Simulation and Uncertainty Analysis of Nuclide Transport Breakthrough in DFN

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Introduction

Geological barrier is the final line of defense against nuclide transport.

The fractures in the geological barrier form the primary pathway for nuclide transport. Groundwater flow in these fractures is the main driver of transporting nuclides to the biosphere.

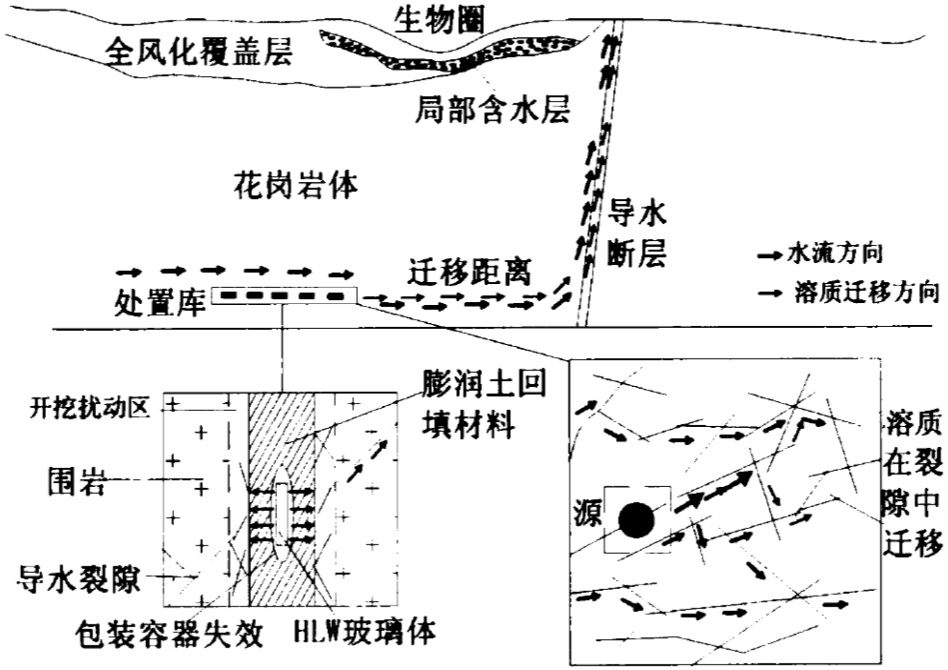


Fig.1. Schematic diagram of solute migration in deep geological disposal reservoirs for radioactive wastes(JNC,2000)

The Challenging - Solution

Difficulties in modeling

Strong inhomogeneity and anisotropy in fractured rocks.

Solution

Discrete fracture networks (DFN)

Define all the geometric parameters of the fracture, each of which determines a distributional species and a statistical characterization. Construct statistically significant stochastic models.

Assessment of uncertainty

DFN describes fracture characterization in detail, which introduces additional uncertainty and result in an underestimation of the uncertainty in the results.

Solution

The Sobol variance-decomposition method

Quantify the contribution of the fracture parameters to the uncertainty in the results of flow and transport distance.

DFN Modeling

The mathematical description of the fracture geometry is the key to modeling.

Assuming that the fracture is a disc model, it can be represented by six parameters: α-dip, β-dip angle, r-radius, and x, y, z-three-dimensional coordinates of the center of the disc of the fracture. The Poisson model was used to define the spatial distribution of fractures locations.

Table1. Fracture geometry parameter distribution law table

Geometric Parameter	Radius	Aperture	Cohesion	Friction Angle	Dip	Dip Angle
Distributed Type	Normal Distribution	Exponential Normal Distribution	Average Distribution	Normal Distribution	Fisher	Fisher

These parameters characterize the geometry of the fracture in three-dimensional space, with each parameter determining a type of distribution and a statistical property, thus establishing a stochastic model of the discrete fracture network.

Simulation of Flow

Construct a planar fracture network model to simulate fluid flow in a fracture network

A single fracture can be regarded as a thin aquifer, which is generally described by the cubic law. The cubic law for a single fracture means that the fracture is represented by two parallel plates with a constant distance between the parallel plates. Then the one-dimensional flow equation is:

$$Q = \frac{1}{f}\frac{b^3}{12\gamma}\Delta p$$

In a fracture network, the fluid flows in three dimensions, but for individual fractures, the fluid flows in a two-dimensional plane. The equations controlling the two-dimensional steady flow are:

$$\frac{\partial}{\partial \mathrm{x}}\left(\mathrm{T}\frac{\partial \mathrm{H}}{\partial \mathrm{x}}\right) + \frac{\partial}{\partial \mathrm{y}}\left(\mathrm{T}\frac{\partial \mathrm{H}}{\partial \mathrm{y}}\right) + Q = 0$$

Simulation of Flow

Mesh Dissection

The disk-shaped fracture can be approximated using regular polygons, which can then be dissected into triangular meshes.

