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

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Abstract: This paper documents current status in the development of a coupled thermal-hydraulic-chemical-geomechanical numerical suite within COMSOL-MATLAB environment to address soil and concrete applications. The mathematical formulations are based on well-established continuum scale models unifying mass conservation, energy conservation, charge conservation, thermodynamic equilibrium and kinetics and stress equilibrium equations. In this instance, four benchmark problems have been selected which shows the ability of the coupled model to handle hydro-mechanical, thermal-hydro-mechanical, chemo-osmotic and reactive transport problems. Results have been discussed in terms of comparisons of pore water pressure, temperature, concentrations, stresses and displacements against alternative numerical codes and experiments. The results are largely encouraging and go to establish that COMSOL can serve as a powerful research tool.

Keywords: Thermal-Hydraulic-Chemical-Geomechanical, Porous media, Geochemical, Nuclear waste.

1. Introduction

In the broad context of geotechnical and geo-environmental problems, the study of coupled thermal, hydraulic, chemical, mechanical behaviour of natural soils and engineered materials has attracted tremendous interest amongst scientific community and industry (e.g. Pusch and Yong, 2005). This is especially the case in the study of feasibility, design, construction and long term performance of nuclear waste disposal facilities. From the point of view of deep disposal studies, the main research questions typically investigated are (i) saturation time, (ii) peak temperature in the near field, (iii) duration of thermal phase, (iii) geomechanical stability and (iv) chemical stability of engineered barriers and host soil together with interactions with waste matrix. Similar questions are investigated in the case of near surface disposal facility but mainly for cementitious materials under isothermal conditions, with specific attention to long term concrete degradation (e.g. Jacques et al. 2010). In order to address these, Belgian Nuclear Research Centre (SCK•CEN) has already made significant advances both in terms of laboratory and in-situ experiments such as ATLAS, PRACLAY projects, etc. at their HADES underground research laboratory (e.g. Chen et al. 2011, Li et al. 2010) and development and applications of complex multiphysics models (e.g. Jacques et al. 2006).

In this context, the paper describes current progress in the feasibility study of a generic numerical suite in COMSOL-MATLAB environment within which the coupled thermal-hydraulic-chemical-geomechanical behaviour of soil and concrete can be investigated (Figure 1).

Due to the complex coupling involved and resultant large number of parameters, coefficients, constitutive laws and internal features, a stepwise approach has been taken to verify different combinations of physics in order to gain confidence in the implementation and quality assurance.

In this paper, the presentation is limited to four benchmark problems based on previously published literatures and SCK•CEN data on an in-situ experiment.

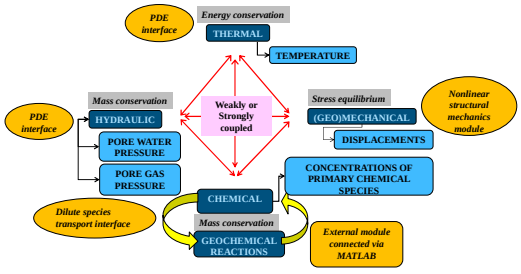

Figure 1. General approach to the coupled COMSOL-MATLAB model.

3. Governing equations

Governing equations for the coupled model are formulated in terms of primary variables: temperature (T), pore water pressure (P_l), pore gas pressure (P_g), pore water chemical concentration (c_i), electrical potential (ψ_e) and displacements (**u**). The theoretical formulation is principally adapted from the work of:

a. Thomas and He (1995) for thermal, hydraulic and mechanical behaviour.
b. Wu and Chieng (1995) for chemo-osmotic flow.
c. Cleall et al. (2006) and Seetharam et al. (2007) for reactive transport and its coupling with the THM variables.
d. Jacques and Šimůnek (2005) for coupling chemical transport with Phreeqc.
e. Seetharam (2003) and Thomas et al. (2012) for Soret effect and Samson and Marchand et al. (2007) for species dependent diffusion coefficient.

These were developed mainly in the context of unsaturated soil, exception being Samson and Marchand et al. (2007) which was for concrete.

The mechanical model and all transport equations are implemented within COMSOL. For performing geochemical equilibrium and kinetic calculations, recourse is made to IPhreeqc (Charlton and Parkhurst, 2011) via Livelink for MATLAB and using the basic MATLAB script of Wissmeier and Barry (2011) as the starting point. As noted below, a combination of in-built COMSOL modules with some modifications and PDE interfaces have been used. Due to limitation of space, not all constitutive relationships used are included in this paper but can be found in the above references and from those mentioned in Section 4. Table 1 provides description of notations.

