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TECHNICAL UNIVERSITY OF LIBEREC
Faculty of Mechatronics, Informatics
and Interdisciplinary Studies

Modeling of Bentonite Hydration Process in a High Level Waste Repository

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Introduction:

We deal with a problem of bentonite behavior during the saturation process in a high level waste repository of KBS-3V conception according to [6], **Figure 1**. Bentonite is a type of clay with specific nonlinear behavior caused by water adsorption and swelling ability in contact with water. It leads to nontrivial problems for a numerical solution. The base of the work was done in a cooperation with Clay Technology AB, Sweden and applied to Task Force on Engineered Barrier System problems [2].

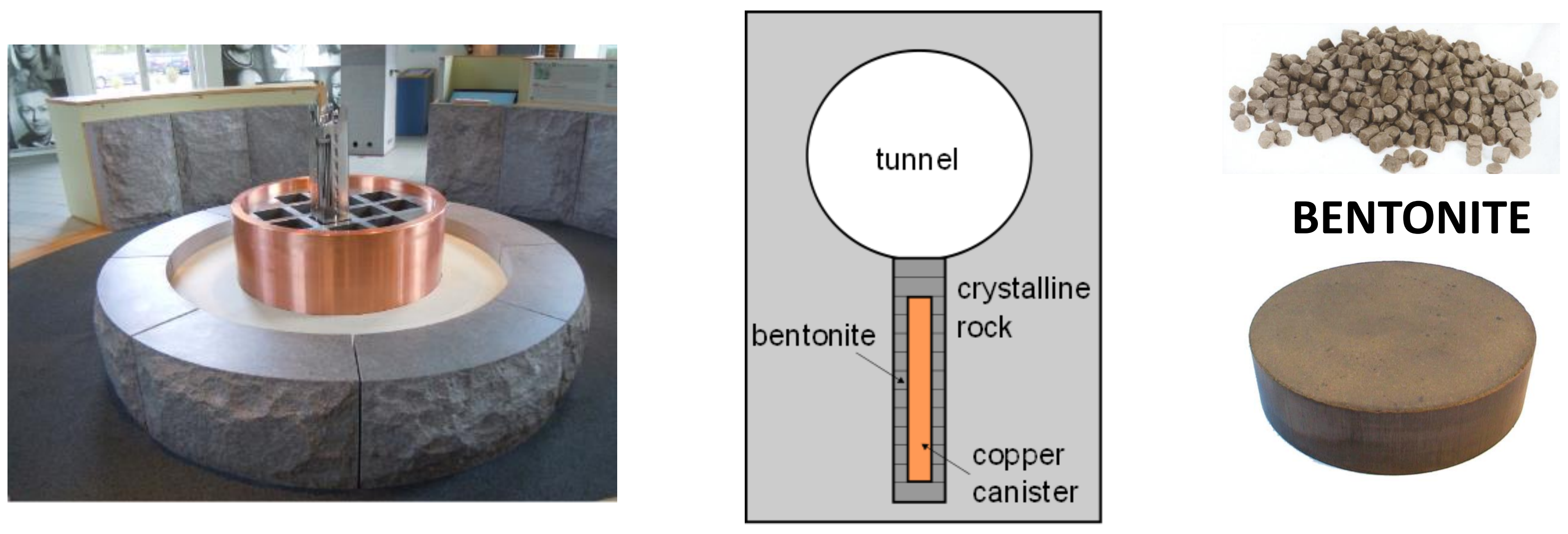

Figure 1. KBS-3V concept – deep repository in compact crystalline rock with bentonite buffer and backfill (as pellets and compacted bentonite), spent nuclear fuel encapsulated in special copper canisters [6], left picture from exhibition in Äspö hard rock laboratories [7], pictures of bentonite from [8].