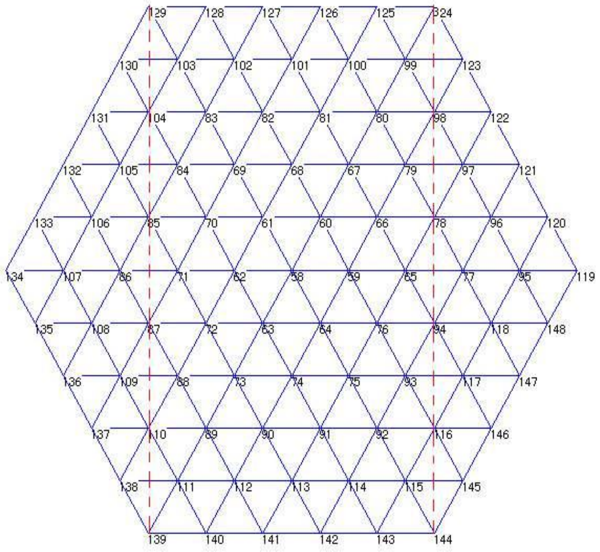


Fig.2. Schematic diagram of a single fracture section and node

Analytic Solution

The conservation equation at node i is:

$$\sum_e \left[T \frac{\overline{pb}}{\overline{ij}} \left(h_j - h_i\right) + T \frac{\overline{qb}}{\overline{ik}} \left(h_k - h_i\right) \right] + Q_i = 0$$

$$\frac{\overline{pb}}{\overline{ij}} = -\frac{1}{4A}\left(b_1 b_2 + c_1 c_2\right)$$

$$\frac{\overline{qb}}{\overline{ik}} = -\frac{1}{4A}\left(b_1 b_3 + c_1 c_3\right)$$

$$A = \frac{1}{2}\left(b_1 c_2 - c_1 b_2\right)$$

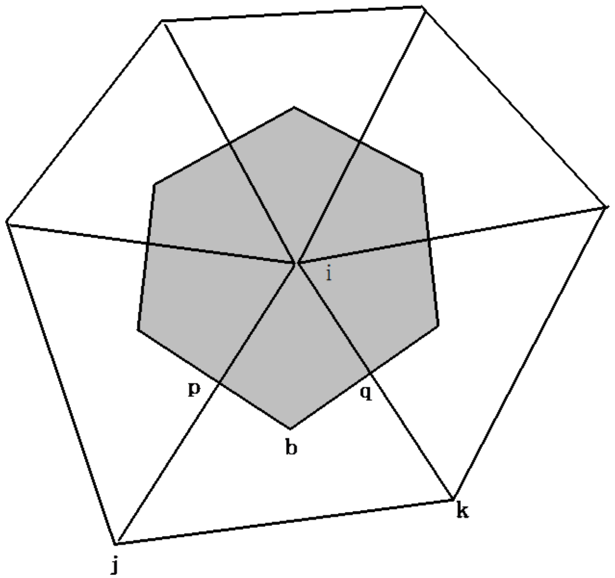


Fig.3. Schematic representation of node i conservation area

Nuclide Transport - Particle Tracking Algorithm

Suppose:

(1) Particle motion is driven by convection and dispersion;

(2) Chemical reactions and adsorption are not taken into account;

(3) Neglect diffusion in fluids and rock matrices.

The transport control equations are:

$$\frac{\partial}{\partial x}[(a_L V)\frac{\partial c}{\partial x}] - V\frac{\partial c}{\partial x} = \frac{\partial c}{\partial t}$$

$$c(\pm\infty, t) = 0$$

$$c(x,0) = \frac{M}{n}\delta(x)$$

$$V(x,t) = \text{ constant}$$

(A drop of tracer-labeled fluid is injected at x = 0.0 into a column of infinite porous media flowing steadily in the x-axis direction.)

Bear gives the solution:

$$c(x,t) = \frac{M/n}{\sqrt{4\pi a_L V t}}\exp[-\frac{(x - Vt)^2}{4a_L V t}]$$

Nuclide Transport - Particle Tracking Algorithm

The velocity of a mass has three components:

Convection (Vf) , Longitudinal dispersion (Vl) , Transverse dispersion (Vd)

$$V_x = Vf_x + Vl_x + Vd_x \qquad V_y = Vf_y + Vl_y + Vd_y \qquad V = \sqrt{V_x^2 + V_y^2}$$

