Developments in a Coupled Thermal-Hydraulic-Chemical-Geomechanical Model for Soil and Concrete

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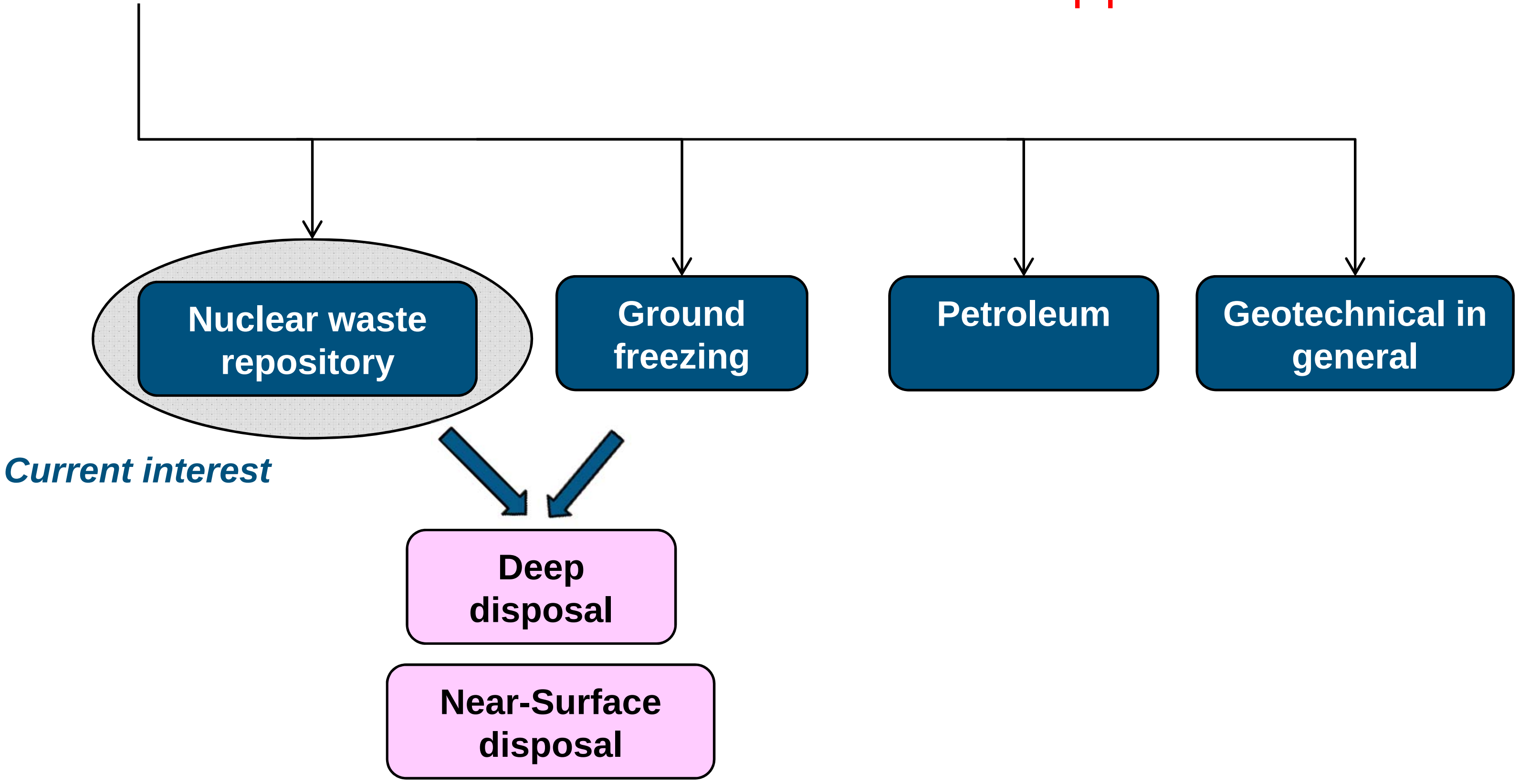
COMSOL CONFERENCE ROTTERDAM 2013

Outline

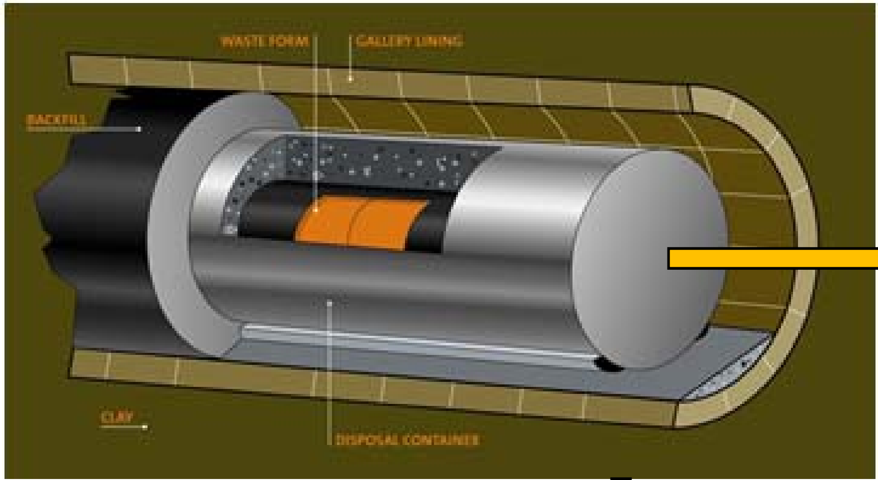
- Potential applications
- Objective
- Governing equations
- COMSOL-MATLAB
- Sample Benchmarks
- Conclusions and perspectives

Potential applications

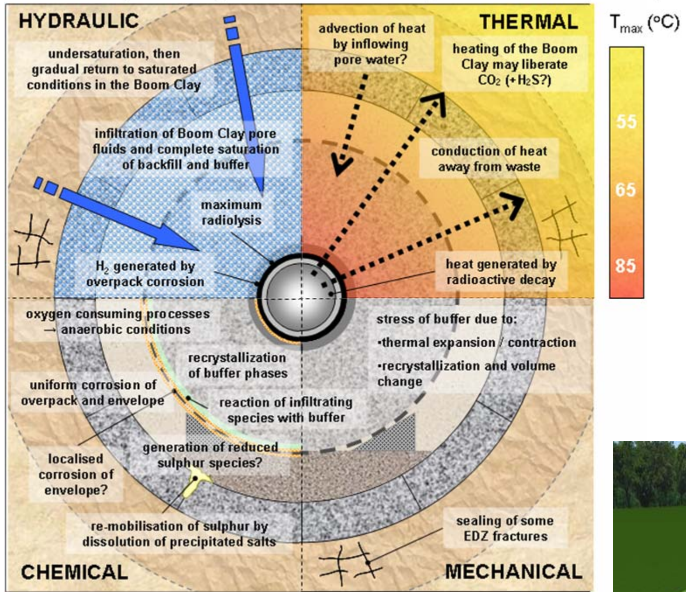
- Significant experimental and numerical research on coupled **THCM** behaviour for soil and concrete applications.



