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Radionuclide Transport through Different Routes near a Deposition Hole for Spent Nuclear Fuel

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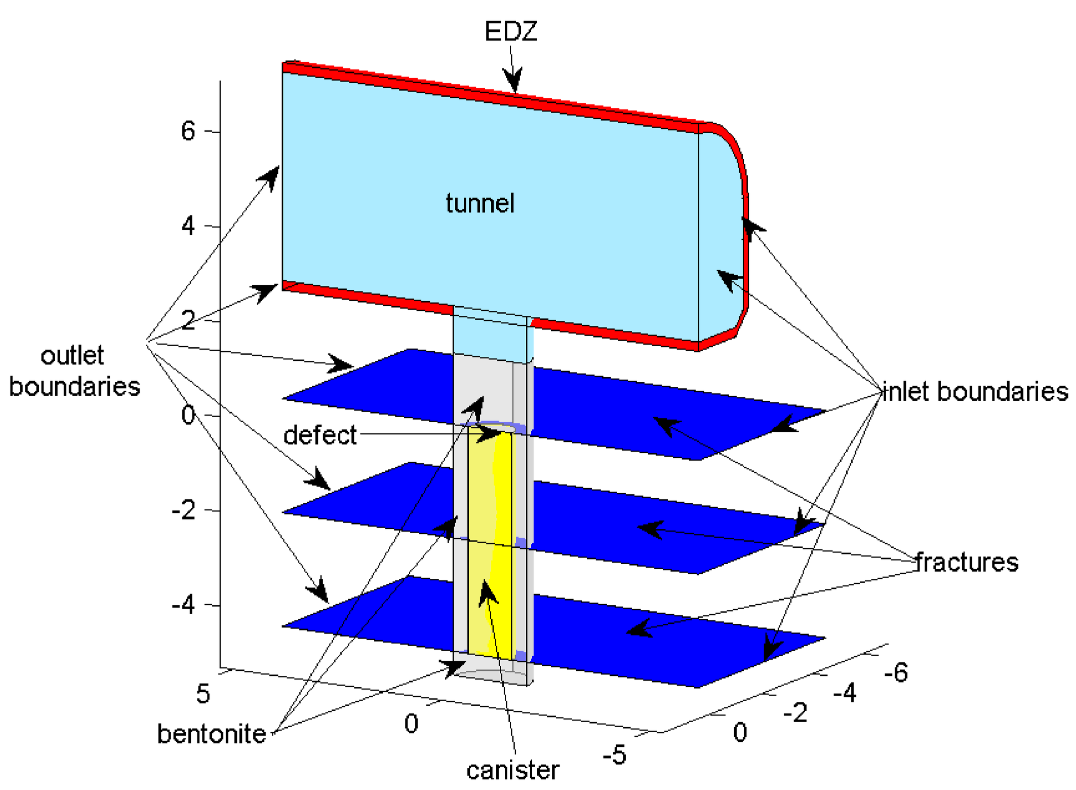
INTRODUCTION