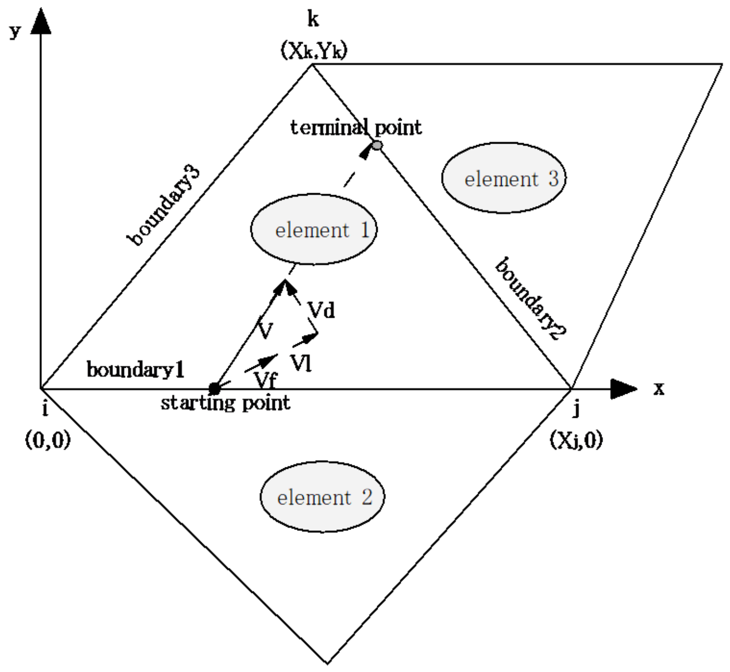


Fig.4. A particle and local coordinate system

$$Vl_x = Vl\cos\alpha$$

$$Vl_y = Vl\sin\alpha$$

$$Vl = Z_1\sqrt{2a_L Vf}$$

$$Vd_x = Vd\sin\alpha$$

$$Vd_y = Vd\cos\alpha$$

$$Vd = Z_2\sqrt{2a_T Vf}$$

$$Vf_x = K(h_i - h_j)/X_j$$

$$Vf_y = K[X_j(h_i - h_k) + X_k(h_j - h_i)]/X_k X_j$$

$$Vf = \sqrt{Vf_x^2 + Vf_y^2}$$

Nuclide Transport - Particle Tracking Algorithm

The particle tracking algorithm consists of the following main steps:

(1) Place a particle on the boundary of the element;

(2) Establish a local coordinate system and calculate the convective velocity;

(3) Generate two random numbers, calculate the longitudinal and transverse dispersion velocities;

(4) Calculate the compound velocity;

(5) The end point depends on the direction of V, determine the end point on the, and calculate the particle distance (L);

(6) Calculate the travel time as the particle passes through the element;

(7) Using the end point as a new starting point, perform the same loop of (2) through (6) until the particle reaches the boundary, or moves for more than a specific maximum time.

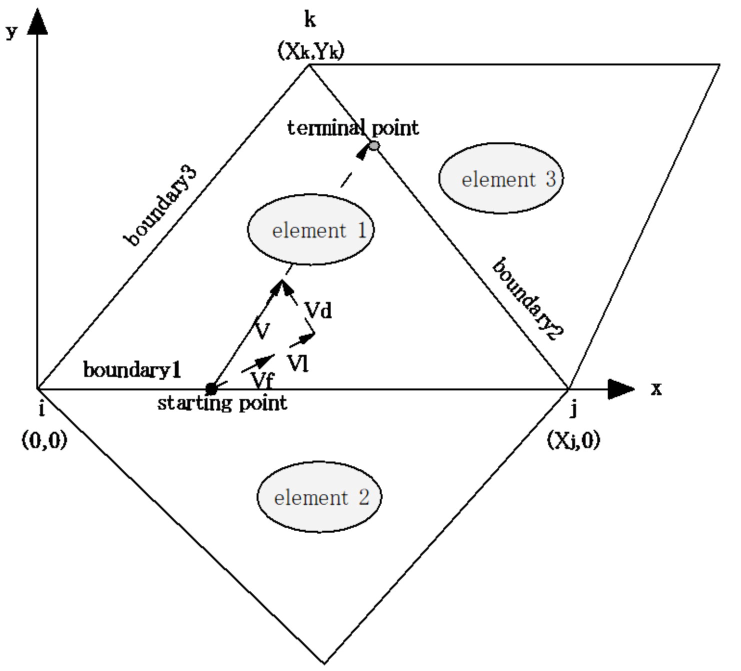
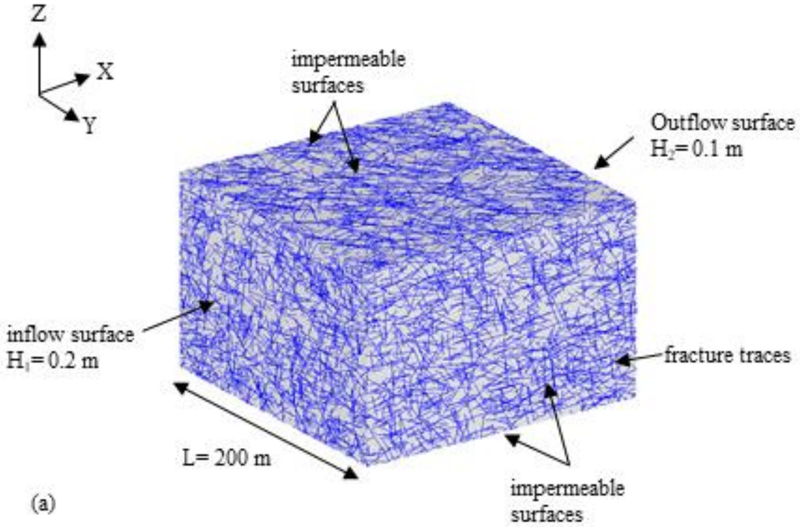


Fig.4. A particle and local coordinate system

Generate Äspö HRL Model

Table.1. Table of the fracture parameters of the Äspö HRL model in three groups

Parameter	Distribution type	First group fractures	Second group fractures	Third group fractures
Radius(m)	log-normal	mean=2;std=2	mean=8;std=2	mean=5;std=4
Dip(°)	\	218.8	126.9	17.9
Dip-angle(°)	\	83.7	86.8	7.5
Density(m^{-3})	\	0.029102	0.002563	0.008027
Aperture(cm)	log-normal	0.000769	0.000769	0.000769
Longitudinal dispersion(m^2/s)	log-normal	1	1	1
Transverse diffusion(m^2/s)	log-normal	0.1	0.1	0.1