Potential applications…

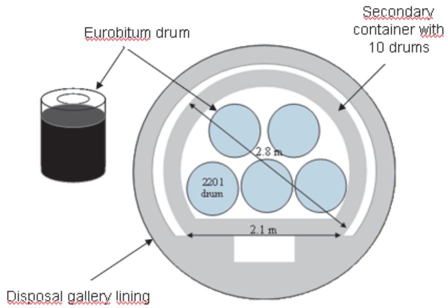


T_0 to T_{+20} (Closure, resaturation and peak thermal phase)



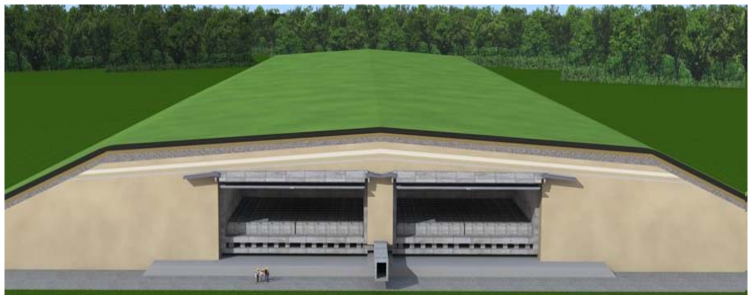
Initially perforated envelope

THCM:
In situ Processes in deep disposal repository in Boom Clay



CHM:
Impact of bitumen waste on Boom clay

THM
Design phase - Half scale test - Supercontainer



H, CM , CH:
Near surface disposal concept based on concrete as predominant material

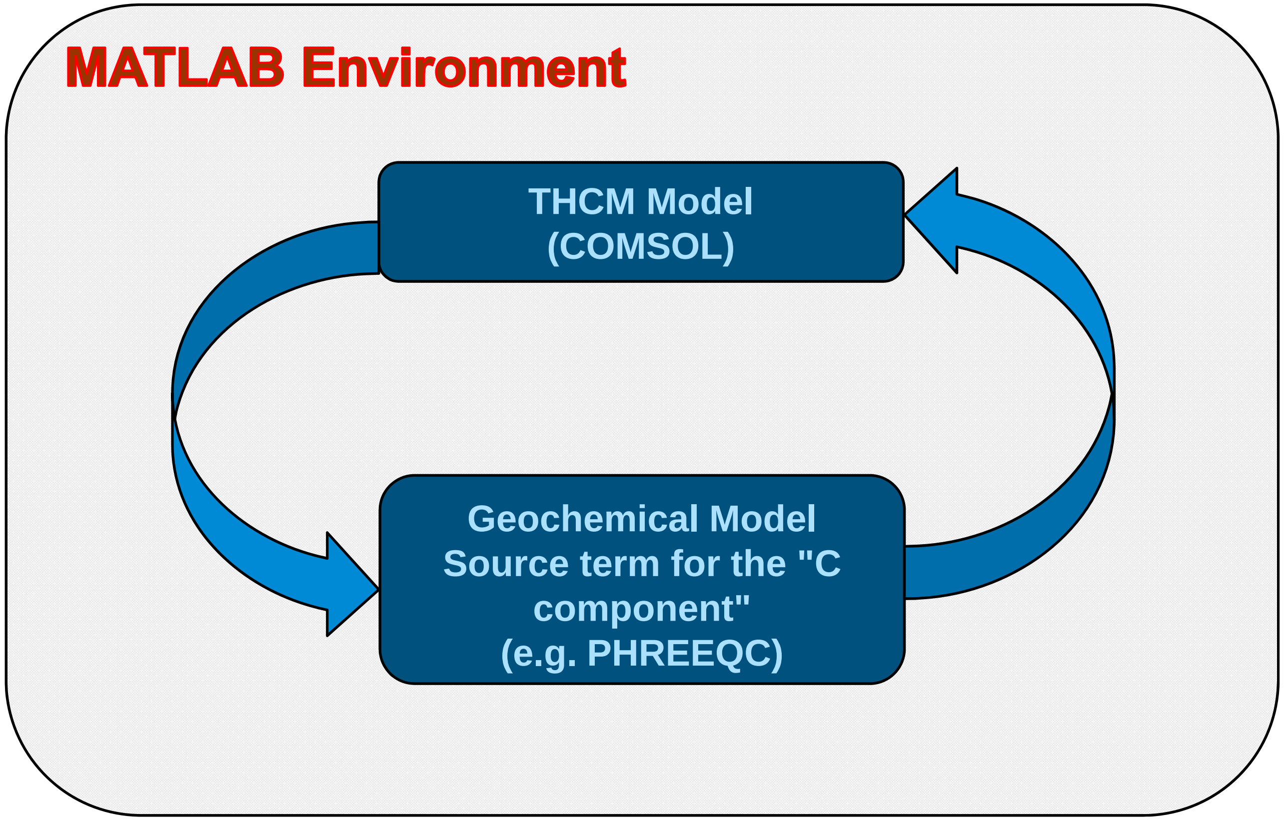
http://science.sckcen.be/en/Institutes_groups/EHS

Well known process interaction matrix for Porous media applications

	Temperature	Hydraulic	Chemical	Mechanical
Temperature	Conduction (Fourier's Law)	Convection	Dufour effect	Volumetric deformation
Hydraulic	Thermal osmosis	Pressure flow (Darcy's law)	Chemical osmosis	Volumetric deformation
Chemical	Soret effect	Advection	Diffusion (Fick's Law)+Reactions	Volumetric deformation
Mechanical	Thermal expansion	Swelling/Shrinkage	Swelling/Shrinkage	Stress/Strain Equilibrium

