Development of a COMSOL application for the efficient evaluation of an engineered barrier system

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Introduction

Radioactive waste repositories include barriers that work to contain the waste, thereby protecting human health and the environment. In deep geological disposal systems, barriers include the natural geological barrier and the engineered barrier system (EBS).

The ability of the EBS to limit groundwater flow is important and optimized design solutions are often sought by means of numerical modelling. For instance, models can quantify flow rates as affected by different assumptions regarding EBS materials and repository location. The present work shows an example of a COMSOL application intended to aid EBS sensitivity studies.

Model Set-up

The Multiphysics model underlying the application simulates groundwater flow through a rock vault in the Swedish final repository for short-lived radioactive waste [1]. The vault geometry is shown in Figure 1.

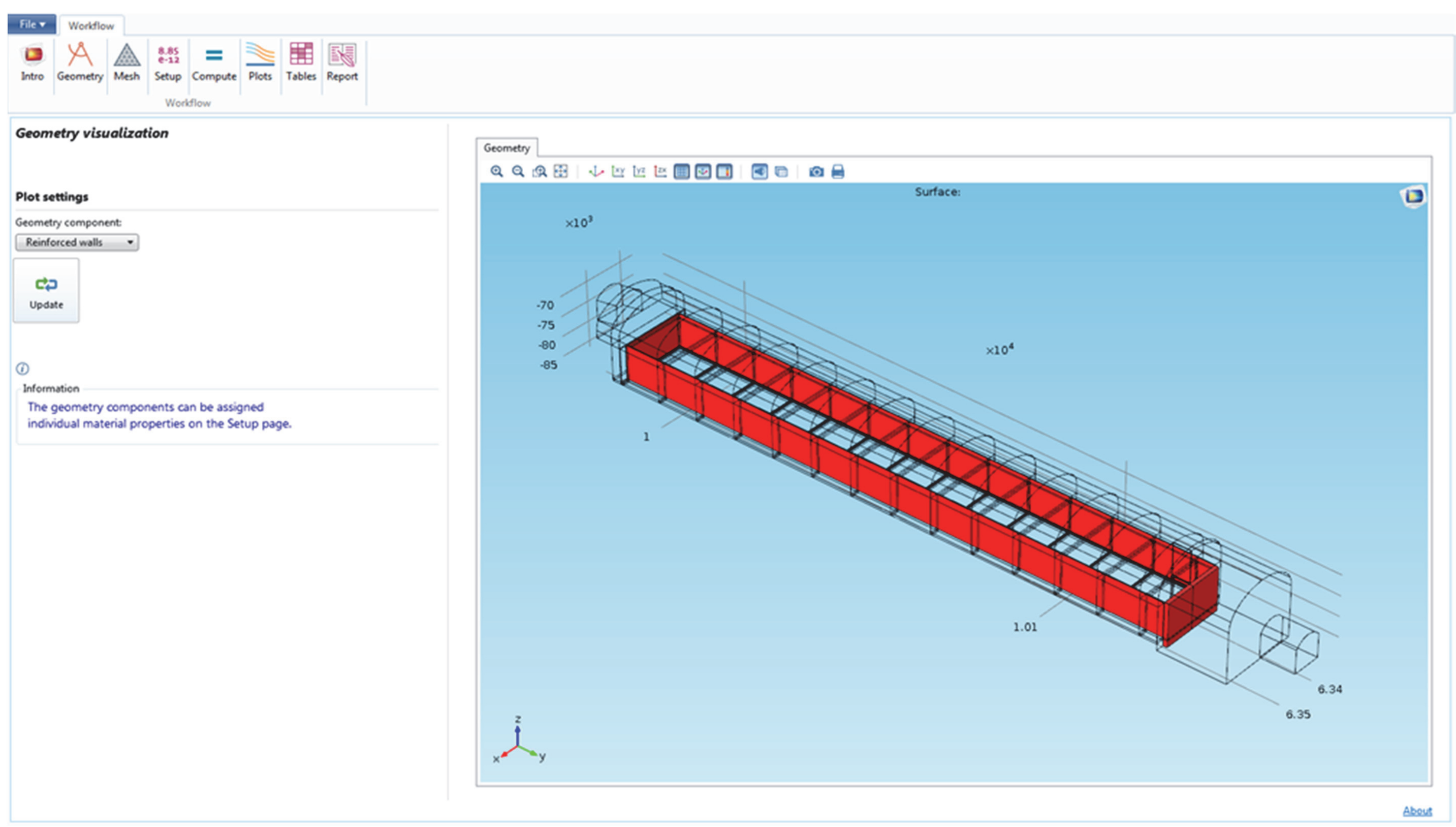

Figure 1. On the Geometry page the user can visualize the different structures and material domains available in the application.

The Darcy's law and Solute Transport interfaces have been applied to calculate groundwater flow rates and residence times in the vault. The residence time is defined here as the spatial distribution of the mean groundwater age, taking into account advection, diffusion and dispersion processes. It is calculated by solving a partial differential equation proposed by Goode et al [2].

