An Alternative Equation-Based Model in COMSOL Multiphysics® for Bentonite Re-Saturation

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Abstract

Bentonite is a versatile clayey material that is, among other things, envisaged in designs for radioactive waste repositories as a geotechnical protection of the waste canisters against groundwater. The thermo-hydraulic-mechanically (THM) coupled process of bentonite re-saturation is commonly simulated using a two-phase flow and a mechanical stress formulation like the Barcelona Basic Model for unsaturated clayey soils.

As an alternative to the numerically demanding THM-formulations, a thermo-hydraulic saturation model for confined conditions (as expected in a repository) based on vapour flow in the pore space has been developed. The conceptual model was experimentally realised in the one-dimensional FORTRAN-code VIPER. While being successfully used, the range of possible applications is inherently limited. The underlying partial differential equations for isothermal water uptake have therefore been transferred to COMSOL Multiphysics® in form of an equation-based model.

The non-linear balance equation was implemented using the coefficient form of the PDE interface. It was linearized by taking the solution from the previous timestep to calculate the parameters that depend on the primary variable.

Subsequently, a model was set up to match earlier calculations with code VIPER concerning a 1D laboratory test of water uptake. Validation of the new implementation in COMSOL was therefore based on a code comparison as well as on matching model results with the real data.

Based on this model, a simple application was developed to provide a reference for subsequent modelling of multi-dimensional problems of the same type. A 2D- and a 3D-model expanding the 1D-problem to two and three dimensions was successfully tested that way.

A last 3D-model of a rod with a quadratic cross-section demonstrates the influence of limited space for water uptake on the uptake dynamics.

Keywords: Bentonite, re-saturation, vapour diffusion, experiment, PDE-model, code comparison

Introduction

Bentonite is envisaged as a buffer and sealing material in many concepts for geological storage of radioactive waste to prevent damage of the waste canisters from groundwater and to impede migration of radionuclides in case of a damaged canister [1],[2]. Incoming water lets the clay particles, major part of the bentonite, swell by hydration and thereby reduces the hydraulic permeability considerably. The water uptake dynamics of bentonite are therefore of considerable interest.

Numerical simulation of bentonite re-saturation is commonly done with the help of thermo-hydraulic-mechanically (THM) coupled models. The swelling of the bentonite from water uptake or the development of swelling pressure if the bentonite is emplaced in a confined space are calculated with the mechanical part which is often represented by the Barcelona Basic Model (BBM). One example of this type of model is given in the COMSOL application library[3].

Assuming that the strain in a bentonite body can be neglected if the bentonite is situated under confined conditions, the mechanical part can be dropped, though. Following moreover a completely different approach for the hydraulics of the re-saturation, an alternative concept was developed including a new balance equation and backed up by laboratory experiments[4]. In order to check the viability of the new approach, the experimental FORTRAN-code VIPER has been developed for one-dimensional problems.

In order to enhance the inherent limited range of possible applications of code VIPER, the underlying partial differential equations in their most basic form are transferred to COMSOL Multiphysics® in an equation-based model. As a validation of this exercise, a one-dimensional COMSOL-model is set up to compare calculation results to the data of the experiments as well as to the results from code VIPER. Secondly, the applicability of the new model to 2D- and 3D-problems is demonstrated by setting up a 2D- and a 3D-model with a point-like water inlet. Here, the results of the transient water content distributions are compared along a straight line through the water inlet that is orthogonal to the model boundary.

Theory and Experimental Set-up

The classic concept for bentonite re-saturation explains the migration of water into the bentonite by advective water flow driven by suction[5]. The alternative model is based on the reflection that water vapour, while having a much lower density than water, is migrating much faster through the pore space by diffusion than by advection of liquid water. The idea had been triggered by water uptake tests performed in the laboratory with water as well as with water vapour that indicated similar uptake dynamics[6]. Initially, the hydrated water had been assumed to be immobile[7]. Later, it was found, though, that a diffusion-like migration mechanism is actually affecting the hydrated water[8].

The tests mentioned above were performed on cylindrical pre-compacted bentonite samples with a length of 100 mm and a diameter of 50 mm as illustrated in Figure 1. The samples were encased in a steel liner to ensure confined conditions and were wetted from one end. The other end was closed. After pre-defined periods of time, the samples were cut into slices to determine the axial distribution of the water content. Many of the tests were repeated to get an impression of the accuracy of the measurements. The data are depicted below in Figure 2 together with numerical results.