Objective

Develop a generic fully coupled THCM model within COMSOL-MATLAB environment



Governing equations

Energy conservation

THERMAL

$$\frac{\partial\left(\left((1-n)C_{ps}\rho_s + n\begin{pmatrix}C_{pl}S_l\rho_l + \\ C_{pv}S_g\rho_v + C_{pda}S_g\rho_{da}\end{pmatrix}\right)(T-T_r) + LnS_g\rho_v\right)}{\partial t} =$$

$$-\nabla\cdot(-\lambda\nabla T) + (\mathbf{v}_v\rho_l + \mathbf{v}_g\rho_v)L + \begin{pmatrix}C_{pl}\mathbf{v}_l\rho_l + C_{pv}\mathbf{v}_g\rho_v \\ + C_{pda}\mathbf{v}_g\rho_{da}\end{pmatrix}(T-T_r)$$

Mass conservation – pore water pressure

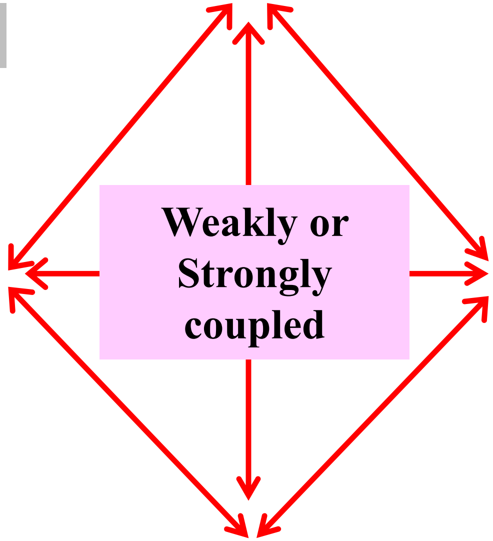
$$\frac{\partial\rho_l\theta_l}{\partial t} + \frac{\partial\rho_v\theta_g}{\partial t} = -\nabla.\rho_l\left(-K_l\left[\nabla\psi_m + \nabla\psi_0 + \nabla z\right]\right)$$
$$-\nabla.(\rho_l\mathbf{v}_v) - \nabla.(\rho_v\mathbf{v}_g)$$

HYDRAULIC

- PORE WATER
- PORE GAS

$$\frac{\partial\theta_g\rho_{da}}{\partial t} = -\nabla.\left[\rho_{da}\mathbf{v}_g - \theta_g\rho_g D_a\nabla\left(\frac{\rho_{da}}{\rho_g}\right)\right]$$

Mass conservation – pore gas pressure



Stress equilibrium

(GEO)MECHANICAL

$$\nabla.\left(\left(\mathbf{C}:(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_{\mathbf{th}} - \boldsymbol{\varepsilon}_{\mathbf{ie}})\right) - \chi P_f\mathbf{I} - P_s\mathbf{I}\right) + \mathbf{b} = 0$$

CHEMICAL

Mass conservation

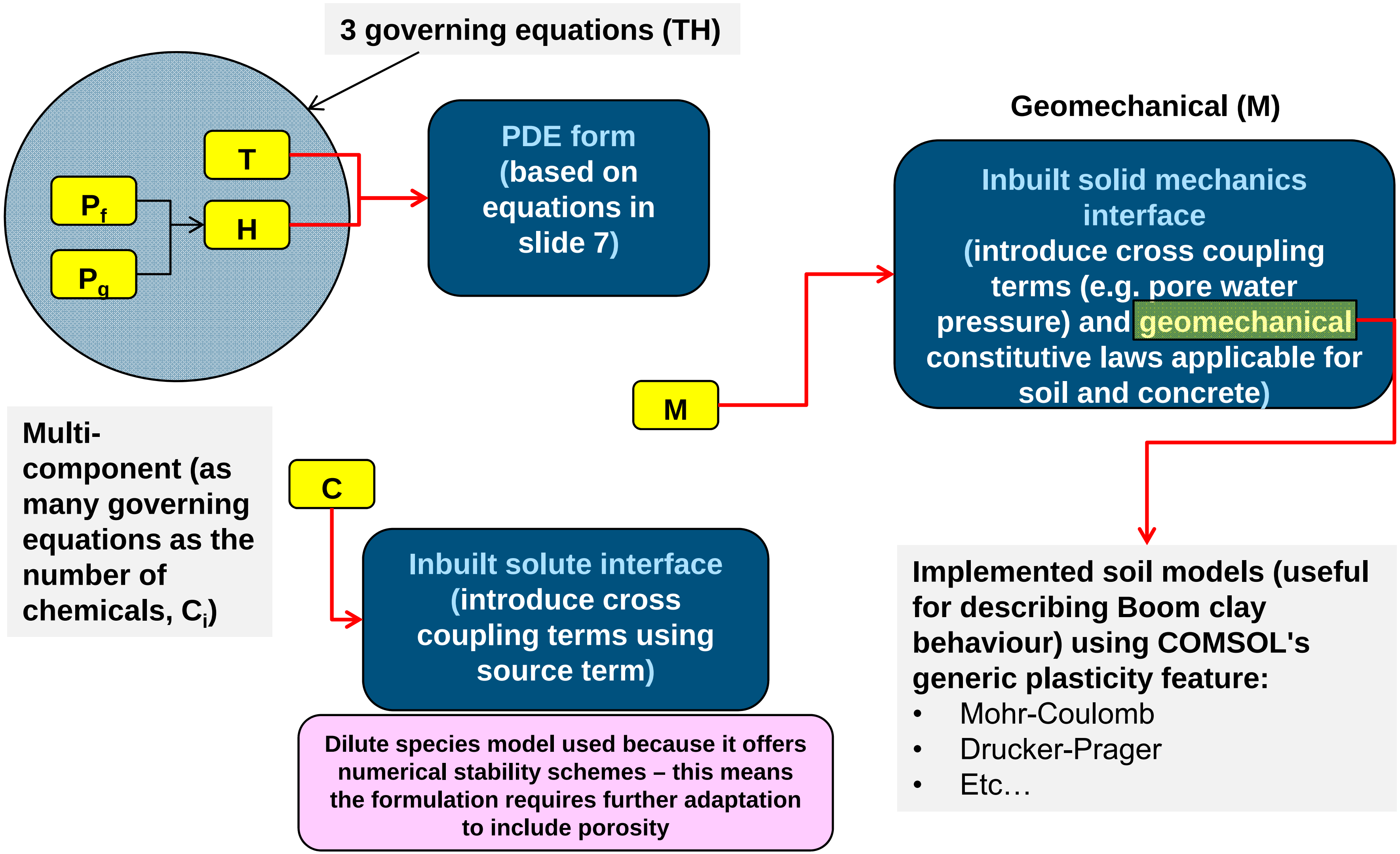
$$\frac{\partial(\theta_l c_i)}{\partial t} = -\nabla.\begin{pmatrix}D_i\nabla c_i + \frac{D_i z_i F c_i}{RT}\nabla\psi_e \\ + D_i c_i\nabla\ln\gamma_i \\ + \frac{D_i c_i\ln(\gamma_i c_i)}{T}\nabla T + c_i\mathbf{v}_l\end{pmatrix} + R_i$$

