Simulation of Radionuclide Transport in Fractured Porous Media

Seminar presentation

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Outline

Introduction & Motivation

- Final disposal of HLW
- Fractured porous media

NCU_TW-Hybrid_FEM

Current Results

- Study subject
- Parameter

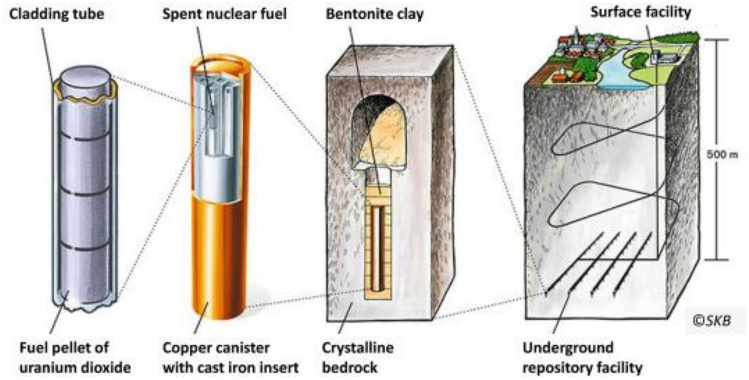
Conclusion & Future work

Introduction

- Final disposal of high-level radioactive waste (HLW)
- Deep geological repository (DGR)
  - Deposit the waste in deep and stable geological formations with multi-barrier system.
  - Isolate waste from the scope of human activities and biosphere.
  - The radionuclides decay over time.
- KBS-3 disposal concept (Swedish Nuclear Fuel Supply Company, 1983)
  - multi-barrier system = engineering barrier + natural barrier

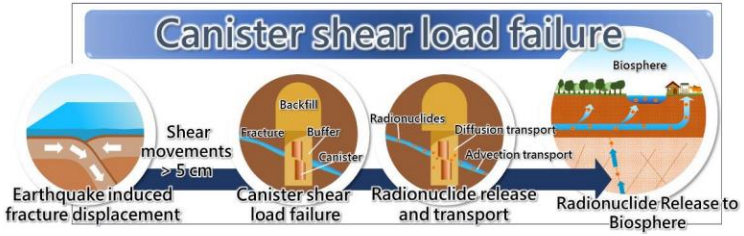
Natural barrier system:
Host rock
(e,g., granite, crystalline rock)

Engineering barrier system:
Canister
Buffer
Backfill



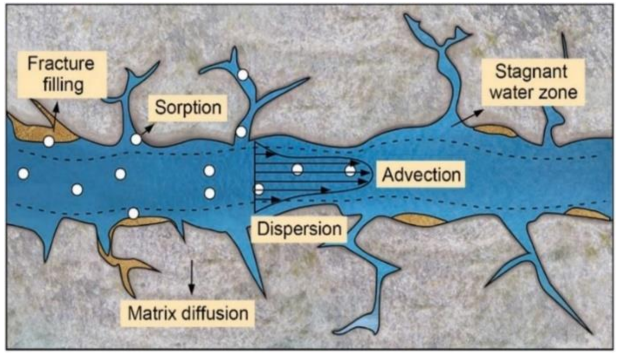
(SKB, 2006)

Radionuclide Transport



(Taiwan Power Company, 2023)

- If the engineering barrier system fail, the radionuclide might migrate into host rock through groundwater.
- Radionuclide transport is one kind of solution transport with chemical reaction, e.g. decay, sorption.
- **Fractures** provide major conduits (or barriers) for fluid. Solution might diffusion into **matrix (porous media)**.
- In solid rock (e.g., granite 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)



(Zhang et al., 2022)

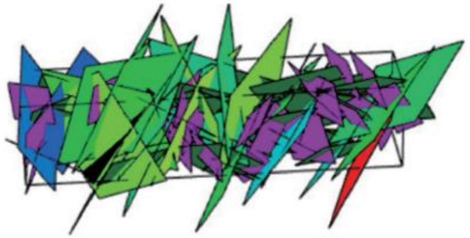
fracture

matrix

Fractured porous media (fracture–matrix system)

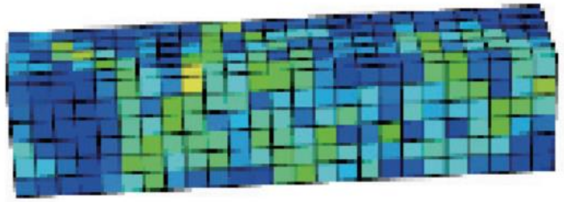
- Conceptual models for characterizing **fractured porous media** systems in numerical model
  - Discrete fracture network (DFN) (only fracture)
  - Equivalent continuum porous medium (ECPM)
  - Dual domain /Hybrid domain