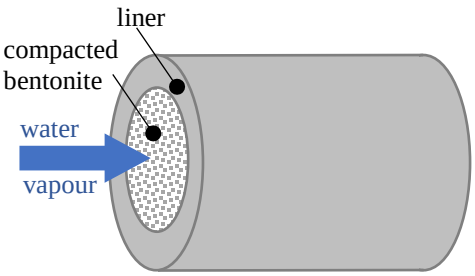

Figure 1. Sketch of the test principle

Numerical Model

An appropriate balance equation for isothermal water uptake via vapour had not been available at the time when the uptake experiments had been performed. A new equation was therefore derived for the mass of water[5] from a general balance equation based on Reynolds' transport theorem[9] with the partial density of the vapour as the primary variable. In the final form of (1) and the first summand in (2), it just includes the physical processes of binary diffusion of vapour in the pore air and instantaneous hydration of vapourous water in the clay particles. In this form, hydrated water is treated as being immobile. Including the second summand in (2) takes care of diffusive migration of hydrated water. A particular difficulty is here that the diffusion coefficient for hydrated water D_{hyd} depends stepwise on the water content w [8] which in turn is a secondary variable depending eventually on the vapour partial density ρ_v. These circumstances make Equation 1 non-linear.

$$\frac{\rho_d}{\rho_{v\,sat}} w_e \frac{\partial \rho_v}{\partial t} - D_a \Delta \rho_v = 0 \qquad (1)$$

ρ_v - partial density of the vapour
$\rho_{v\,sat}$ - vapour saturation density
ρ_d - dry density of the bentonite
w_e - water content at full saturation
D_a - apparent vapour diffusion coefficient (see (2))
t - time

$$D_a = D_{mol} \cdot \varphi \cdot \tau + \rho_d \cdot \frac{\partial w}{\partial r_h} \cdot \frac{1}{\rho_{v\,sat}} D_{hyd} \qquad (2)$$

D_{mol} - molecular diffusion coefficient for vapour
φ - porosity
τ - tortuosity
w - water content
r_h - relative humidity
D_{hyd} - diffusion coefficient for hydrated water

The balance equation was implemented using the coefficient form of the PDE node. Because of the stepwise dependence of the diffusion coefficient D_a on the water content w, a step function distinguishing between three different water content ranges has been implemented. The water content is evaluated using the calculated partial vapour density ρ_v of the previous timestep. Therefore, the calculated ρ_v needs to be saved and used as input for the next time step.

This procedure was realised by using the previous solution operator, as explained in the COMSOL blog[10]. In addition to this operator, also the Domain ODEs and DAEs interface is needed. In this interface, the nojac command was used to write the saved value from the last solution in a new variable. At this stage, the model input was chosen to be compatible with the older VIPER-model.

Only the mathematics interface was used for the present model. At a later stage, however, coupling with other physic interfaces, particularly the temperature interface, is envisaged and has already been prepared.

After validating the results of the 1D-model by comparing the calculated water content distributions with the measured ones, a simple COMSOL-application was developed. It was not very complex, because it was only intended to make the validation for the higher-dimensional models more efficient and compatible among each other.

The model for the water uptake tests is quite simple as it consists only of a straight one-dimensional domain with a constant cross-section. The inflow side is represented by a Dirichlet boundary condition for the vapour partial density ($\rho_v(x=0) = \rho_{v\,sat}$) on the left-hand side and a no flow boundary condition on the right-hand side of the model. The initial vapour partial density is set consistent with the initial water content of 10 %.

Experimental and Simulation Results

The new COMSOL-model was validated by comparing the calculated water content distributions for several test periods (4d, 13d, 20d, 55d, 90d, 120d, 185d) with the experimental data. For some periods, only one dataset is available, all others have been tested twice, though. A graphical comparison is given in Figure 2. The experimental data are plotted as symbols that are

connected by black dotted lines. The curves from the COMSOL-model are depicted in blue. The match between experimental and model results is very good.

Additionally, also the model output from the original VIPER-model is included in Figure 2. Note that based on these data, the first balance equation for code VIPER had been formulated. The results calculated with VIPER are plotted in orange showing an excellent match of the results from the COMSOL- and the VIPER-model.