Charge conservation

ELECTROCHEMICAL

$$\nabla\cdot(\tau\theta_l\nabla\psi_e) + \frac{F\theta_l}{\varepsilon}\sum c_i z_i = 0$$

Implementation



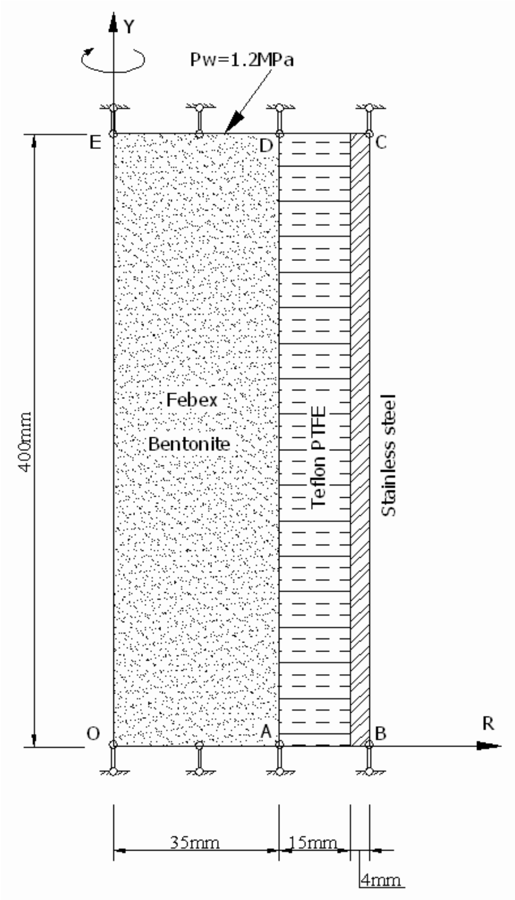
Benchmark 1

Infiltration under isothermal conditions (Hydro-mechanical coupling)

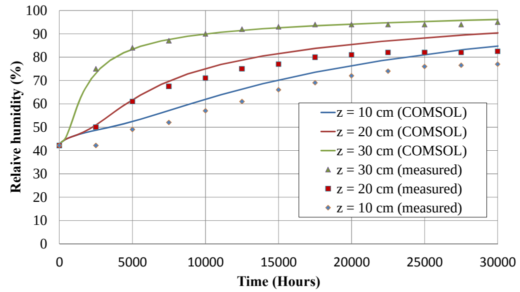
$$\frac{\partial \rho_l \theta_l}{\partial t} = -\nabla.\rho_l\left(-K_l\left[\nabla \psi_m + \nabla z\right]\right)$$

$$\nabla.\left(\left(\mathbf{C}:\boldsymbol{\varepsilon}\right) - \chi P_f \mathbf{I} - P_s \mathbf{I}\right) + \mathbf{b} = 0$$

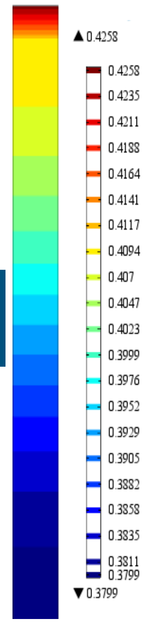
Infiltration under isothermal conditions…



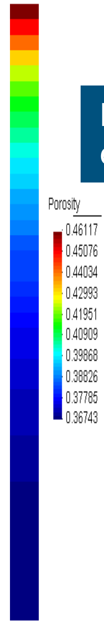
Test equipment (CIEMAT, Spain) and model idealisation for the infiltration experiment under isothermal conditions



Degree of saturation



Linear elasticity



Nonlinear elasticity

Porosity: COMSOL (left) and Chen et al. (right) – scale not same

Benchmark 2

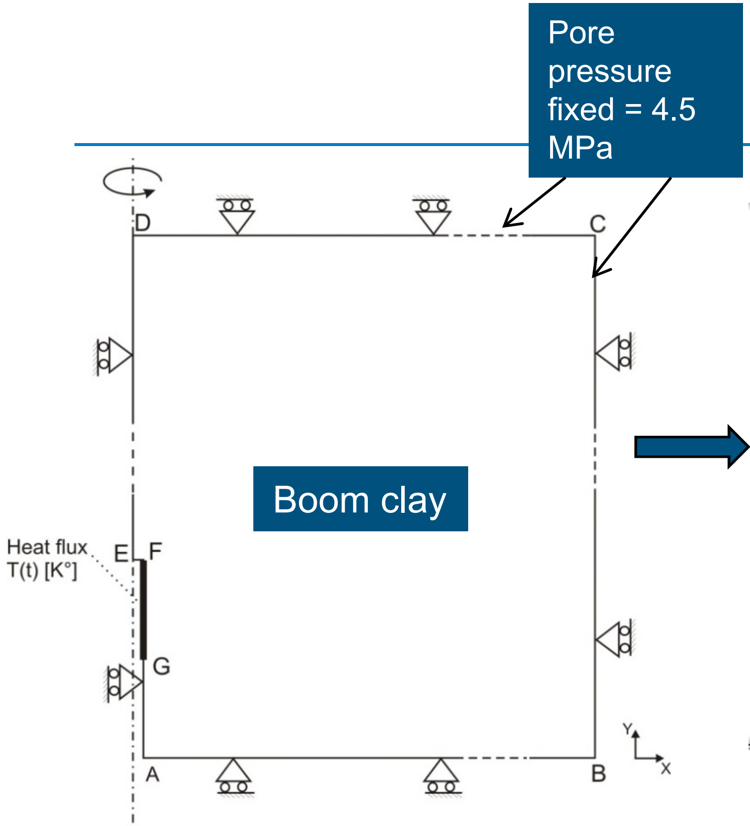
THM response of the in-situ ATLAS III Experiment