Theory and used interfaces:

– flow of water in partly saturated conditions (according to [4] which corresponds to Richards' equation – **water mass balance in liquid phase**)

$$\underbrace{n\left(\frac{\partial S_l(p_l)}{\partial p_l}\rho_l(p_l)+\frac{\partial \rho_l(p_l)}{\partial p_l}S_l(p_l)\right)\frac{\partial p_l}{\partial t}}_{\text{time change in water content in liquid phase}}-\nabla\cdot\underbrace{\left(\frac{kk_r\rho_l(p_l)}{\mu}\nabla p_l\right)}_{\text{advective flux of liquid water}}=0$$

p_l …liquid pressure
k… permeability
n… porosity
k_r …rel.permeability
ρ_l …water density
μ…viscosity
S_l …degree of saturation for liquid phase

– flow in partly saturated conditions **with diffusion of water vapour** (water mass balance in liquid and gas phase)

$$\underbrace{n\left([\rho_l(p_l)-\theta_g^w(p_l)]\frac{\partial S_l(p_l)}{\partial p_l}+S_l(p_l)\frac{\partial \rho_l(p_l)}{\partial p_l}+[1-S_l(p_l)]\frac{\partial \theta_g^w(p_l)}{\partial p_l}\right)\frac{\partial p_l}{\partial t}}_{\text{time change in water content in gas and liquid phase}}-\nabla\cdot\left(\left[\underbrace{\frac{kk_r\rho_l(p_l)}{\mu}}_{\substack{\text{advective flux of}\\ \text{liquid water}}}+\underbrace{\left(nS_gD_g^w\right)\left(\frac{\partial\theta_g^w}{\partial p_l}-\frac{\theta_g^w}{\rho_g}\frac{\partial\rho_g}{\partial p_l}\right)}_{\text{diffusive flux of water vapour}}\right]\nabla p_l\right)=0$$

θ_g^w …mass content of gas
ρ_g …gas density
D_g^w …diffusion coefficient
S_g … degree of saturation (gas phase)

– used Comsol interfaces: **Richards' equation** (mass balance in liquid phase) and **General form PDE** (for problems with water vapour)
– models follow up on problems solved by diffusion equation with nonlinear diffusivity [2], [3] (corresponding approach) in Ansys [1]

– 2D axisymmetric model test case:

- mass balance approach corresponds with results of Richards' eq. interface (**Figure 2.**)
- the obvious influence of water vapour (**Figure 4.**)

Material properties

	P$_0$ [MPa]	λ [1]	k [m^2]	n [1]	μ [Pa·s]
Bentonite	9.23	0.3	$9.5\cdot10^{-21}$	0.438	10^{-3}
Rock	1.74	0.6	$9.0\cdot10^{-22}$	0.003	10^{-3}
Fracture	1.74	0.6	$2.5\cdot10^{-15}$	0.003	10^{-3}