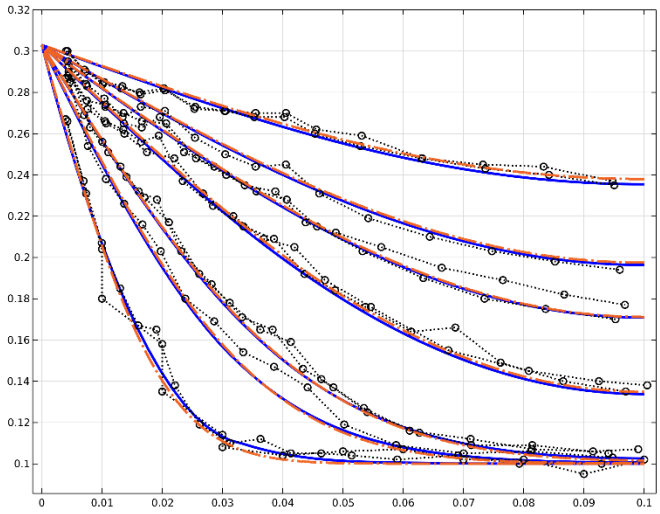

Figure 2. Numerical results from the 1D COMSOL-model (blue), experimental results (black), numerical results from VIPER (orange dash-dotted curves)

After establishing the 1D-model of the water uptake experiment, the model was expanded to a 2D-model. The new model geometry was a square with a side length of 10 cm. In order to create a basis for a comparison of results from the 1D- and the 2D-model, a cutline through the middle of the square was defined where one end of the line was aligned with the inflow. The inflow was assigned to one entire side of the square, the rest of the boundary was set to be impermeable. Water content distributions were calculated at the same model times as for the 1D-model. In this case the resulting curves for the water content distribution matched the corresponding curves from the 1D-model.
In order to demonstrate the influence of two-dimensional uptake the inflow was concentrated to a point like inflow at the middle of the side. This means of course that because of transversal diffusion the results of the 2D-model must deviate from those of the 1D-model. As expected, the diffusion orthogonal to the cutline lead to an ever-increasing distance between the corresponding curves of the two models as depicted in Figure 3. The water content distributions from the 1D-model are plotted in coloured dash-dotted curves while the results from the 2D-model are plotted in coloured solid curves.

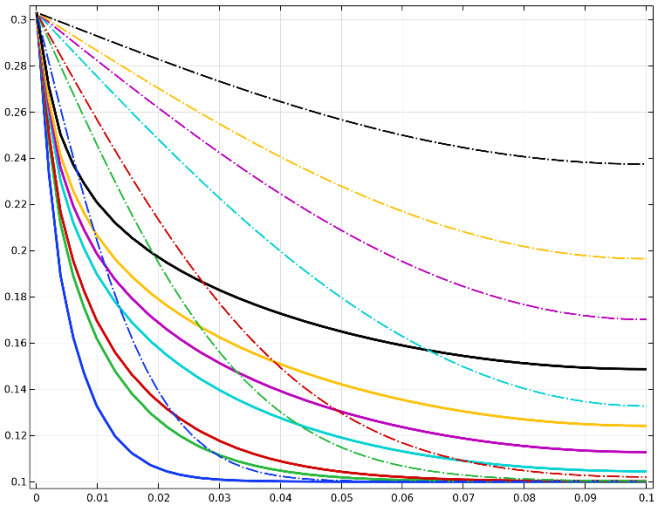

Figure 3. Numerical results from the 2D model (solid curves) in comparison to the 1D model (dash-dotted curves); distributions for 4 days (blue), 13 days (green), 20 days (red), 56 days (cyan), 90 days (violet), 120 days (orange), 185 days (black)

An analogous observation was made when the 2D-model was expanded further to a 3D-model with pointwise inflow. In the 3D-model, the domain was defined to be a cube with a side length of 10 cm, to make it comparable to the previous two models. For comparability there was also a cutline defined, this time through the middle of the cube. In Figure 4, the results of the 3D-model are plotted in coloured solid curves while the results of the 2D-model are represented by coloured dash-dotted curves. The water content curves from the 3D-model are lying closely together demonstrating the strong influence of the transversal diffusion in 3D.