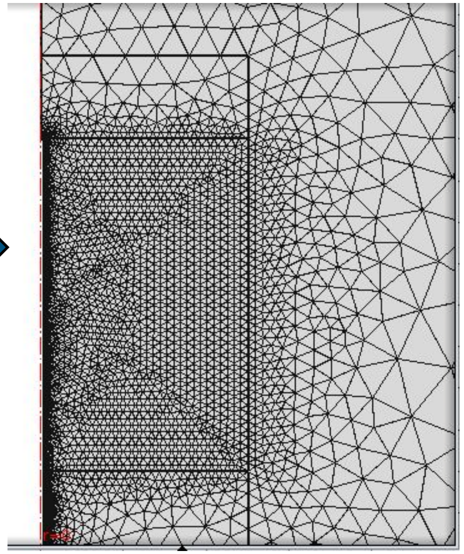
$$\frac{\partial\left(\begin{pmatrix}(1-n)C_{ps}\rho_s \\ +n\left(C_{pl}S_l\rho_l(T)\right)\end{pmatrix}(T-T_r)\right)}{\partial t} = -\nabla\cdot(-\lambda\nabla T)+\left(C_{pl}\mathbf{v_l}\rho_l\right)(T-T_r)$$

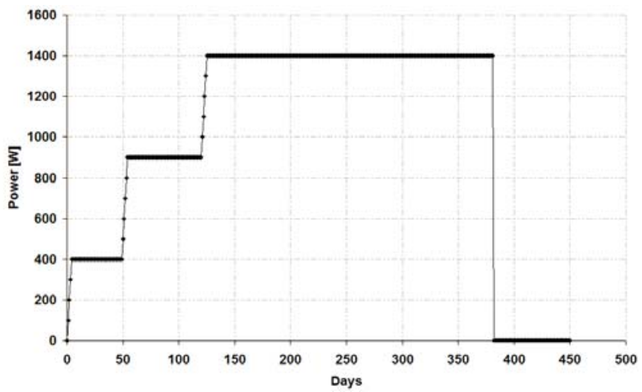
$$\frac{\partial\rho_l(T)\theta_l}{\partial t} = -\nabla.\rho_l\left(-K_l(T)\nabla\psi_m\right)$$

$$\nabla.\left(\left(\mathbf{C}:\left(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}_{\mathbf{th}}-\boldsymbol{\varepsilon}_{\mathbf{ie}}\right)\right)-P_s\mathbf{I}\right)=0$$

Conceptual model and data







Chen and Li, 2009

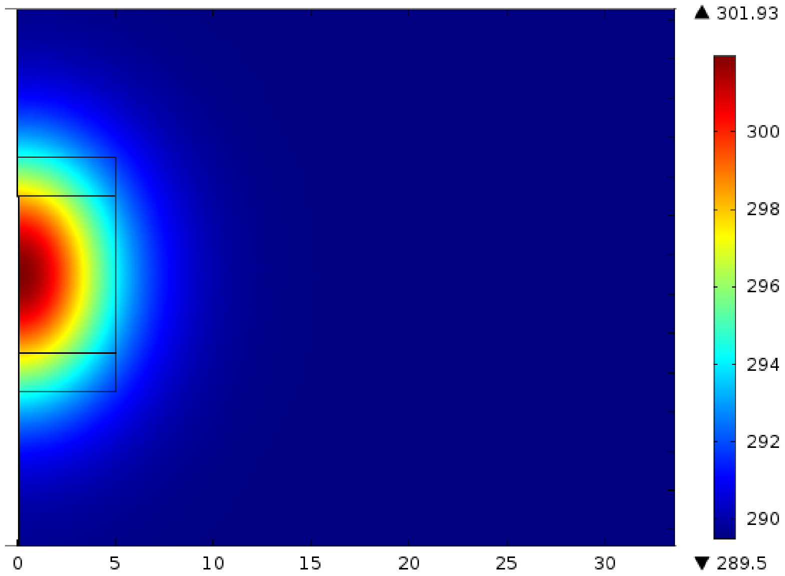
$$f \equiv J + \frac{2\sqrt{3}\sin\varphi}{3-\sin\varphi}\left(p - c\cdot ctg\varphi\right)$$

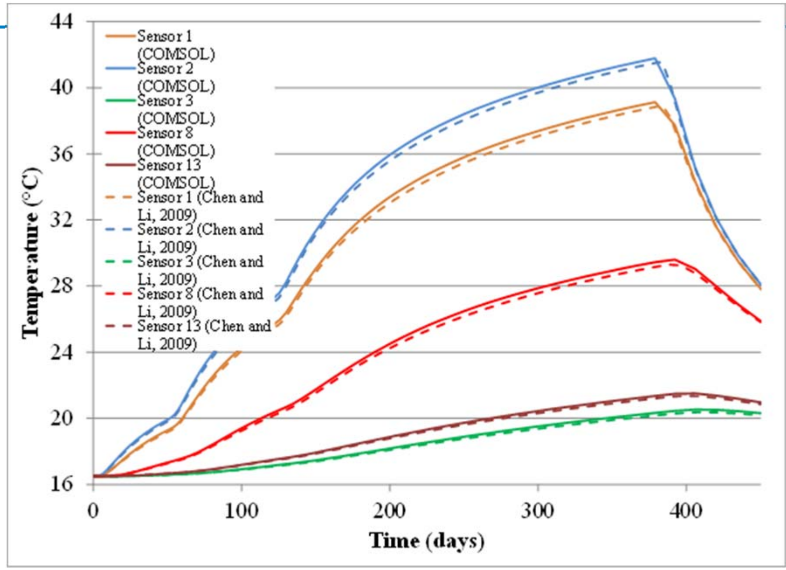
$$g \equiv J + \frac{2\sqrt{3}\sin\psi}{3-\sin\psi}\left(p - c\cdot ctg\varphi\right)$$