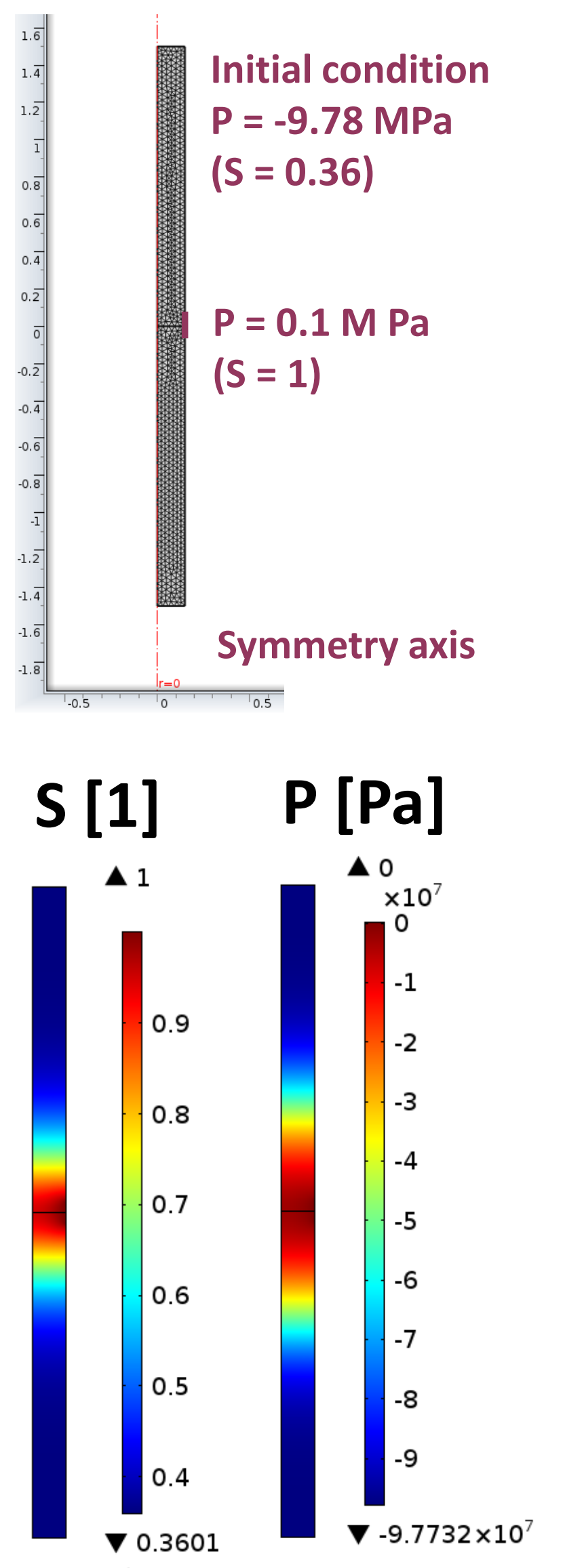

Figure 3. Distribution of degree of saturation and pressure (t = 3.17 year)