3.1 Heat transfer (PDE interface)

The heat transfer formulation considers the standard conduction, convection and latent heat of vapourisation in the energy conservation equation as follows:

$$\frac{\partial \Omega}{\partial t} = -\nabla \cdot \mathbf{Q} \tag{1}$$

$$\Omega = H_c \left(T - T_r\right) + LnS_g\rho_v \tag{2}$$

$$H_c = \left(1-n\right)C_{ps}\rho_s + n\left(\begin{matrix} C_{pl}S_l\rho_l + \\ C_{pv}S_g\rho_v + C_{pda}S_g\rho_{da} \end{matrix}\right) \tag{3}$$

$$\mathbf{Q} = -\lambda\nabla T + \left(\mathbf{v_v}\rho_l + \mathbf{v}_g\rho_v\right)L + \left(\begin{matrix} C_{pl}\mathbf{v_l}\rho_l + C_{pv}\mathbf{v}_g\rho_v \\ +C_{pda}\mathbf{v}_g\rho_{da} \end{matrix}\right)\left(T - T_r\right) \tag{4}$$

where T_r is the reference temperature, L is the latent heat of vapourisation, n is the porosity, S is the degree of saturation, ρ is the density, C_p is the specific heat capacity, λ is the thermal conductivity and **v** is the velocity vector. Subscripts l, v, g and da stand for liquid, vapour, gas and dry air, respectively.

3.2 Moisture transfer (PDE interface)

The moisture transfer formulation combines liquid and vapour flow including osmotic flow in the mass conservation equation as follows:

$$\frac{\partial \rho_l\theta_l}{\partial t} + \frac{\partial \rho_v\theta_g}{\partial t} = -\nabla.\rho_l\mathbf{v_l} - \nabla.\left(\rho_l\mathbf{v_v}\right) - \nabla.\left(\rho_v\mathbf{v}_g\right) \tag{5}$$

$$\mathbf{v_l} = -K_l\left[\nabla\psi_m + \nabla\psi_0 + \nabla z\right] \tag{6}$$

where θ is the volumetric content of a given phase, K_l is the hydraulic conductivity, ψ_m is the matric potential, ψ_0 is the osmotic potential and z is the elevation that pertains to gravitational potential.

3.3 Dry air transfer (PDE interface)

The dry air transfer formulation considers advection, diffusion and appropriate source terms in the mass conservation equation as follows.

$$\frac{\partial \theta_g\rho_{da}}{\partial t} = -\nabla.\left[\rho_{da}\mathbf{v}_g - \theta_g\rho_g D_a\nabla\left(\frac{\rho_{da}}{\rho_g}\right)\right] \tag{7}$$

where D_a is the atmospheric diffusivity of vapour defined as a function of temperature. Note that the final form of the above equation (not shown here) is expressed in terms of total pore gas pressure, P_g.

3.4 Multicomponent chemical transport (i^{th} chemical) (Dilute species transport)

The multicomponent chemical transport formulation considers the standard advection, diffusion and reaction equation in the mass conservation equation as follows (i^{th} chemical).

$$\frac{\partial\left(\theta_l c_i\right)}{\partial t} = -\nabla.\left(\begin{array}{l} D_i\nabla c_i + \dfrac{D_i z_i F c_i}{RT}\nabla\psi_e \\ +D_i c_i \nabla \ln\gamma_i \\ +\dfrac{D_i c_i \ln\left(\gamma_i c_i\right)}{T}\nabla T + c_i \mathbf{v_l} \end{array}\right) + R_i \quad (8)$$

Additional components include gradients of temperature and electrical potential terms to account for Soret effect and species dependent diffusion coefficient both of which are more relevant for diffusion dominated problems. The reaction term, R_i, is evaluated through the external geochemical module (section 3.6). D_i is the effective diffusivity, z_i is the valence, F is Faraday's constant, R is the universal gas constant, ψ_e is the electrical potential and γ_i is the activity coefficient of primary species, c_i.

3.5 Electrical potential (Poisson's interface)

The electrical potential formulation essentially is a Poisson's equation (see Samson and Marchand, 2007)).

$$\nabla\cdot\left(\tau\theta_l\nabla\psi_e\right) + \frac{F\theta_l}{\varepsilon}\sum c_i z_i = 0 \quad (9)$$

where ε is the permittivity of the liquid phase.

