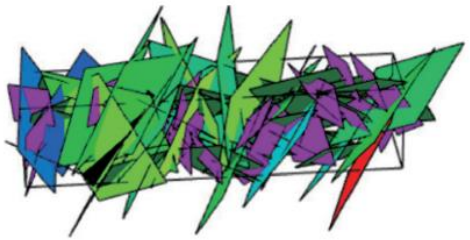
The radionuclide might migrate into host rock through groundwater.



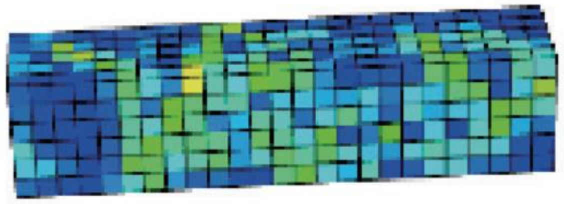
(Taiwan Power Company, 2023)

Fractured porous media (fracture–matrix system)

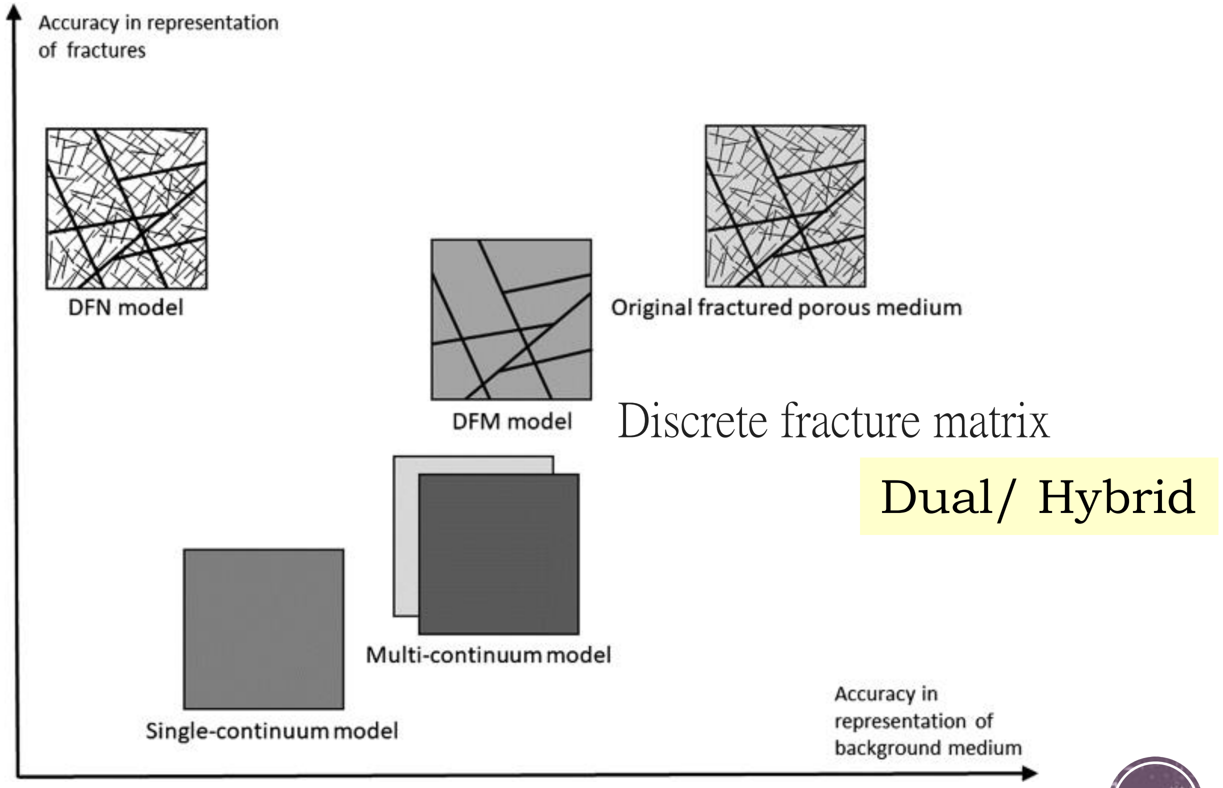
- Conceptual models for characterizing **fracture** systems in numerical model
  - Discrete fracture network (DFN) (only fracture)
  - Equivalent continuum porous medium (ECPM)
  - Dual domain /Hybrid domain



discrete



continuum



(Wu et al., 2017)

(Berre et al., 2019)

Numerical simulation

- Verification benchmarks for single-phase flow in 3D fractured porous media (Berre et al., 2021)