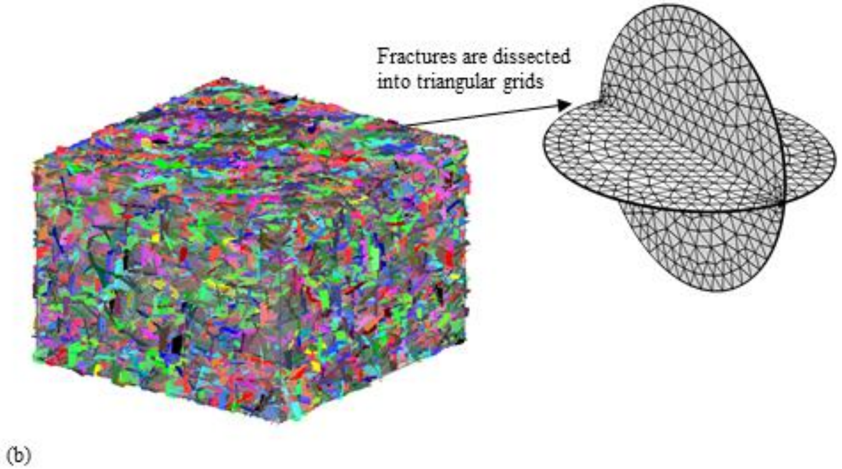


Fig.5. (a) the surface trace and boundary condition setup of the Äspö HRL 3D DFN model
(b) triangular meshes of the dissected fracture network.

Results of Äspö HRL Model

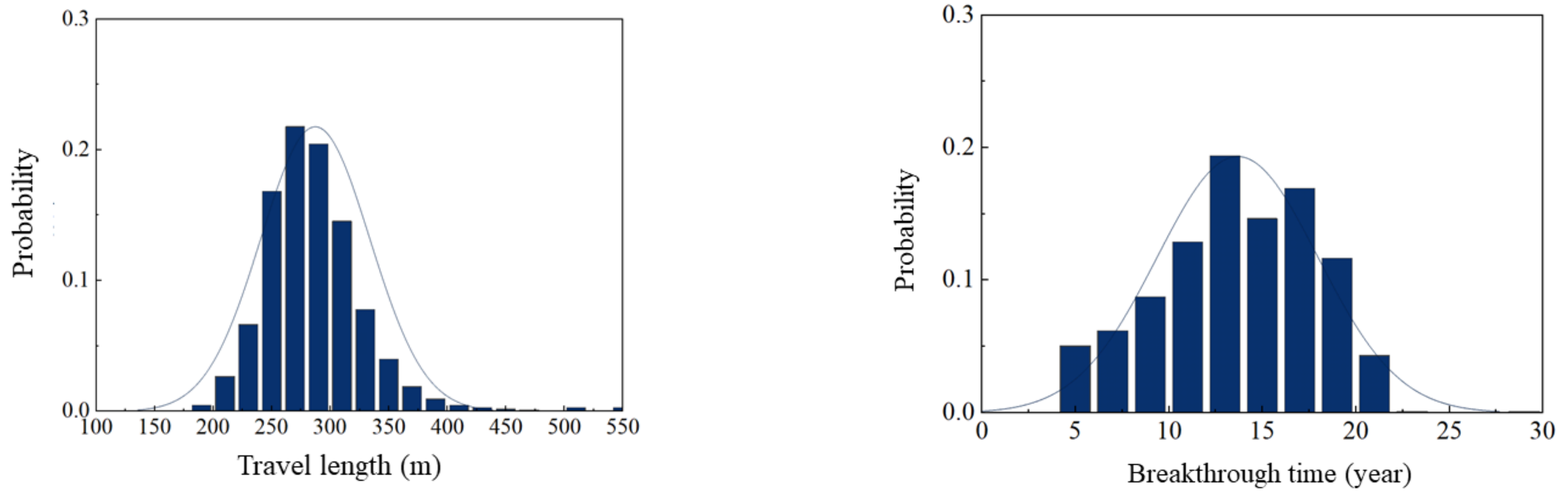


Fig.6. Probabilistic statistics of 3171 nuclide particles breakthrough time and travel length

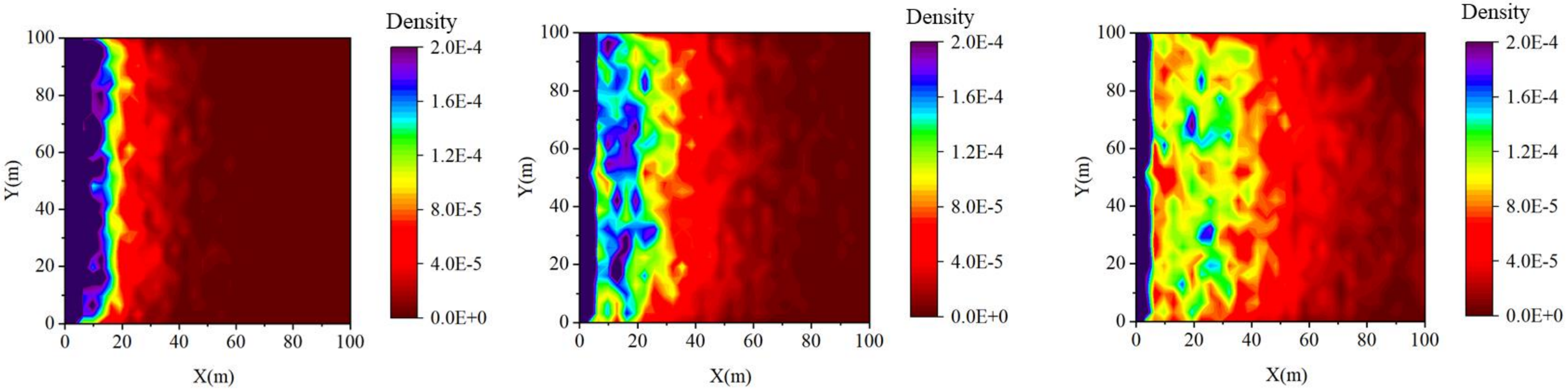


Fig.7. Density distribution of nuclides in the XY plane separately after 1, 7, and13 years of travel

Uncertainty Analysis

The DFN model has the advantage of characterizing the fracture in detail, but introduces additional uncertainty.