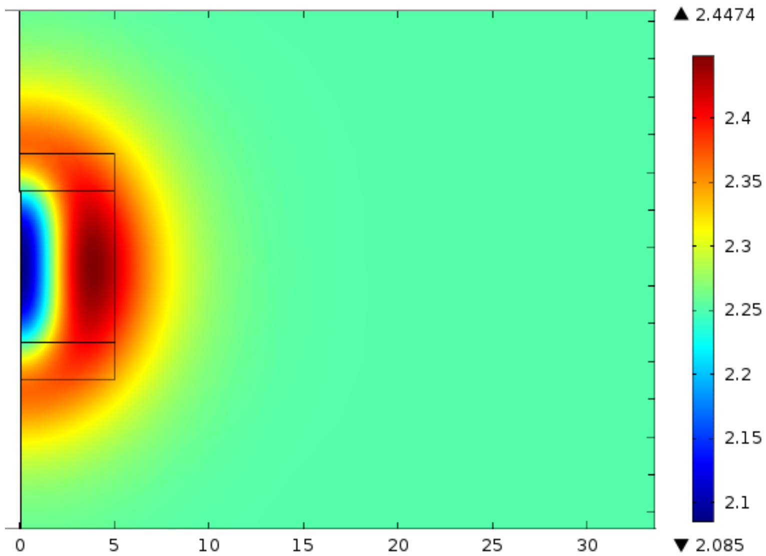
Key features:

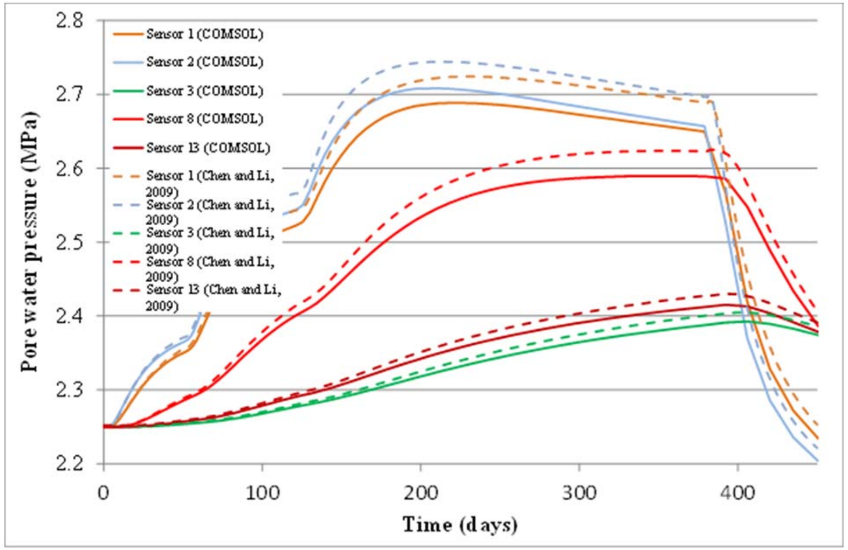
- **Fully coupled THM**
- **Axisymmetric**
- **Fully saturated**
- **Viscosity and density as a function of temperature**
- **Thermo-Elasto-plastic (Drucker Prager) model**
- **Two materials = steel + boom clay**
- **COMSOL computation time = 0.5 hours**