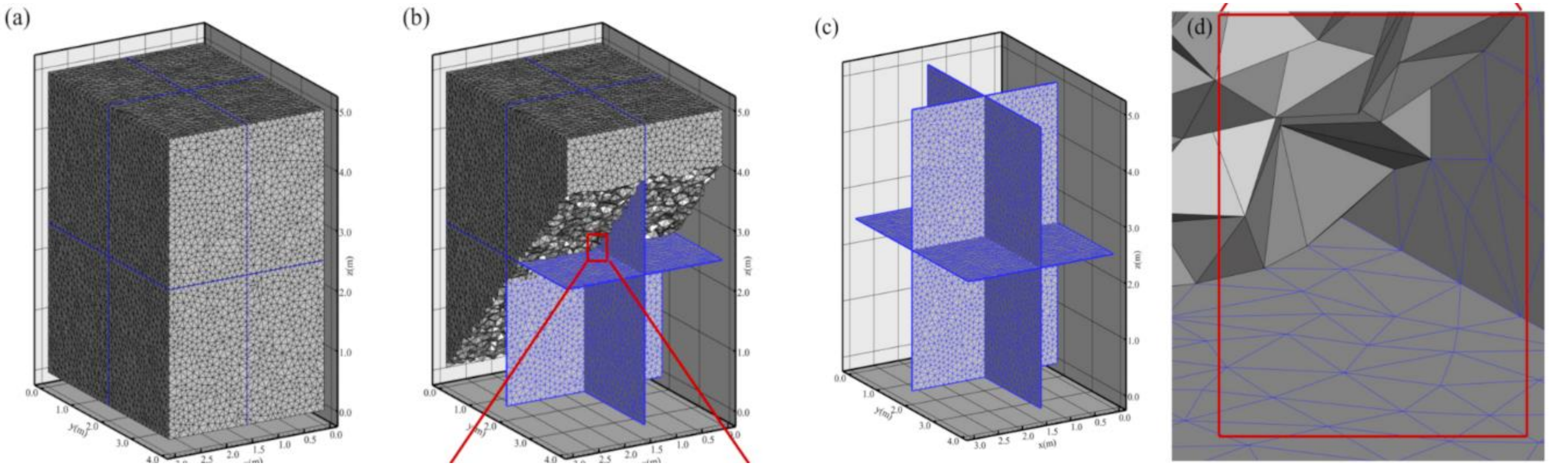
	Name/Acronym	Method
1	UiB-TPFA	Two-point flux approximation
2	UiB-MPFA	Multi-point flux approximation
3	UiB-MVEM	Lowest order mixed virtual element method
4	UiB-RT0	Lowest order Raviart-Thomas mixed finite elements
5	USTUTT-MPFA	Multi-point flux approximation
6	USTUTT-TPFA_Circ Koch	Two-point flux approximation
7	LANL-MFD	Mimetic Finite Differences
8	NCU_TW-Hybrid_FEM	Hybrid finite element method
9	UNICE_UNIGE-VAG_Cont	Vertex Approximate Gradient continuous hydraulic head
10	UNICE_UNIGE-HFV_Cont	Hybrid Finite Volumes continuous hydraulic head
11	UNICE_UNIGE-VAG_Disc	Vertex Approximate Gradient discontinuous hydraulic head
12	UNICE_UNIGE-HFV_Disc	Hybrid Finite Volumes discontinuous hydraulic head
13	ETHZ_USI-FEM_LM	Lagrange multiplier - L2-projection finite elements
14	UNICAMP-Hybrid_Hdiv	Hybrid H(div)
15	UNIL_USI-FE_AMR_AFC	Flux-corrected finite element method and adaptive mesh refinement
16	INM-EDFM	Embedded discrete fracture method
17	DTU-FEM_COMSOL	First-order Lagrangian finite elements (COMSOL)

(Modify from Table 1 in the paper)

Numerical simulation

- A hybrid approach for simulating three-dimensional flow and advective transport in fractured rocks (Lee et al., 2019, Yu et al., 2021)
- The hybrid domain (HD) model uses 2D triangular mesh for fractures and 3D tetrahedron mesh for the rock matrix, and allows the system of equations to be solved at the same time.

The 2D meshes share the nodes and faces of 3D meshes



(Yu e al., 2021)

Hybrid domain

Numerical simulation

(Yu e al., 2021)

incompressible fluid

Flow equation

$$u + K\nabla h = 0, \qquad in\ \Lambda$$
$$\nabla \cdot u = q, \qquad in\ \Lambda$$

boundary conditions on the boundaries $\partial\Lambda$

$$h\Big|_{\partial\Lambda_h} = \bar{h}, \qquad on\ \partial\Lambda_h$$
$$u \cdot n\Big|_{\partial\Lambda_h} = \bar{u}, \qquad on\ \partial\Lambda_u$$

u = Darcy velocity (m/s)
K = hydraulic conductivity (m/s),
h = hydraulic head (m),
q = source/sink term (1/s),
Λ = is the equidimensional model domain (m^3).