3.6 Geochemical equations (external module)

The formulation is detailed in Parkhurst and Appelo (2013) and in its most basic form solves mass action, mass balance and charge balance equations for primary chemical species.

3.7 Stress-strain equilibrium (nonlinear structural mechanics)

This essentially follows a standard poroelastic model with an additional term to include the effect of swelling pressure. Plasticity and thermo-elasticity is invoked by activating the respective features within the solid mechanics interface in COMSOL.

$$\nabla.\left(\sigma - \chi P_f \mathbf{I} - P_s\mathbf{I}\right) + \mathbf{b} = 0 \quad (10)$$

where σ is the total stress, χ is the effective stress parameter attaining zero value if the medium is unsaturated and one if it is saturated, P_f is the pore water pressure, P_s is the swelling pressure defined as a function of degree of saturation (e.g. Nowak, 2007) and **b** is the body force. The above formulation needs a modification to include pore gas pressure (as in Thomas and He, 1995) when net mean stress is used as the stress state (Alonso et al. 1990).

4. Verification

Due to limitation of space, four benchmark problems have been selected in order to demonstrate a stepwise verification of the COMSOL model.

4.1 Hydro-mechanical behaviour

The purpose of this exercise is to test the model against an isothermal hydro-mechanical experiment on a swelling clay (Villar et al. 2005). This benchmark will test the model's ability to handle coupled unsaturated flow and mechanical behaviour. A 2D axi-symmetric model was used with initial and boundary conditions as described in Figure 2. Material parameters were obtained from Chen and Ledesma (2006) and Nowak (2007). Note that the Teflon and stainless steel layers were not considered and hence a no-flow boundary condition is imposed.

Figure 3 shows a comparison of relative humidity at various points in the specimen. Since water is allowed to enter the initially unsaturated specimen from the top, saturation

front progresses from the top end. This is reasonably captured by the linear swelling elastic strain model. A better match with experimental results can be achieved by considering an alternative approach such as the nonlinear elastic approach adopted by Chen and Ledesma (2006).

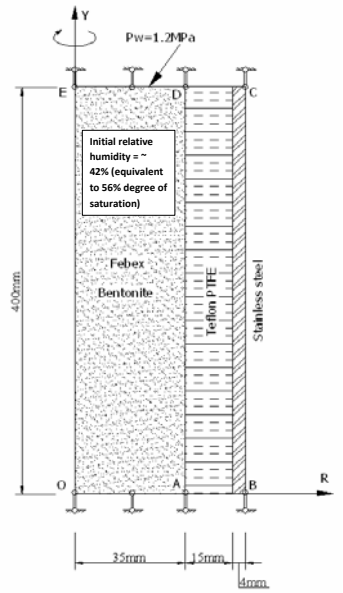

Figure 1. Model set-up for an isothermal infiltration experiment (Chen and Ledesma, 2006).

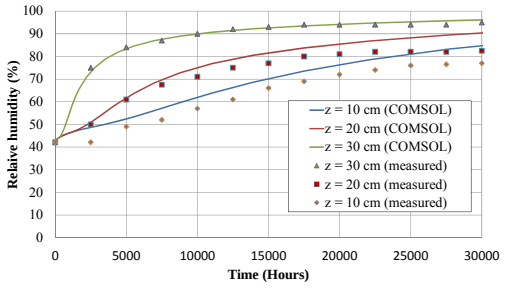

Figure 2. Comparison of relative humidity history for three observation points.

4.2 Thermo-hydro-mechanical behaviour

The purpose of this exercise is to test the thermo-hydro-mechanical component of the model. For this purpose, simulations carried out by Chen and Li (2009) on an in-situ test, ATLAS III, in the HADES underground research laboratory at Belgian Nuclear Research Centre is considered. The ATLAS III small scale in situ heating test is aimed at assessing the thermo-hydro-mechanical (THM) effects on the Boom clay due to heat-emitting wastes. The model solves for heat transfer, saturated flow and elasto-plastic mechanical behaviour. The yield surface is defined by a Drucker–Prager criterion. A non-associative elastoplastic constitutive law has been employed. Note that the second term of equation (10) which considers swelling effect is not applicable.