DFN

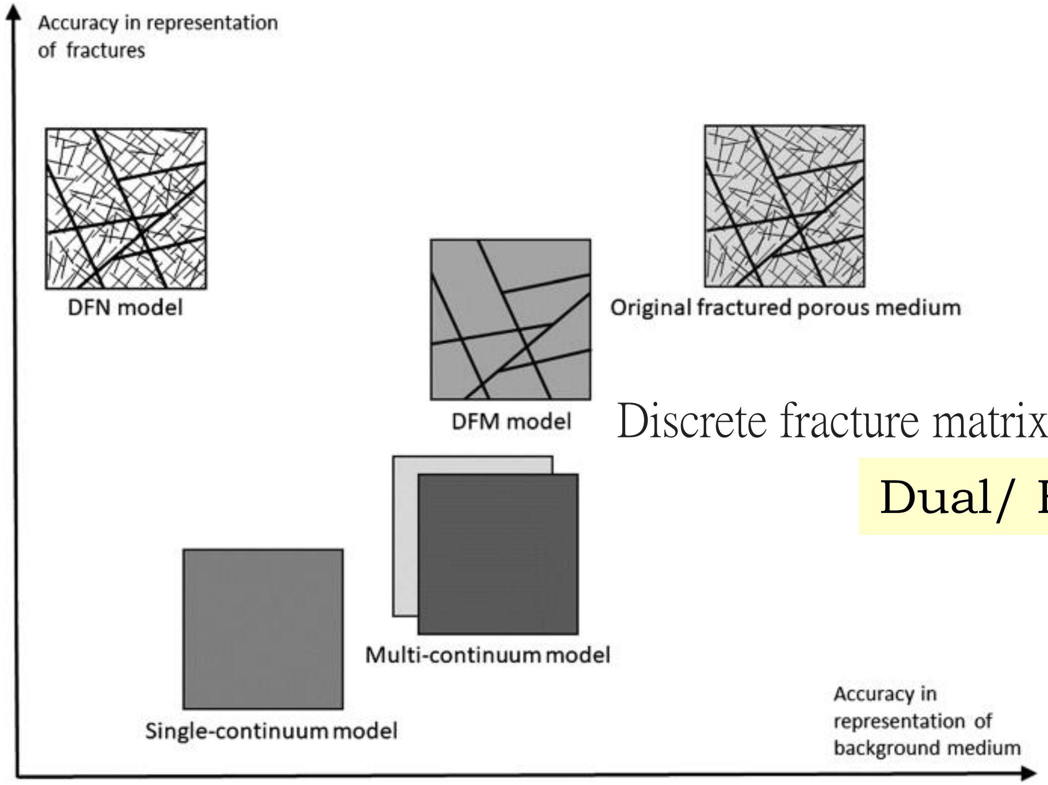


discrete

ECPM



continuum



Discrete fracture matrix

Dual/ Hybrid

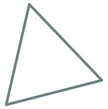
(Wu et al., 2017)

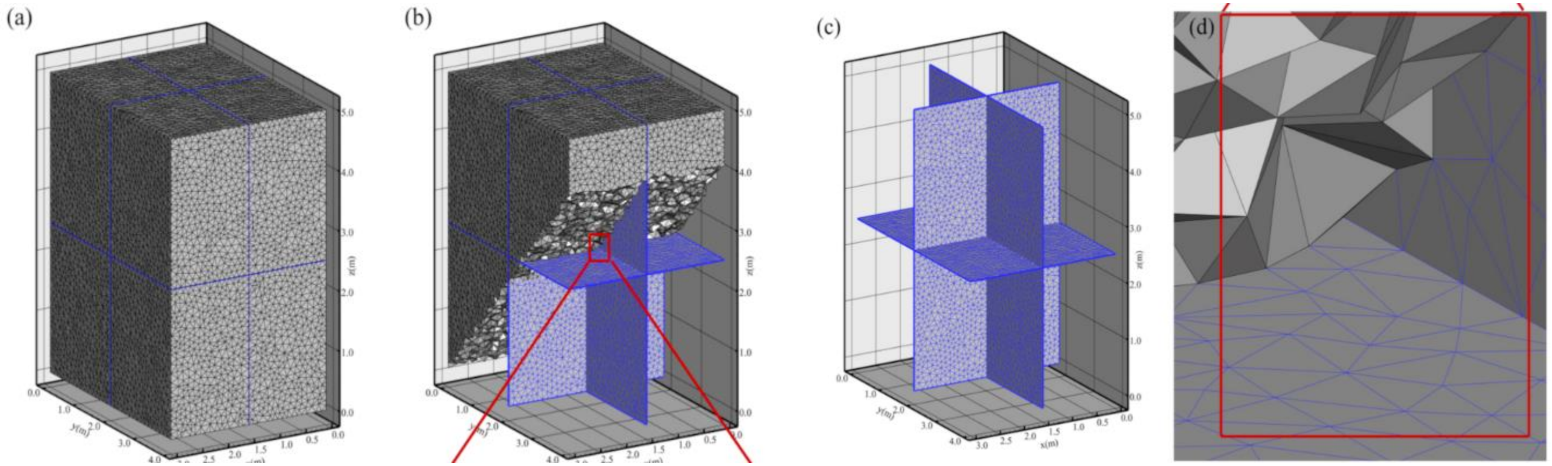
(Berre et al., 2019)