$\bar{h}$ = the hydraulic head on the boundary $\partial\Lambda_h$ (m)
$\bar{u}$ = the Darcy velocity perpendicular to the boundary surface $\partial\Lambda_u$ (m/s) concerning the outer unit normal vector n (-).

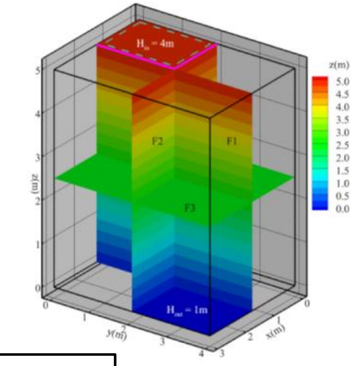
the flow parallel to the fracture

Assumption for fracture: (1) fracture aperture is uniform and << fracture size
(2) hydraulic conductivity of fracture >> matrix

$$\frac{1}{\varepsilon_2} u_2 + K_2^{eq} \nabla_2 h_2 = 0, \qquad in\ \Omega_2$$
$$\nabla_2 \cdot u_2 - \sum \left(u_3 \cdot n\Big|_{\Gamma_2} \right) = q_2, \qquad in\ \Omega_2$$

u_2= Darcy velocity (m/s),
K_2^{eq}= effective hydraulic conductivity perpendicular to the fracture plate (m/s),
h_2 = pressure head (m),
∇_2 =the gradient in the tangent direction (-),
q_2= the source/sink term (1/s).

cases(1)



Numerical simulation

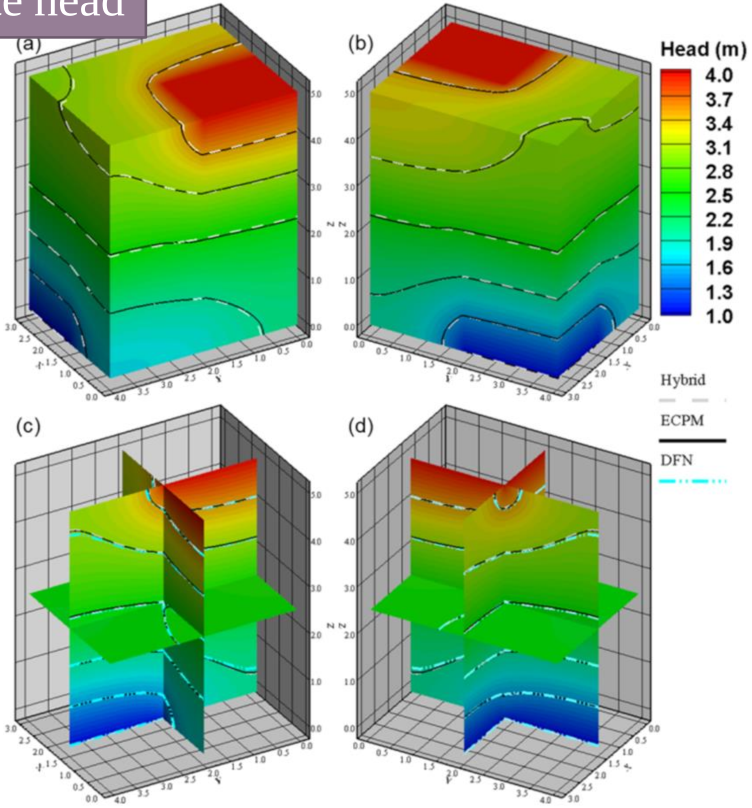
(Yu e al., 2021)

Comparison between HD, DFN method (FracMan) and ECPM method (DarcyTools)