$$\frac{\partial A}{\partial t} = 1 + \nabla \cdot (\mathrm{D} \cdot \nabla A) - \nabla \cdot \frac{q}{\theta} A + \frac{F}{\theta \rho}$$

Above, A is the water age (s), q is the Darcy velocity field (m/s), D is the hydrodynamic dispersion tensor (m^2/s), θ is the porosity, ρ is the water density (kg/m^3) and F is a source term.

Application description

Figure 2 shows the ribbon at the top of the application graphical user interface. Clicking the buttons, from left to right, provides a workflow that guides the user through the application.

Intro	Geometry	Mesh	Setup	Compute	Plots	Tables	Report
▪General view of the app ▪Open user's guide ▪Open report related with the app	▪Visualize the geometry ▪Differentiate materials	▪Visualize the mesh	▪Select values of parameters ▪Select or import boundary conditions (BC) ▪Visualize the new parameters and BC	▪Compute Groundwater flow and residence time	▪Customize Plot 2D and 3D ▪Flow and RT tables		▪Customized Report with the different figures and tables contained in the app.

Workflow

Figure 2. The application ribbon provides the workflow to guide the user.

The user can change model inputs on the Setup page. This involves assigning values to the porosity, hydraulic conductivity and effective diffusivity of different materials and engineered structures.

The user can also select among predefined pressure fields to prescribe the boundary conditions for the groundwater flow (Figure 3). As an option, pressure boundary conditions can be imported from file.