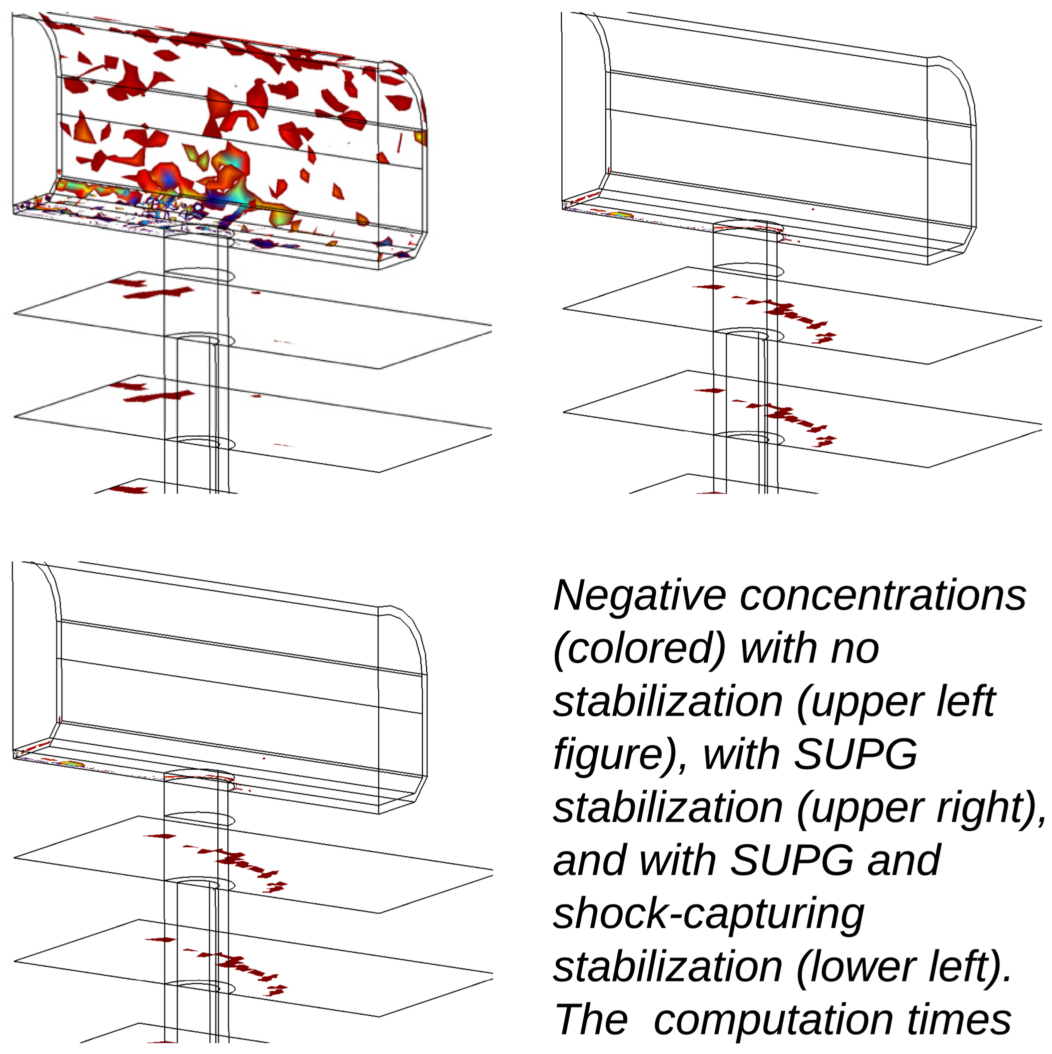
Radionuclide transport modeling is a part of the research concerning the geological disposal of spent nuclear fuel. Typically, the transport models focus on the reactions of nuclides, while model geometry and ground-water flow are often simplified. Here, instead, a radionuclide transport model in a detailed 3D geometry with no reactions is introduced. The aim is to study the effects of the geometry and realistic flow fields on nuclide trans-port. This presentation focuses on the development of the model instead of the final results.



The model geometry. Water flows in the fractures (blue), in the tunnel section (light blue) and in the excavation damaged zone, EDZ (red). The scale is meters.

USE OF COMSOL MULTIPHYSICS

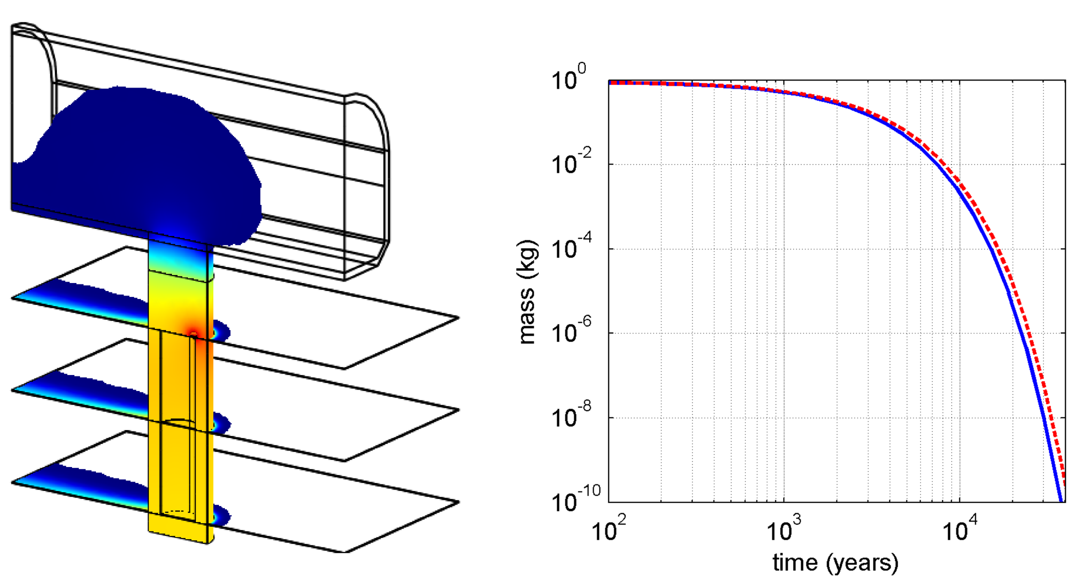
- The Chemical Engineering Module
  - includes numerical stabilization options
  - includes porous medium flow equations (Darcy's law in this case)
  - the convection-diffusion equation in porous medium can be modified to fit straight into the module
- The COMSOL Multiphysic main module
  - Boundary Weak Form application mode
  - needed when describing the interior of the deposition canister with an equation on the defect surface