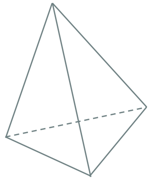
NCU_TW-Hybrid_FEM

- The hybrid domain (HD) model, NCU_TW-Hybrid_FEM, can simulate 3-D flow, advective transport, and diffusion in fractured porous rocks. (Lee et al., 2019, Yu et al., 2021)
- This HD model uses 2D triangular mesh for fractures and 3D tetrahedron mesh for the rock matrix, and allows the system solved equations at the same time.

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







(Yu e al., 2021)

Hybrid domain

Governing equations

(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).

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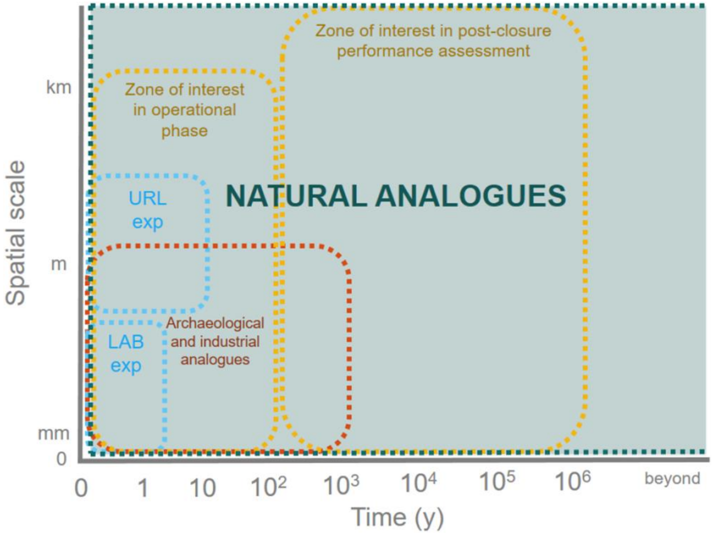
Current results

Natural Analogues



(Reijonen et al., 2023)

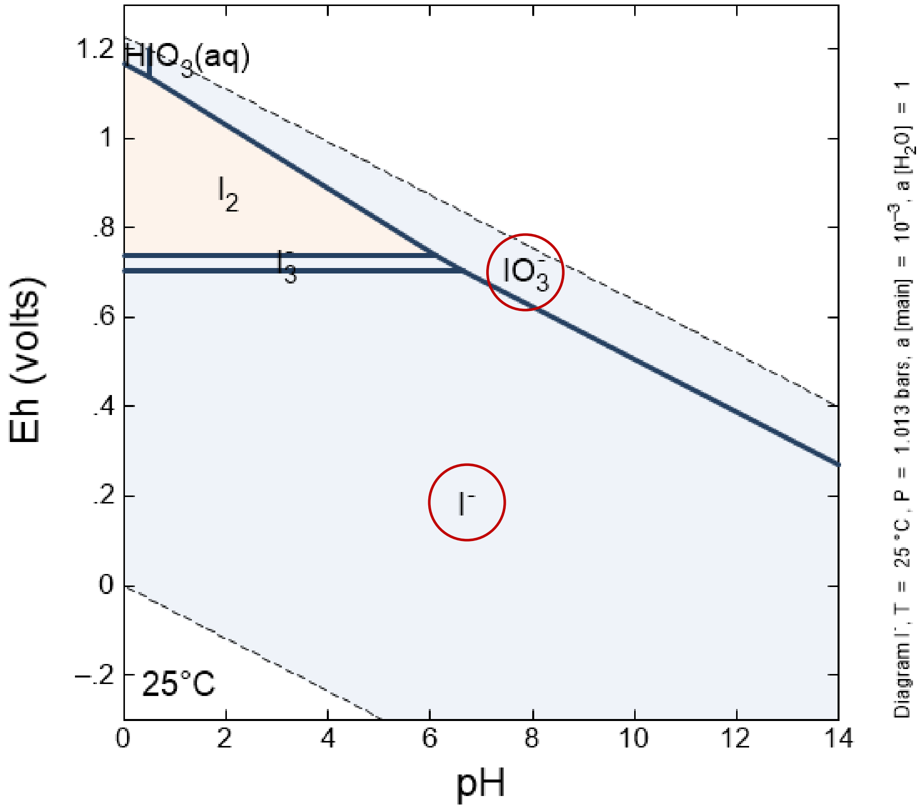
- “Natural Analogues” (NAs) refers to natural events or processes (usually geological and anthropogenic) similar to those in DGR systems, which helps people understand the long-term behavior of these systems, enhancing confidence in safety and performance assessments.
- NAs can provide data to calibrate models/simulation results used in safety and performance assessment.
- NAs can be used for public communication, since it’s easy to understand.