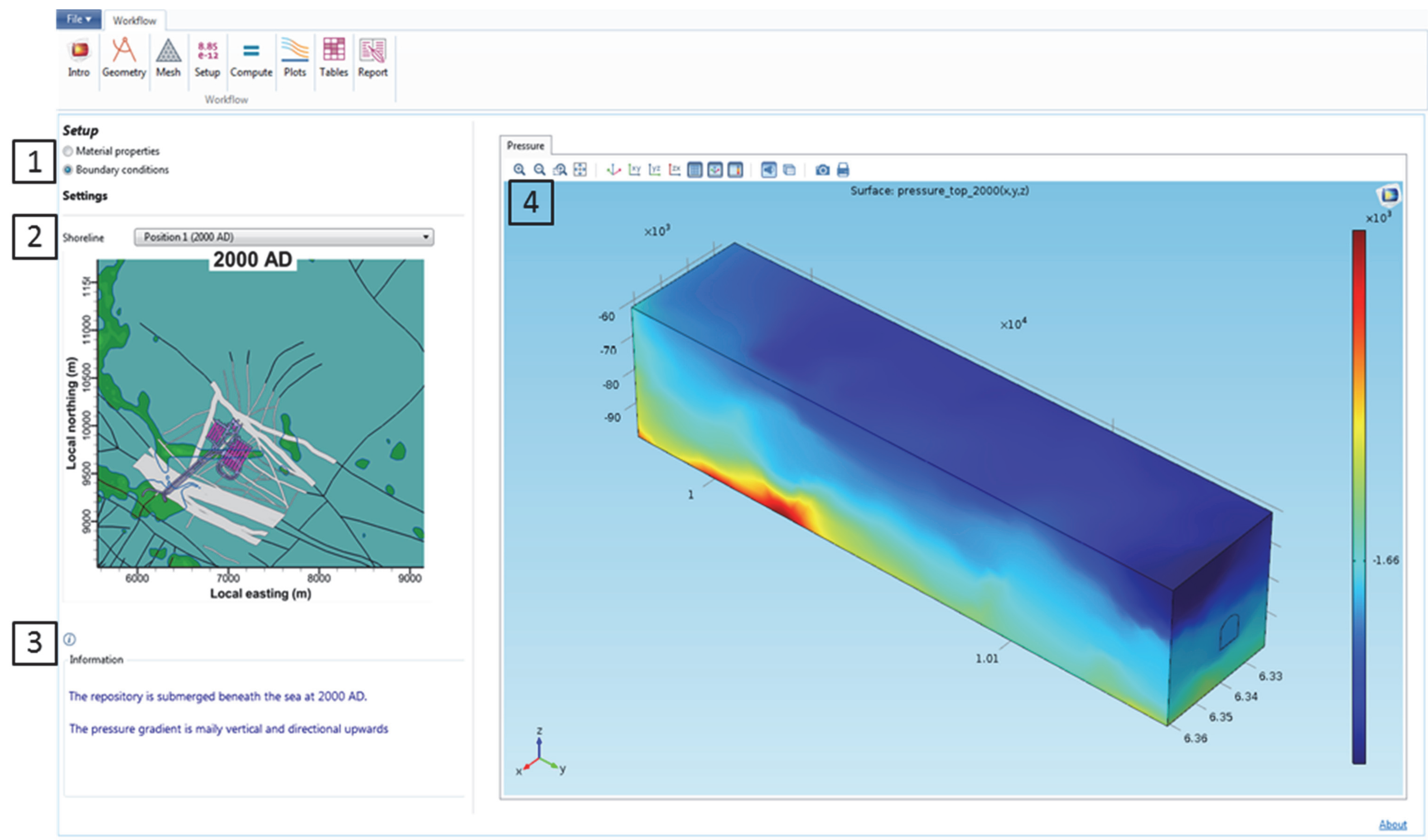

Figure 3. On the Setup page the user can modify the material transport properties and the boundary conditions (1). Selecting from the list of shoreline positions (2) updates the information graphics and text (3) as well as the displayed pressure field (4).

After model setup the user can compute the groundwater flow and the residence time in the rock vault. Results can be analyzed through a set of predefined plots in 2D and 3D (Figure 4). Numerical values can be output in table exports. Formats are standardized such that quantitative simulation results can be used directly in connected modelling activities.