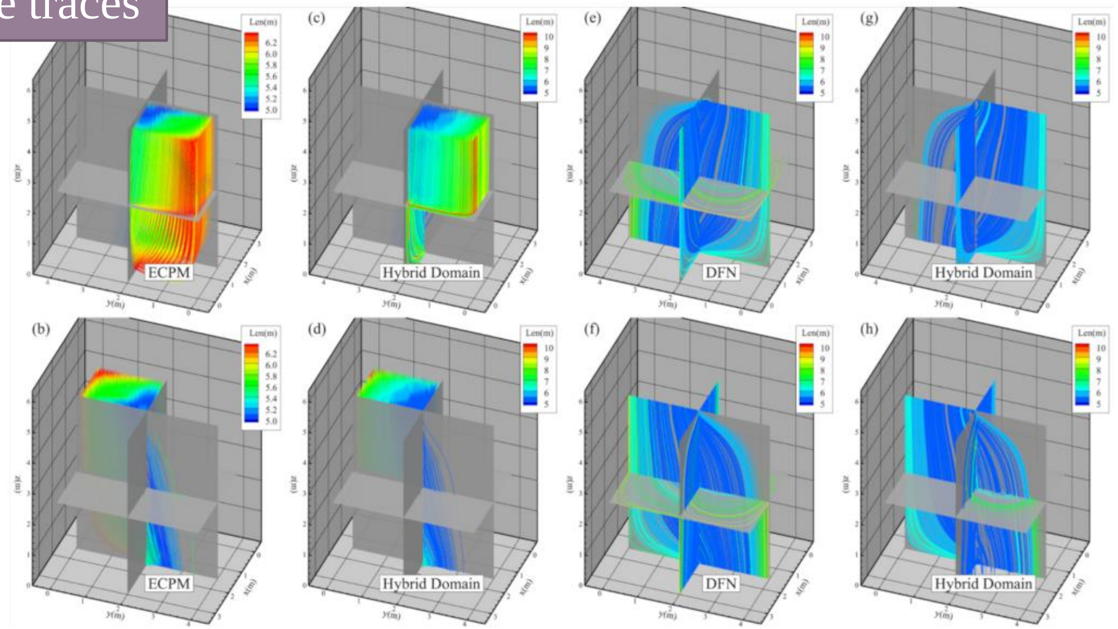
steady-state head

HD and ECPM

HD and DFN



particle traces



the mean trace length: ECPM < HD , HD < DFN
the mean trace time: ECPM > HD , HD > DFN
the mean velocity: ECPM < HD, HD < DFN

Conclusion

- In the issue of radionuclide transport in solid host rock, we need to consider solute transport and chemical reactions in fractured porous media.
- In the issue of solute transport in fractured porous media, the interaction between fractures and matrix needs to be considered.
- One way of hybrid domain (HD) model is introduced, which use 2D triangular mesh for fractures and 3D tetrahedron mesh for the rock matrix, and allows the system of equations to be solved at the same time.
- According to the simulation results, the HD model is flexible in considering the concepts of DFN, ECPM, or both. And the HD model is feasibility to do the simulations of flow and advective transport in complex fractured porous media.

Reference

- Apted, M. J., & Ahn, J. (Eds.). (2017). *Geological repository systems for safe disposal of spent nuclear fuels and radioactive waste*. Woodhead Publishing.
- Swedish Nuclear Fuel Supply Company/Division KBS. “Final storage of spent nuclear fuel – KBS-3 repository, Sweden”, 1983.
- SKB, “Long-term Safety for KBS-3 Repositories at Forsmark and Laxemar – a First Evaluation, Main Report of the SR-Can Project”, Swedish Waste Management Company, Sweden (2006) Report: TR-06-09
- Zhang, X., Ma, F., Dai, Z., Wang, J., Chen, L., Ling, H., & Soltanian, M. R. (2022). Radionuclide transport in multi-scale fractured rocks: A review. *Journal of hazardous materials*, *424*, 127550.
- Taiwan Power Company, "Spent Nuclear Fuel Final Disposal Program--Preliminary Development of Pre-Siting Safety Case", TPC-SNFD2021-V1
- Berre, I., Doster, F., & Keilegavlen, E. (2019). Flow in fractured porous media: A review of conceptual models and discretization approaches. *Transport in Porous Media*, *130*(1), 215-236.
- 吳宛庭, 倪春發, 李奕賢. (2017). 三維裂隙網路升尺度方法推估等效參數之差異評估. *農業工程學報*, *63*(1), 35-41.
- Berre, Inga, et al. "Verification benchmarks for single-phase flow in three-dimensional fractured porous media." *Advances in Water Resources* 147 (2021): 103759.
- Lee, I. H., Ni, C. F., Lin, F. P., Lin, C. P., & Ke, C. C. (2019). Stochastic modeling of flow and conservative transport in three-dimensional discrete fracture networks. *Hydrology and Earth System Sciences*, *23*(1), 19-34.
- Yu, Y. C., Lee, I. H., Ni, C. F., Shen, Y. H., Tong, C. Z., Wu, Y. C., & Lo, E. (2021). Numerical Assessment of the Hybrid Approach for Simulating Three-Dimensional Flow and Advective Transport in Fractured Rocks. *Applied Sciences*, *11*(22), 10792.

Thank you for your attention!

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