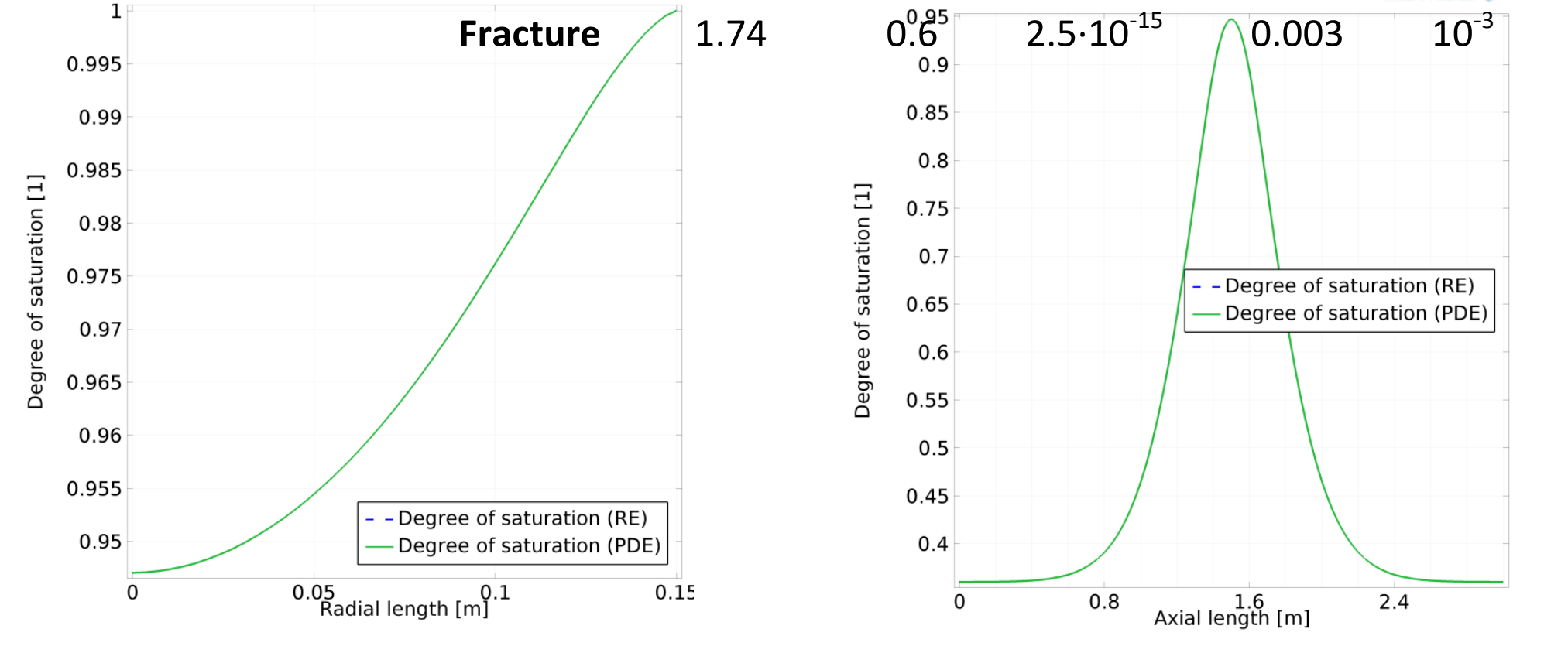

Figure 2. Radial and axial dependence of degree of saturation (t = 3.17 year) for Richards' equation interface and PDE interface **without vapour diffusion**

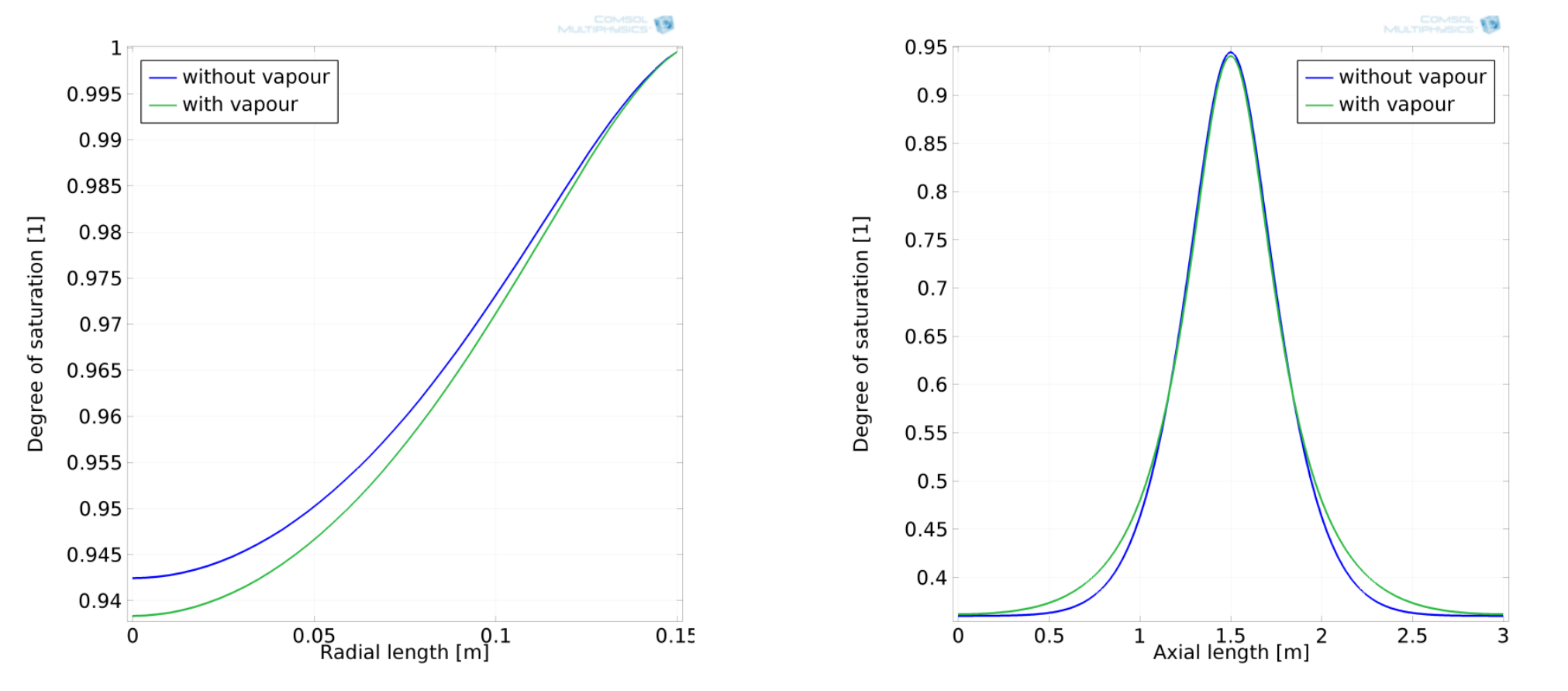

Figure 4. Radial and axial dependence of degree of saturation (t = 3.17 year) for PDE interface **without and with vapour diffusion**