Quantify the degree of contribution of fracture parameters to the uncertainty in the flow and transport distance by the Sobol variance decomposition method.

First-order sensitivity indicator:

$$S_i = \frac{V[E(Y|X_i)]}{V(Y)}$$

Second-order sensitivity indicator:

$$\mathrm{V_{ij}} = \mathrm{V}\left(\mathrm{f_{ij}}(\mathrm{X_i}, \mathrm{X_j})\right) = \mathrm{V}\left(\mathrm{E}(\mathrm{Y}|\mathrm{X_i}|\mathrm{X_j})\right) - \mathrm{V}(\mathrm{E}(\mathrm{Y}|\mathrm{X_i})) - \mathrm{V}\left(\mathrm{E}(\mathrm{Y}|\mathrm{X_j})\right)$$

Total sensitivity indicator:

$$\mathrm{S_{Ti}} = \frac{\mathrm{V}[\mathrm{E}(\mathrm{Y}|\mathrm{X_{-i}})]}{\mathrm{V}(\mathrm{Y})}$$

Uncertainty Analysis

Construct stochastic parametric models:

Random parameters were generated by LHS (Latin Hypercube Sampling) sampling method based on the parameters of the most developed set of fractures in the Äspö HRL prototype repository.

Table 2. Range of fracture parameters for stochastic parametric models

Parameter	minimum	maximum	cov(%)
Radius(m)	2.13	10.57	38.01
Dip(°)	0.0006	0.002	24.41
Dip-angle(°)	0.0015	0.0353	60.39
Density(m^{-3})	1.05	3.92	34.35
Aperture(cm)	0.1	0.59	41.09
Longitudinal dispersion(m^2/s)	4.92	354.04	64.95
Transverse diffusion(m^2/s)	1.47	89.77	57.61