What the results presented so far do not show is the complexity of the spreading pattern in three dimensions of the water that has been taken up by the bentonite. To get an impression of the spreading patterns, another 3D case was modelled. The model domain is defined to represent a rod with a quadratic cross-section with the dimensions of 0,5m x 0,5m x 1,0m. Water inflow was arranged in the middle of one face of the rod, again in a pointwise manner. The results are given as a set of isosurfaces at a certain model time as shown in Figure 5. This set-up leads of course to longer saturation times, but was a first demonstration of a 3D calculation based on the conceptual model of code VIPER.
In a true half-space point-like inflow would lead to semi spherical water migration. But in the rod the available space is limited. The initially semi-spherical water spreading pattern changes therefore to a basically one-dimensional progress towards the end of the model. This is reflected in the isosurfaces shown in Figure 5. Note that the first isosurface to the left that is not semi-spherical, illustrates nicely the complexity with which the water fills the rod at the inflow side.

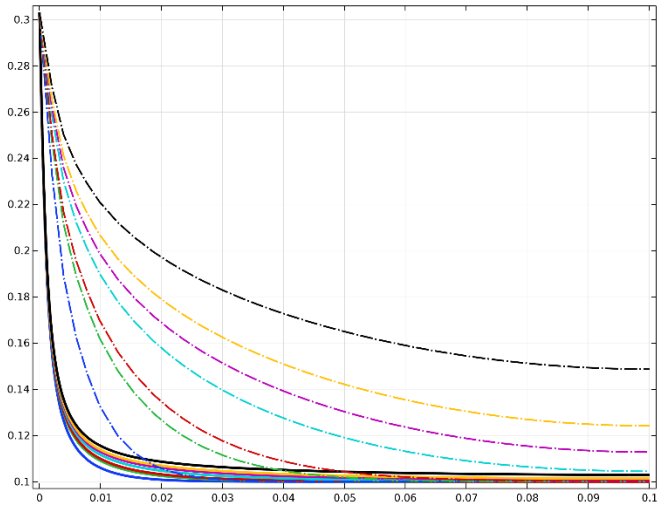

Figure 4. Numerical results from the 3D model (solid curves) in comparison to the 2D-model (dash-dotted curves); distributions for 4 days (blue), 13 days (green), 20 days (red), 56 days (cyan), 90 days (violet), 120 days (orange), 185 days (black)

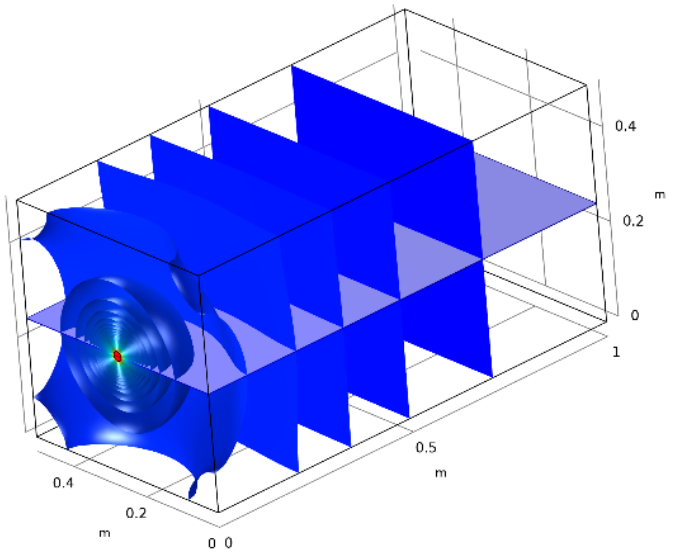

Figure 5. Calculated water content distribution in a 3D-rod with pointwise injection after 75 years

Conclusions and Outlook

The conceptual model and the referring mathematical model for isothermal bentonite re-saturation underlying code VIPER have successfully been transferred to an equation-based formulation in COMSOL. This allows now for the first time for applications of this concept to higher dimensional water uptake problems.

This is, however, only the first in several steps on the way to a complete transfer. Two general lines of work should be followed in the future. One line would be concerned with the refinement of the isothermal model. In the present form of the model, the constitutive equations, particularly the adsorption isotherm (or the equivalent retention curve) are incorporated in their most simple form. More complex forms or analytical formulations should be implemented as well. Another point is the adaption of the model to low inflow rates which are more realistic in the framework of nuclear waste repositories but require principally different inflow boundary conditions.

The second line of possible future work concerns the expansion of the model in terms of multiphysics, especially with respect to non-isothermal water uptake. This requires on the one hand coupling of the heat flow interface to the present model. On the other hand, many parameters in the isothermal formulation such as the vapor saturation density or the molecular diffusion coefficient are actually temperature-dependent and need to be treated as functions instead.

A complete transfer from VIPER to COMSOL is still quite some way away. However, the work presented here marks a successful and encouraging first step on this way.

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