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Modeling Contaminant Diffusion in Highly Complex Rock Structures

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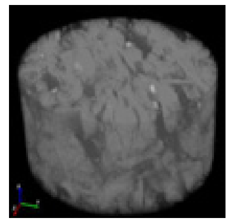
Opalinus Clay is currently being proposed as a potential host rock for radioactive waste repository in deep geological formation. It is then important for performance assessments to understand the transport properties of such rocks. Clay materials are characterized by low hydraulic conductivities and **diffusion** is assumed to be the main transport mechanism. The studied rock is a complex assembly of several minerals and the influence of the **microstructure** (spatial distribution of the minerals in the rock) on solute transport is still an open issue.

Microstructure investigation (Spatial resolution : 15 µm)

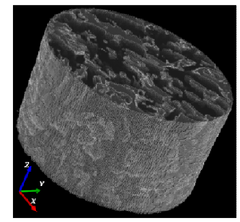
The microstructure was investigated with synchroton based X-ray microtomography provided by the 'TOMCAT' beam line at the Swiss Light Source (SLS, Villigen PSI Switzerland). After tomographic reconstruction and segmentation, three main domains are selected representing the three main minerals in the rock (clay minerals, calcite, oxydes). Only the clay fraction is considered as porous.

Due to the scale of mineral heterogeneities in the rock, the simulation of a contaminant diffusion cannot be implemented with the original data.



Segmentation

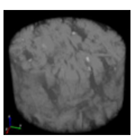
Clay fraction of the rock



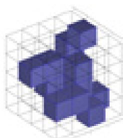
Size : 252x252x136 = 8 636 544 voxels

① Data reduction procedure

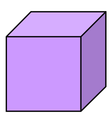
An appropriate data reduction procedure is needed in order to simulate the diffusion of a contaminant in the defined clay domain with COMSOL Multiphysics™. The goal of data reduction is to extract a subset of data from a massive dataset while maintaining the properties and characteristics of the original data in the reduced set.



Extraction of 4x4x4 voxels subvolumes



Averaging of the transport properties (D_e, α)



Homogeneous anisotropic sub-volume

Reduced set of data

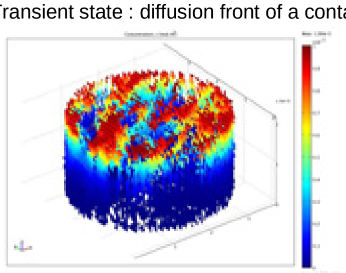
Transport parameters : D_e^{sv}, α^{sv}

Size : 63x63x34 =134 946 voxels)

③ Diffusion calculation

- Mesh : - tetrahedral elements (271 536 elements)
  - clay minerals domain
- Transport parameters defined as interpolated functions (Nearest neighbor method)

Transient state : diffusion front of a contaminant



Cross-section (30 vertical planes) plot of the concentration (time = 50 days)

- Diffusion simulated by maintaining fixed concentration gradient throughout the sample
- Heterogeneous contaminant distribution ➔ influence of the spatial heterogeneities due to the rock microstructure

Conclusion

By implementing a data reduction procedure, we were able to simulate the diffusion of a contaminant in the rock without losing severe information about the microstructure.

Outlook

By adjusting the transport parameters of the clay fraction of the rock and comparing the calculated diffusion front of a contaminant with experimental data, it is then possible to deduce its transport properties.

② Averaging the characteristics of the sub-volume

Transport parameters : - Effective diffusion coefficient D_e
- Rock capacity factor α (solid/solution interaction)

Effective diffusion coefficient calculated with COMSOL Multiphysics™ in the three direction of the space (D_e^X, D_e^Y, D_e^Z) by modeling the diffusion of a contaminant throughout the sub-volume in the chosen direction.

System equation

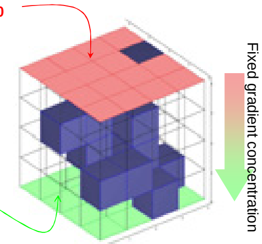
Blue domain : non porous mineral ➔ inactive domain

White domain : clay fraction ➔ diffusive domain

$$\frac{\partial c}{\partial t} = \frac{1}{\alpha}\nabla(-D_e^{clay}\nabla c)$$

C = C_0

C = 0



Boundaries conditions

Upper boundary : C=C_0

Lower boundary : C = 0

⇨ Fixed concentration gradient throughout the defined subvolume

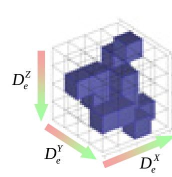
Sides boundaries and inter-domain boundaries : $\vec{J}.\vec{n} = 0$

Effective diffusion coefficient D_e

At the lower boundary, the averaged contaminant flux J at the permanent state is related to the effective diffusion coefficient in the chosen direction following **Fick's first law**

$$J = -D_e \frac{\Delta c}{\Delta l} \text{ with } \begin{cases} \Delta c = C_0 \\ \Delta l \text{ the side length of the sub-volume} \end{cases}$$

For each sub-volume, an anisotropic diffusion coefficient is calculated.



$$D_e^{sv} = \begin{pmatrix} D_e^X & 0 & \\ 0 & D_e^Y & \\ & & D_e^Z \end{pmatrix}$$

Rock capacity factor α

$$\alpha = \varepsilon + \rho K_d$$

ε porosity of the sub-volume
ρ dry density of the sub-volume
K_d distribution coefficient of the sub-volume

For the sub-volume

$$\alpha^{sv} = \%_v^{clay}\alpha^{clay}$$

α_{sv} rock capacity factor of the sub-volume
$\%_v^{clay}$ volumic clay percentage
α^{clay} rock capacity factor of the clay fraction