Uncertainty Analysis

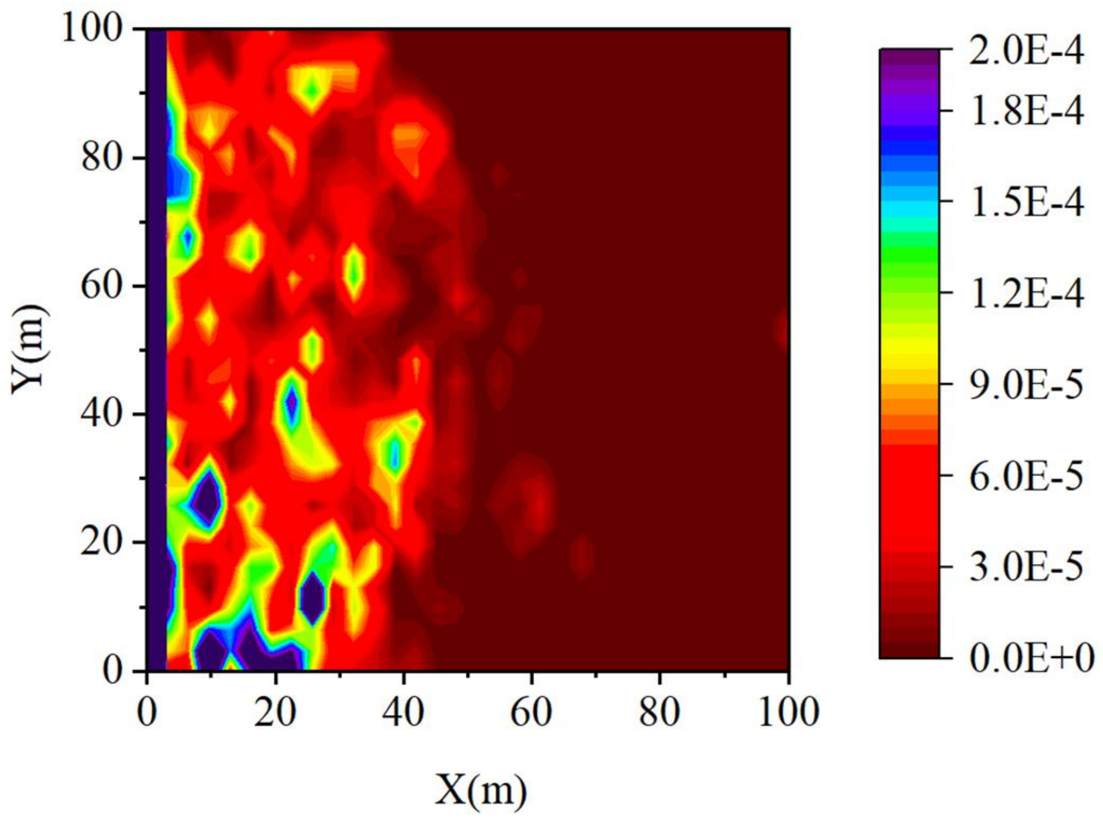


Fig.8. An example of stochastic parametric models with dominant flow phenomena

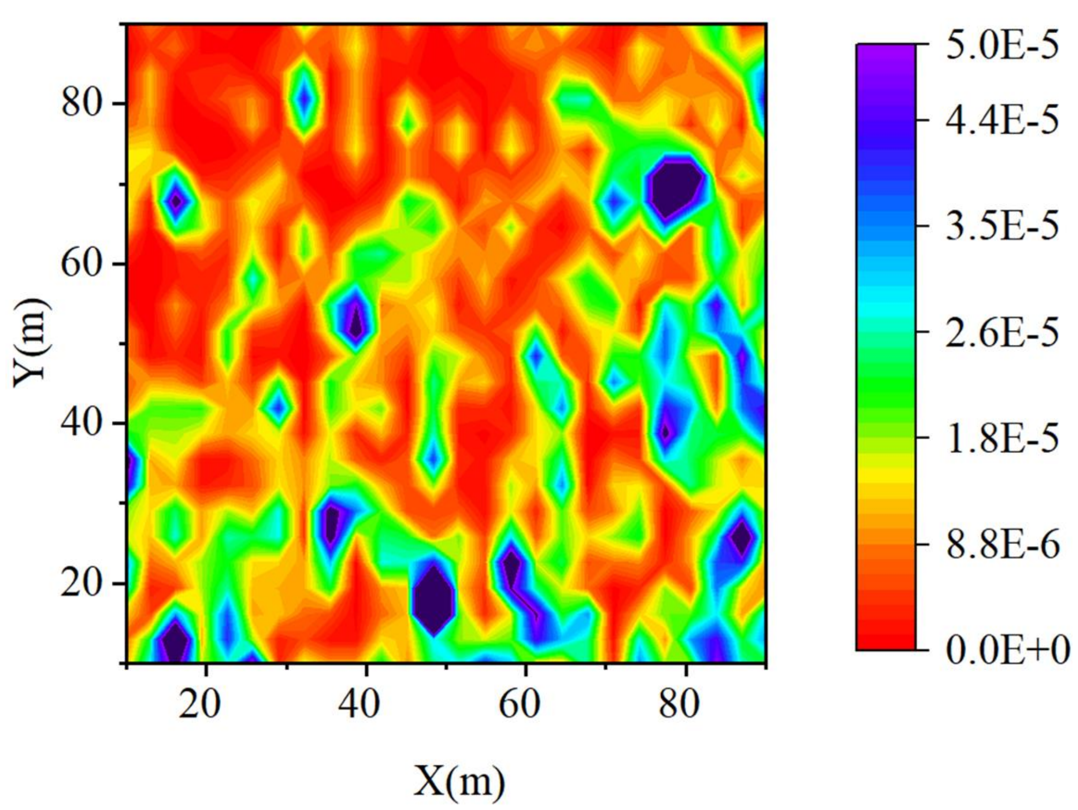


Fig.9. An examples of stochastic parametric models with stagnant water zone phenomena