2D axisym. model of borehole in the rock:

– borehole filled with bentonite with surrounding rock matrix and fracture
– initial state: saturated rock and fracture and low hydrated bentonite
– fracture with permeability which is 7 orders of magnitude lower than rock permeability
– values of material properties in the table:

	P$_0$ [MPa]	λ [1]	k [m^2]	n [1]	μ [Pa·s]
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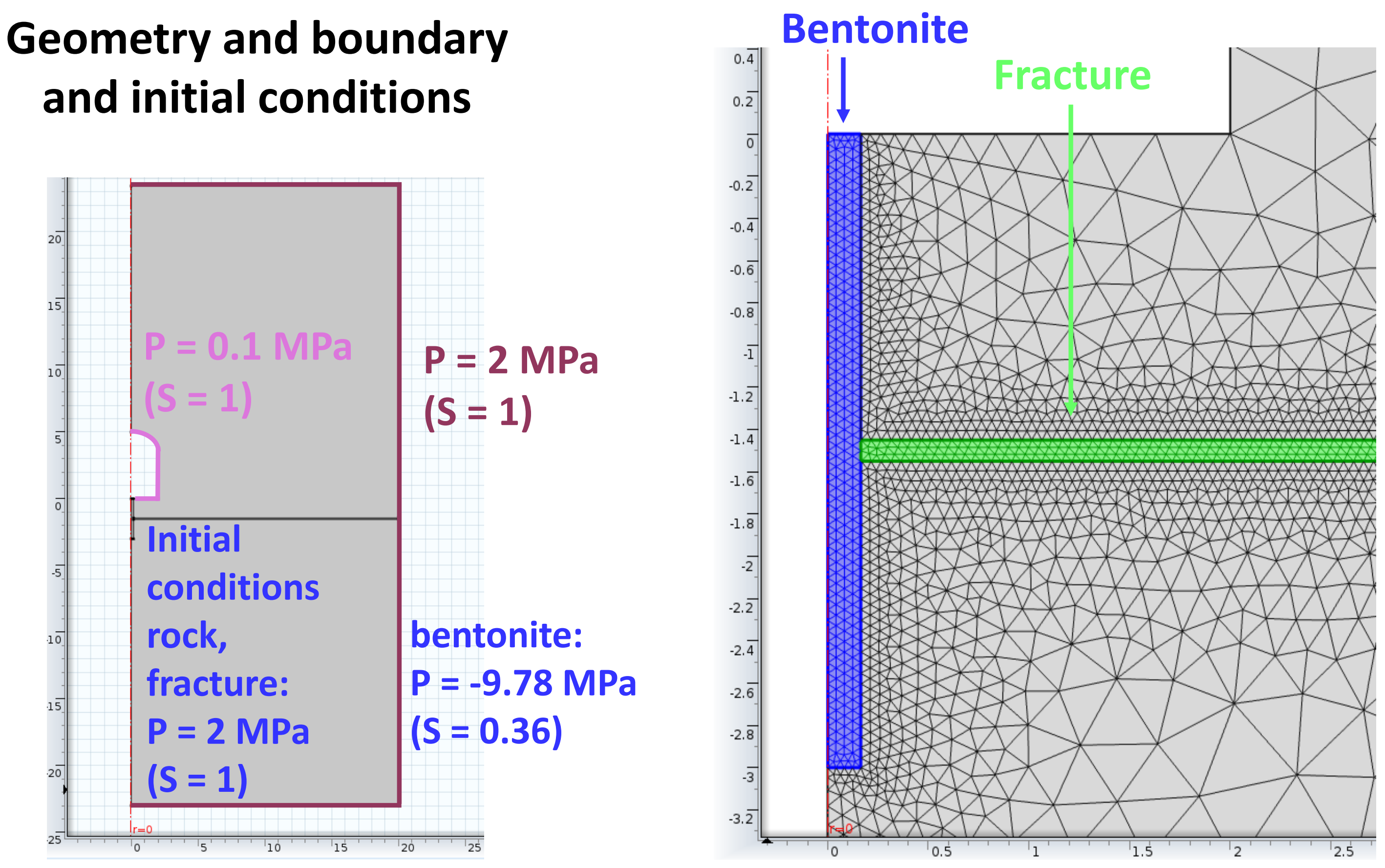
Geometry and boundary and initial conditions