Negative concentrations (colored) with no stabilization (upper left figure), with SUPG stabilization (upper right), and with SUPG and shock-capturing stabilization (lower left). The computation times were 73, 65 and 95 minutes.

NUMERICAL METHODS

- Tested elements
  - various order Lagrange elements
  - the 3rd order Hermite element
- Stabilization techniques
  - streamline upwind/Petrov-Galerkin (SUPG)
    - stabilizes in the streamline direction
    - constant and variable stabilization parameter
  - shock-capturing
    - stabilizes in the crosswind direction
    - makes the problem nonlinear
- Time-dependent solver
  - Backward Differentiation Formula (BDF) solver: maximum order 2 or 5
- Linear equation solvers
  - direct solvers: Umfpack or Pardiso



Examples of the results. The left figure shows the concentration profile at $2.4 \cdot 10^5$ years. The right figure is a comparison of the Lagrange (red slashed line) and the Hermite (solid blue line) elements. The total mass of a radionuclide in the bentonite is monitored in a test case where the nuclide is initially placed in the bentonite above the canister and the tunnel section is excluded from the model.

GROUNDWATER FLOW EQUATIONS

The equation describing the flow of ground-water is obtained by combining the stationary continuity equation in porous medium with Darcy's law. The resulting problem is to find $p=p(\mathbf{x})$ such that

$$\begin{cases} \nabla \cdot \left(-\frac{\boldsymbol{\kappa}}{\mu} (\nabla p - \rho \mathbf{g}) \right) = 0 & \text{in } \Omega_{flow} \\ p = p_{in} & \text{on } \partial\Omega_{inlet} \\ p = p_{out} & \text{on } \partial\Omega_{outlet} \\ \mathbf{n} \cdot \left(-\frac{\boldsymbol{\kappa}}{\mu} \nabla p \right) = 0 & \text{elsewhere on } \partial\Omega \end{cases}$$

MASS TRANSPORT EQUATIONS

The mass transport problem is to find $c=c(\mathbf{x},t)$ such that

$$\begin{cases} \theta \dot{c} + \nabla \cdot (D_e \nabla c) + \mathbf{u} \cdot \nabla c = 0 & \text{in } \Omega_{flow} \\ \theta \dot{c} + \nabla \cdot (D_e \nabla c) = 0 & \text{in } \Omega_{bento} \\ -\mathbf{n} \cdot (-D_e \nabla c) = \frac{D_e}{l} (c_c - c) & \text{on } \partial\Omega_{defect} \\ \mathbf{n} \cdot (-D_e \nabla c) = 0 & \text{on } \partial\Omega_{outlet} \\ \mathbf{n} \cdot (-D_e \nabla c + \mathbf{u} c) = 0 & \text{elsewhere on } \partial\Omega \\ c(\mathbf{x}, t=0) = 0 & \text{in } \Omega = \Omega_{flow} \cup \Omega_{bento} \end{cases}$$

where the canister interior concentration $c_c=c_c(t)$ solved from the initial value problem

$$\begin{cases} \dot{c}_c = -\frac{D_e A}{Vl} (c_c - c) & \\ c_c(0) = c_{c0} & \text{on } \partial\Omega_{defect} \\ \dot{c}_c(0) = -\frac{D_e A}{Vl} (c_c(0) - c(\mathbf{x}, 0)) & \end{cases}$$

CONCLUSIONS

- Non-reactive radionuclide transport problems in realistic geometry can be solved effectively with COMSOL Multiphysics.
- The need for computational resources can be reduced by using special techniques for unimportant parts of the model.
- The numerical stabilization techniques improve solution quality but may also reduce the computation time. The choice of the technique and the stabilization paremeter, however, affects greatly the benefits of the stabilization.
- The use of Matlab interface enhances the sequencing capabilities of COMSOL.

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