Temperature and pore water pressure evolution

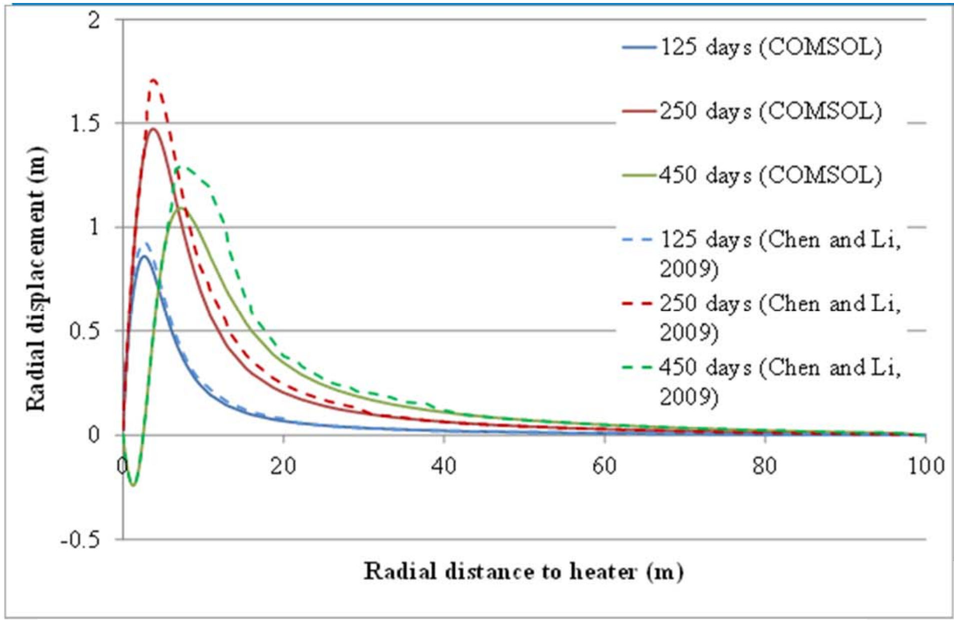


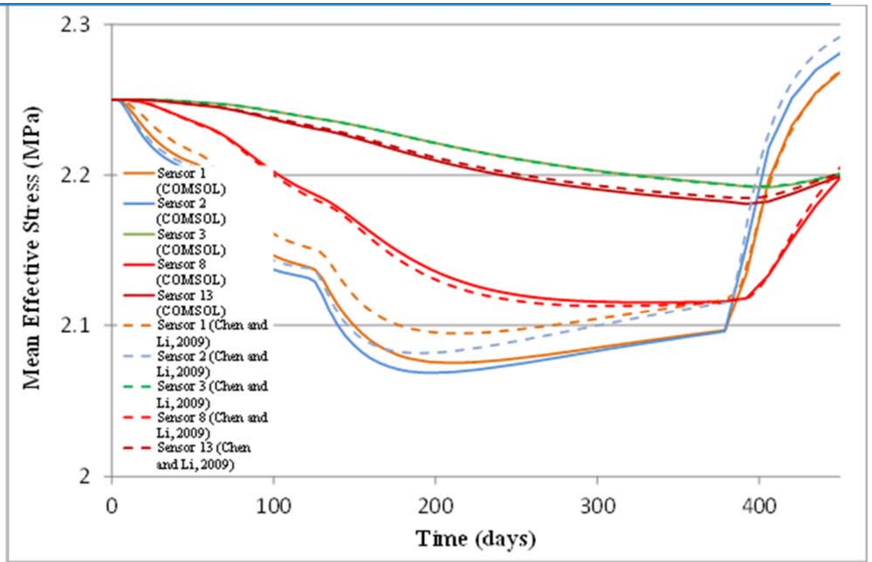


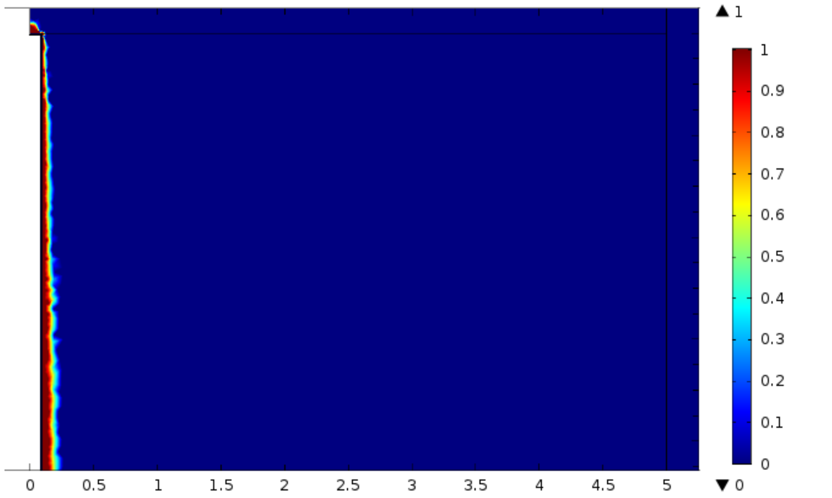




Radial displacement, mean effective stress and plastic strain







Note: Plastic region is insignificant and hence not shown (limited to few elements in the domain.

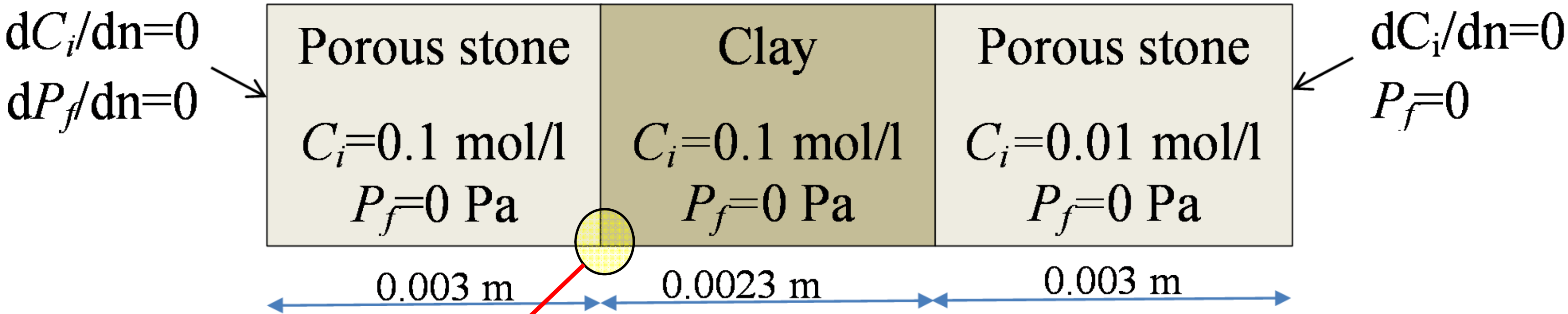
Benchmark 3

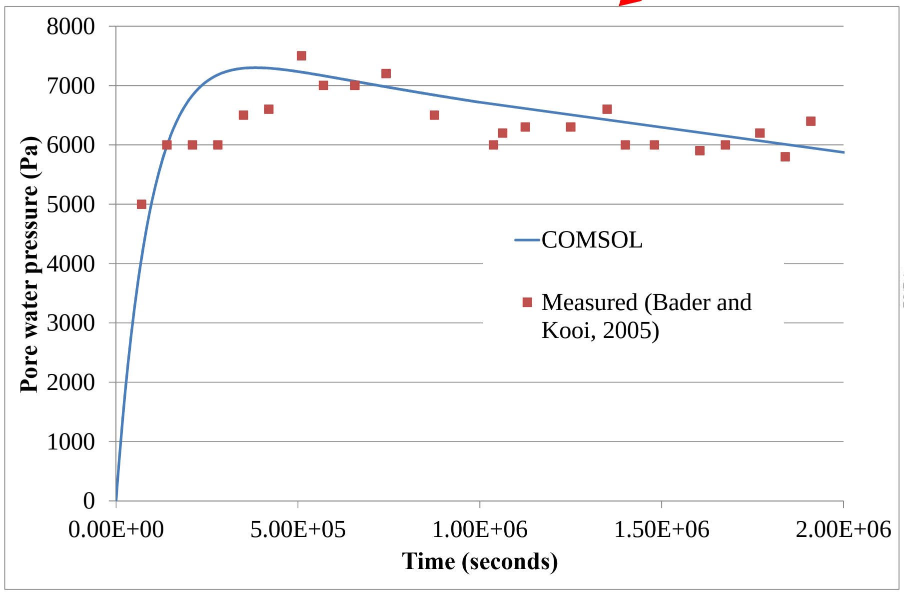
Chemo-osmotic flow

$$\frac{\partial \rho_l \theta_l}{\partial t} = -\nabla . \rho_l \left(-K_l \left[\nabla \psi_m + \nabla \psi_0 \right] \right)$$