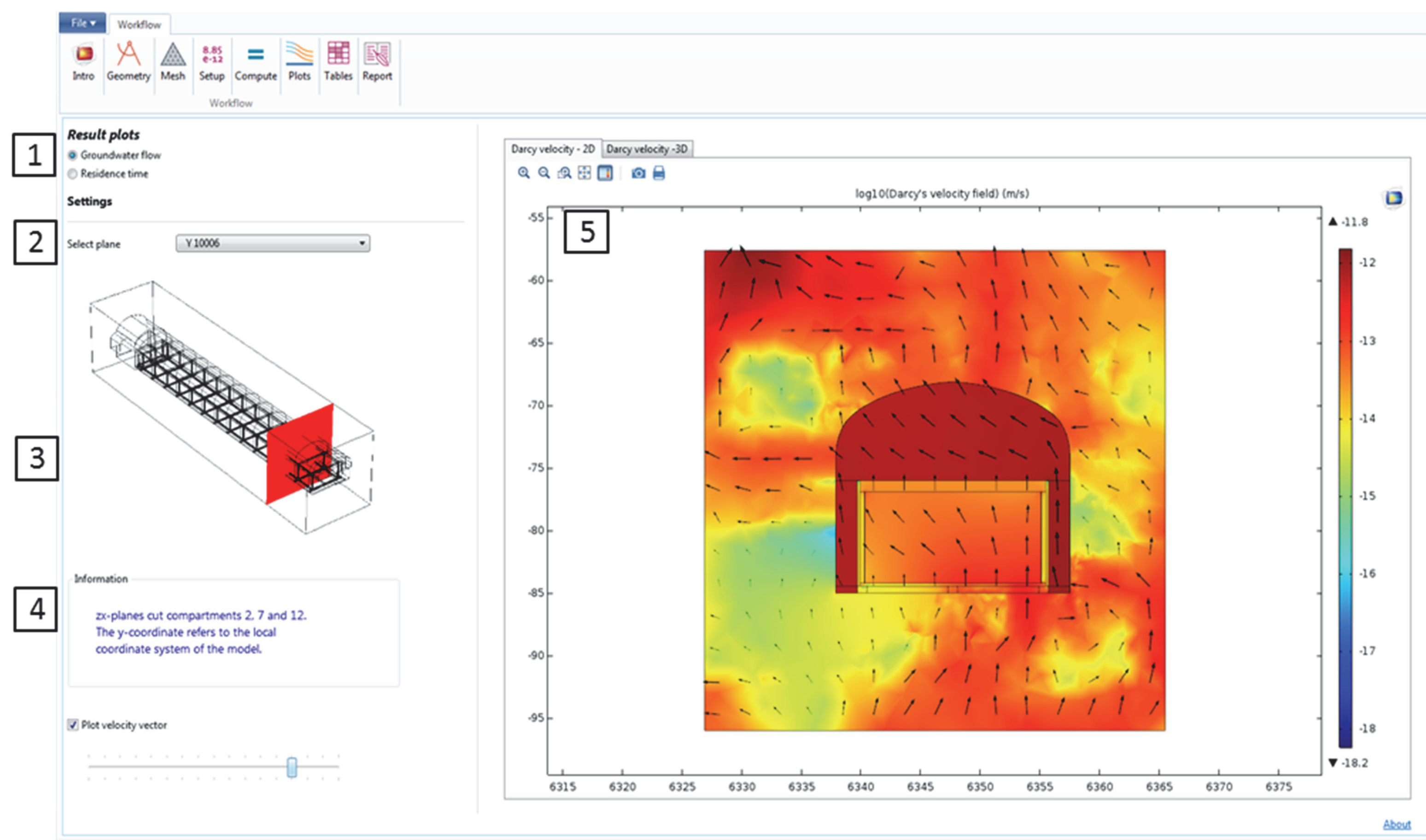

Figure 4. On the Plots page the user can select between flow or residence time results (1) displayed in 2D and 3D. Flow results presented in 2D use predefined cutplanes (2). Selecting from the list updates the information graphics and text (3 and 4) as well as the displayed results (5).

After simulation, modelling reports can be generated automatically, summarizing the model setup and results.

Perspective

The COMSOL Application Builder has been used to rework a coupled Multiphysics model in 3D into a ready-to-use simulation application. The application provides the opportunity for non-modelling experts and engineers to perform extended simulation trials and production runs. The accessibility of the application format furthermore facilitates review and quality control work associated with the model development process itself.

References

[1] http://www.skb.com/our-operations/sfr/

[2] Goode D J, 1996. *Direct simulation of groundwater age*. Water resources research, vol 32. N.12, pages 289-296.