Uncertainty Analysis

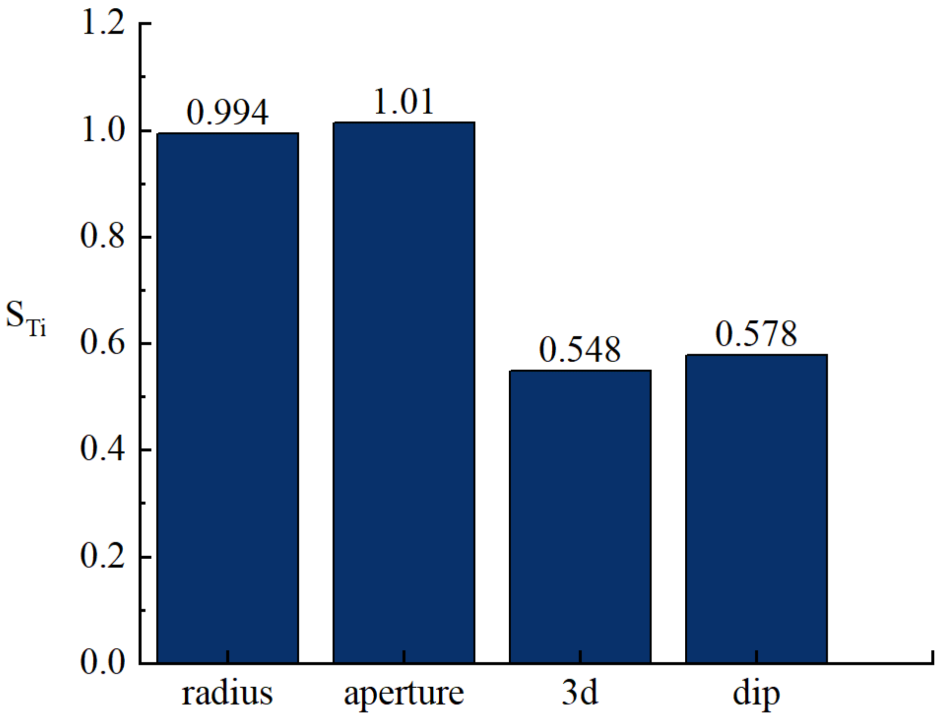


Fig.10. Total sensitivity index of parameters to flow

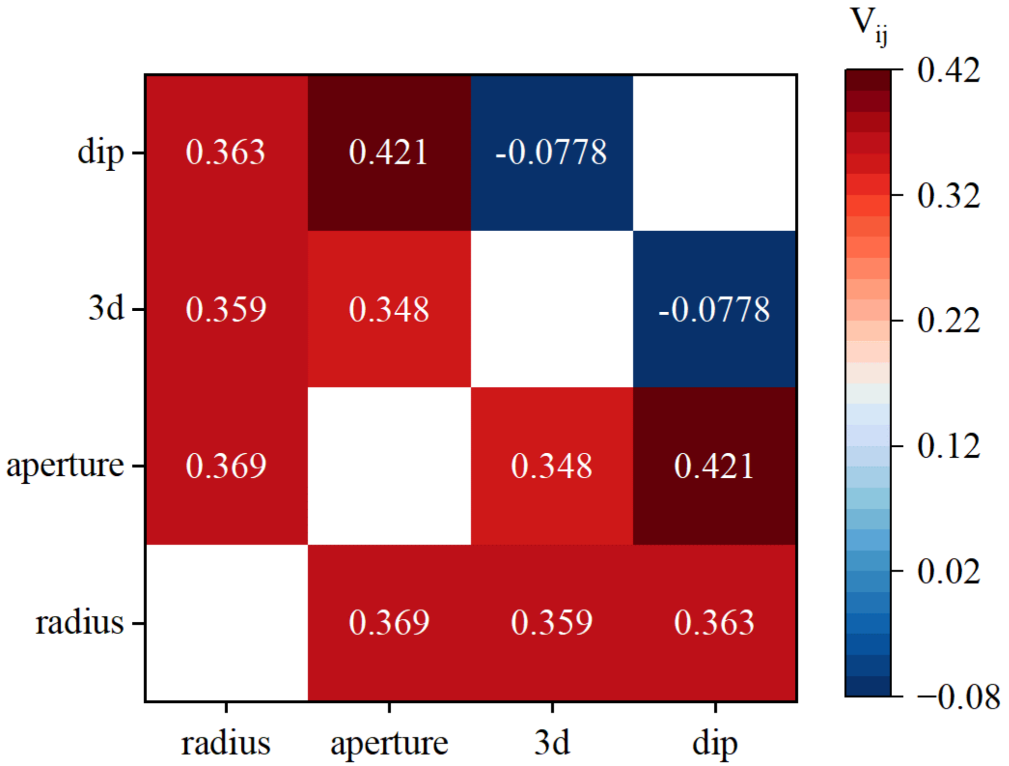


Fig.11. Second-order sensitivity index of parameters to flow

Uncertainty Analysis

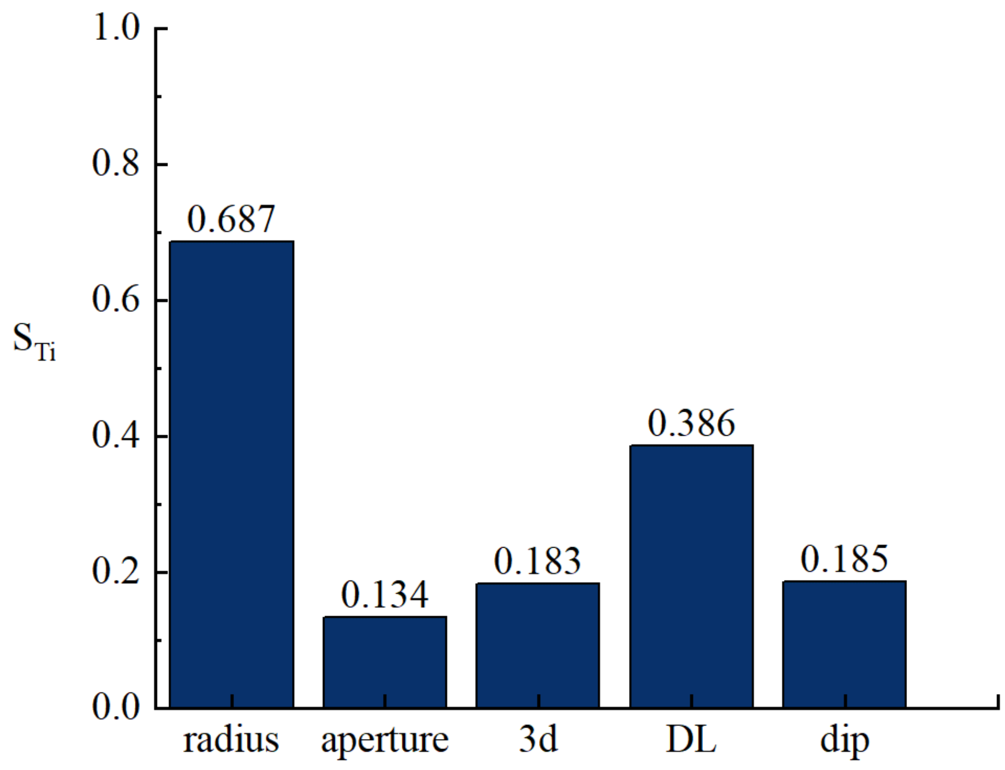


Fig.12. Total sensitivity index of parameters to distance

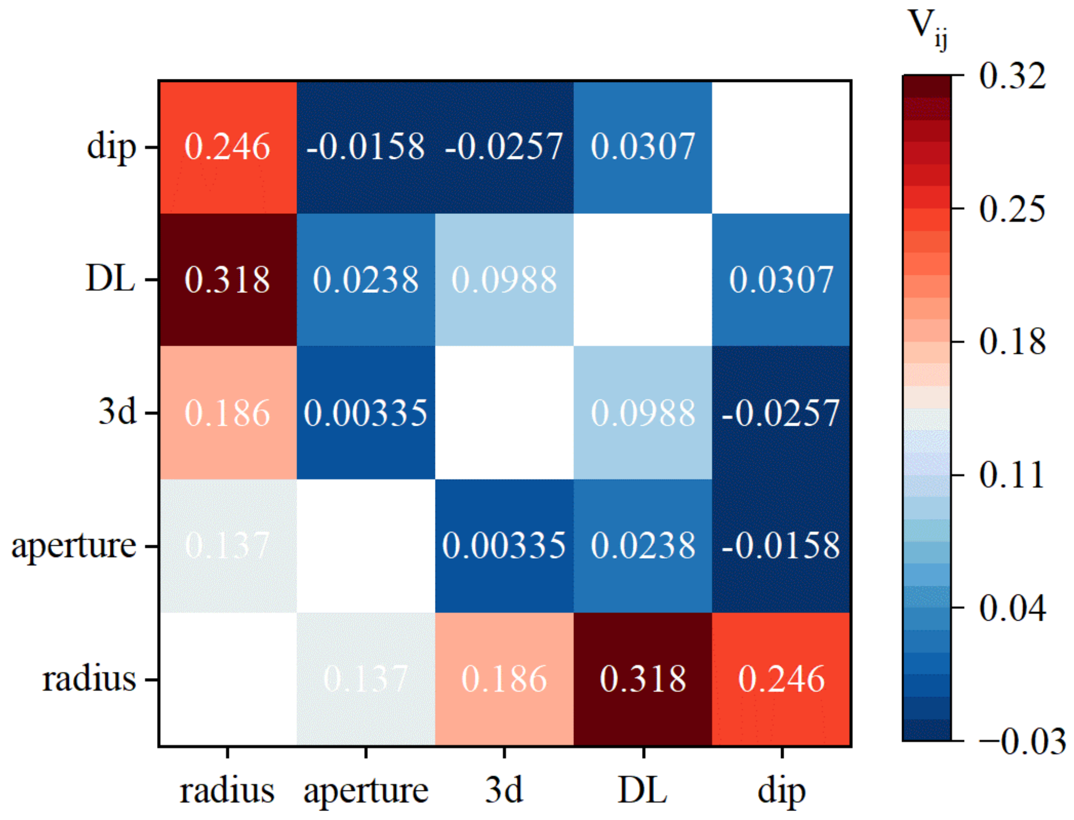


Fig.13. Second-order sensitivity index of parameters to distance

Conclusion

1. In Äspö HRL, the first breakthrough time is 4.19 years, and the shortest transport distance is 187.392 m.
2. In the early stage of transport, the nuclides penetrate into the rock in an explosive way, with the hydraulic gradient as the main driving force. In later stages of transport, the influence of dispersion on nuclide transport increases, resulting in a strong inhomogeneous anisotropy in nuclide distribution and the phenomenon of stagnation and dominant flow.
3. In low density rocks, the flow channels are determined by the X-intersection density and the T-intersection density. Dense X and T fractures can cause nuclides to break through the geologic barrier early from the dominant channel.
4. Stagnant water zones are critical for nuclide transport in fractured rocks. The dispersion coefficient and fracture width control the formation of stagnation zones. The larger the dispersion coefficient, the easier it is for nuclides to enter the stagnant zone formed by the wider fracture under the influence of molecular diffusion.
5. The dead end of the fracture has a certain blocking effect on the transport of nuclides. Nuclides at the dead end are difficult to migrate with water convection, mainly due to molecular diffusion migration attenuation. Different intersection angle of the dead end of the fracture on the nuclide transport blocking effect there is a certain difference.

Conclusion

6. Flow is determined by radius and fracture width, with STi of 0.994 and 1.01, respectively. Fracture radius is the main parameter independently controlling flow without considering interaction effects. The single factor of fracture width has a negligible effect on flow, but strong interactions with other parameters lead to a particularly significant effect when interaction effects are considered.
7. Radius has the largest combined effect on transport distance, with an overall sensitivity index of 0.687. Radius controls nuclide transport distance through flux variations, resulting in a high statistical correlation between transport distance and flux.
8. The interaction between radius and longitudinal dispersion is the strongest of all parameter combinations, with Vij of 0.318. This strong interaction accounts for 82% of the total contribution of the longitudinal dispersion coefficient to the variance of transport distances, and is the main reason for the influence of the longitudinal dispersion coefficient on transport distances.
9. The total sensitivity indexes of 3D density and fracture dip-angle to transport distance are 0.183 and 0.185, respectively. The 3D density may promote nuclide transport by enhancing the connectivity of the fracture network. The average angle parameter of the fracture promotes the formation of dominant flow or stagnant zones by influencing the way of fracture intersection in the network, which promotes or inhibits nuclide transport, leading to increased uncertainty of nuclide breakthrough time.

Thank you!

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