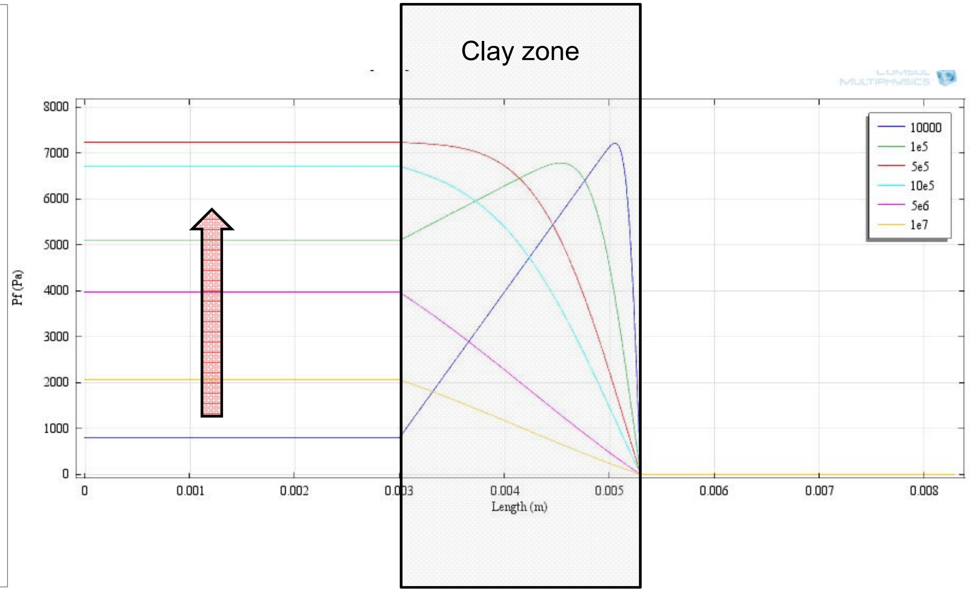
$$\frac{\partial \left(\theta_l c_i \right)}{\partial t} = -\nabla . \left(D_i \nabla c_i + c_i \mathbf{v_l} \right)$$

Keijzer's experiment





Pressure evolution at the interface between the left porous stone and the clay



Transient pressure profile

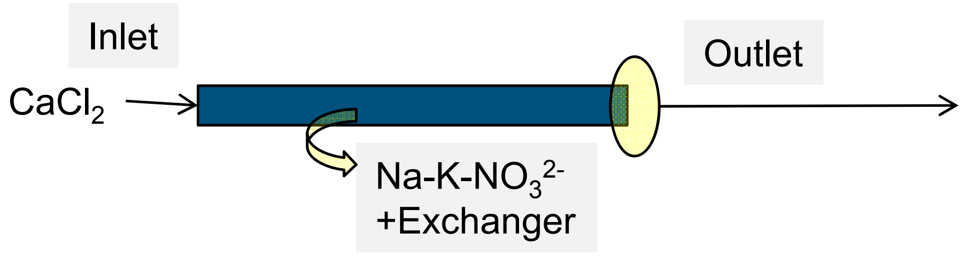
Benchmark 3

Reactive transport (COMSOL-MATLAB)

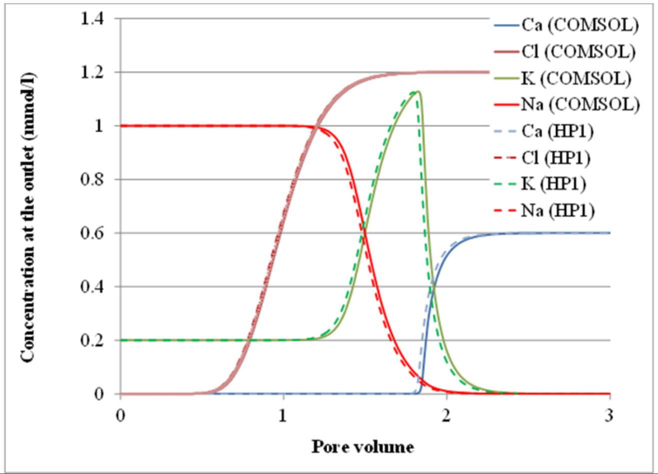
$$\frac{\partial(\theta_l c_i)}{\partial t} = -\nabla.(D_i \nabla c_i + c_i \mathbf{v_l}) + R_i$$

Phreeqc coupling via MATLAB – use sequential non-iterative approach (other approaches also tried, no difference for the specific problems chosen)

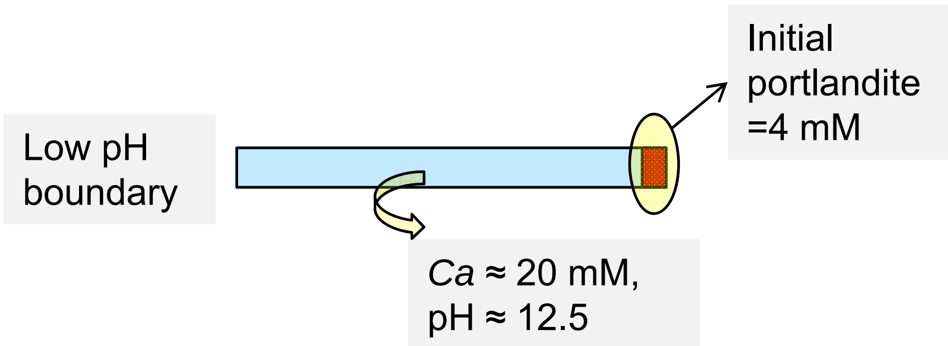
Ion exchange, Mineral dissolution verifications



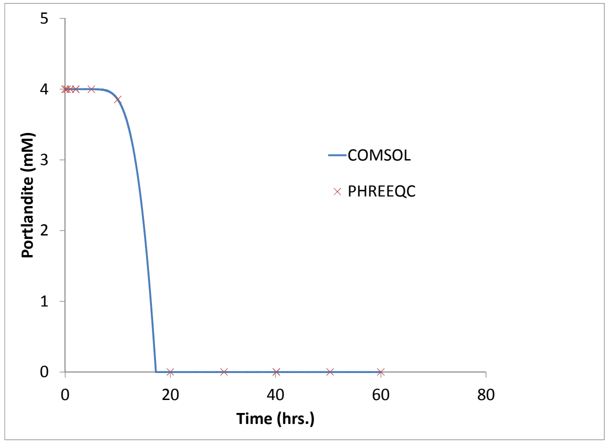
Advection-diffusion



Comparison made with open source code HP1, developed at SCK-CEN



Diffusion only



Portlandite dissolution

Input data: Patel, R.A., Perko, J., Jacques, D., De Schutter, G., Breugel, K. V., Ye, G. , 2013. A versatile pore-scale multicomponent reactive transport approach based on Lattice Boltzmann Method: Application to cementitious systems. Jour. Phy. and Chem. of the Earth (submitted)

Note: More complex chemistry successfully demonstrated in a forthcoming journal publication

Conclusions and perspectives

- Model implementation and benchmark results highly encouraging.
- Further work ongoing in terms of chemo-mechanical coupling, plus more and more verifications/validations.
- Computational constraints especially iterating between COMSOL-MATLAB. Perhaps COMSOL can consider this in future versions.
- COMSOL: easy to implement and serves as a powerful research tool.

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