(Miller et al., 2006)

Near-field component	Fabrication material	Analogue
Wasteform	Spent fuel	Cigar Lake uranium orebody
Canister	Copper	Bronze Kronan cannon
Buffer	Compressed bentonite	Dunarobba fossil forest
Near-field rock	Granite	Osamu Utsumi mine

Geochemistry for Iodine

- Iodine exists in both reduced (I^-) and oxidized (IO_3^-) forms, and can also complex with organics and adsorb to soils and ferric oxides.
- Organic matter is the main factor responsible for iodine fixation in soils, leading to higher concentrations in reducing environments and topsoil layers.
- In groundwater, iodide (I^-) is dominant and does not easily sorb onto minerals due to their negative surface charge.



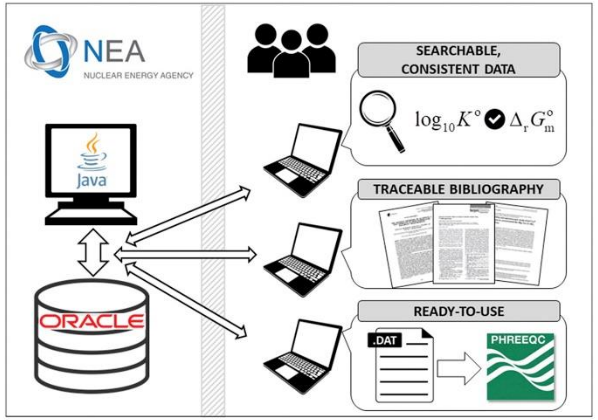
Chemical Reaction Parameters

- For the chemical reaction parameters of iodine, we refer to NEA-TDB.
- The Nuclear Energy Agency (NEA) Thermochemical Database Project (TDB) represents a reference point with regard to high standard thermochemical data for the radioactive waste management community. (Martinez et al., 2019)

```
SOLUTION_SPECIES
+ 6.0 H+ - 3.0 H2O + 1.0 IO3- + 6.0 e- = 1 I-
     log_k      111.563 #+/-
     #delta_h   No data+/-No data
     analytical_expression    1.115630E+02 0 0 0 0
     # delfG0m = -51.724 +/- 0.112(kJ/mol)
     # delfH0m = -56.780 +/- 0.050(kJ/mol)
     # S0m = 106.450 +/- 0.300(J/K/mol)
     # Cp0,m = No data
     # Phreeqc-conformed reaction

+ 1.0 H+ + 1.0 IO3-  = 1 HIO3
     log_k      0.788 #+/-0.029
     #delta_h   No data #+/-No data
     analytical_expression    7.880000E-01 0 0 0 0
     # delfG0m = -130.836 +/- 0.797(kJ/mol)
     # delfH0m = No data
     # S0m = No data
     # Cp0,m = No data
     # [2020GRE/GAO]
```

```
SOLUTION_MASTER_SPECIES
#element        species        alk          gfw_formula    element_gfw
I               IO3-            0           I              126.9045
I(+5)           IO3-            0           IO3
I(-1)           I-              0           I
```



https://www.oecd-nea.org/jcms/pl_22166/thermochemical-database-tdb-project

(Martinez et al., 2019)

Conclusion and Future Work

- In the issue of radionuclide transport in solid host rock, we need to consider solute transport and chemical reactions in fractured porous media.
- A hybrid domain (HD) model, NCU_TW-Hybrid_FEM, is introduced. The model use 2D triangular mesh for fractures and 3D tetrahedron mesh for the rock matrix, and allows the system solved equations at the same time.
- This study focuses on the transport of Iodine-129. Preliminary study has been conducted on geological structure, iodine's chemical properties and relevant simulation tools.
- Future work will involve literature review to identify key parameters, such as hydraulic conductivity, porosity, and diffusion rates, and to develop a conceptual model for Iodine-129 transport.

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Thank you for your attention!

Seminar presentation

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