Figure 5. Model geometry with schematic representation of boundary and initial conditions and detail picture of the mesh near the bottom of the tunnel and the borehole and the fracture

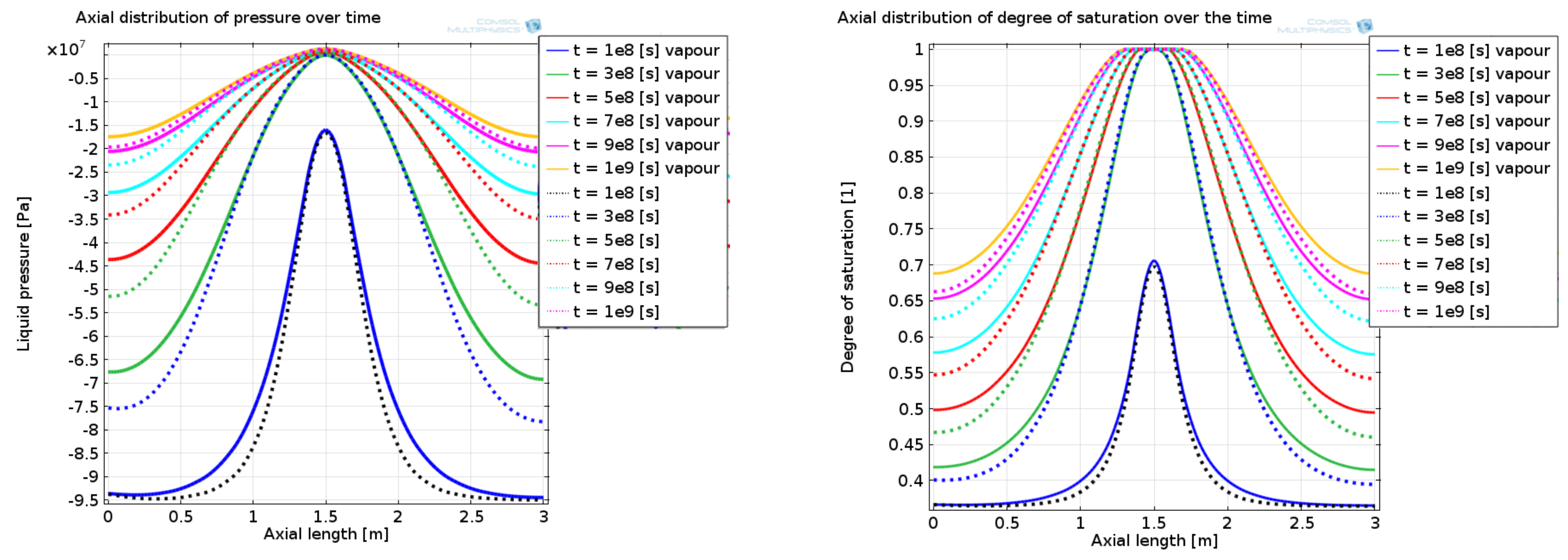

Figure 6. Axial distribution of pressure and degree of saturation over time (along borehole symmetry axis). Obvious differences between cases without and with diffusion of water vapour

Conclusions:

– identical results for Richards‘ equation interface model and model solved in General Form PDE interface according to water mass balance in liquid phase
– implementation Richards' equation with diffusion of water vapour in PDE inteface for bentonite (higher temperature in our models because diffusion of water vapour strongly depends on temperature)
– not so good convergence for 2D axisymmetric models with the surrounding rock (due to very different initial conditions, solution: slightly modificated boundary conditions)

Acknowledgments:

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