A 2D axisymmetric model is considered as shown in Figure 3. The initial conditions and boundary conditions are also shown. Material parameters and constitutive laws for the thermo-hydro-mechanical equation system can be found in Chen et al. (2011) and Chen and Li (2009). Note that the gravity effect is ignored. In this problem, the domain remains fully saturated at all times. The pore pressure builds up close to the heater because of temperature effect on liquid viscosity and density. The buildup of both temperature and pore pressure will affect the mechanical behaviour which is analysed in terms of stresses and displacements via an elastoplastic law.

Only limited results are presented for brevity. Figure 4, 5, 6 and 7 presents numerical comparisons between the COMSOL model and the model by Chen and Li (2009) for temperature, pore water pressure and mean effective stresses at various observation points (1.52,15; 1.32,15; 2.72,9; 2.62,15; 2.35,9.32 m) in the domain, including radial displacements along the midplane of the heater (Figure 3). As seen from the comparisons, temperature is captured very well. However, there are some noticeable differences in the pore water pressure which in turn affects mean effective stresses and displacements, especially close to the heater where the dynamics are high. Further, investigations are therefore warranted. These discrepancies may be attributed to the use of different numerical models, mesh discretization, or tolerances. Note that in this problem plasticity is not predominant and limited to a few elements in the vicinity of the heater and hence not shown. In fact, similar results can be achieved using merely thermo-elasticity.

Successful comparison of results with respect to experimental behaviour can be achieved in the COMSOL model by considering material anisotropy as suggested in Chen et al. (2011).

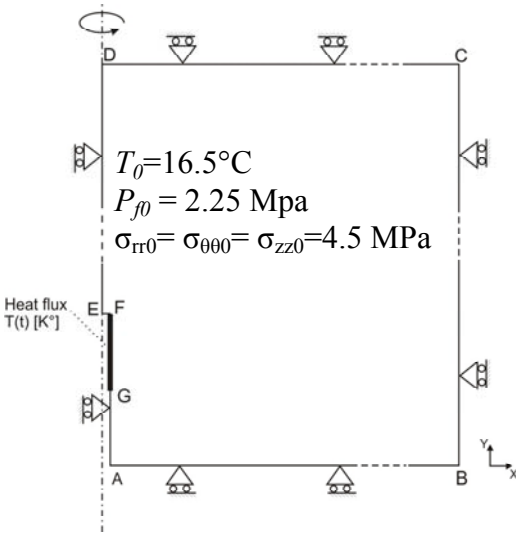

Figure 3. 2D axisymmetric model (Chen and Li, 2009).

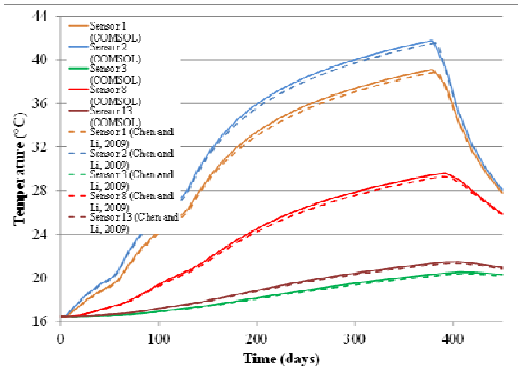

Figure 4. Temperature evolution with time at various observation points.

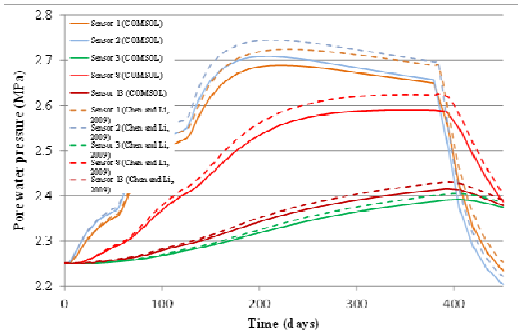

Figure 5. Pore water pressure evolution with time at various observation points.

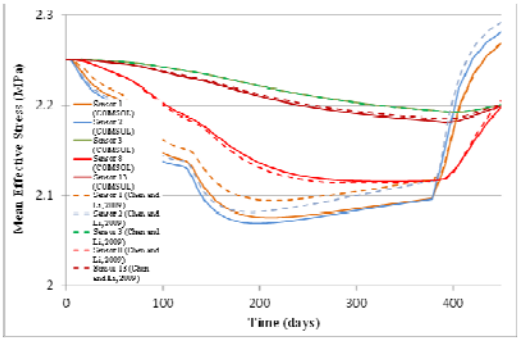

Figure 6. Mean effective stress evolution with time at various observation points.

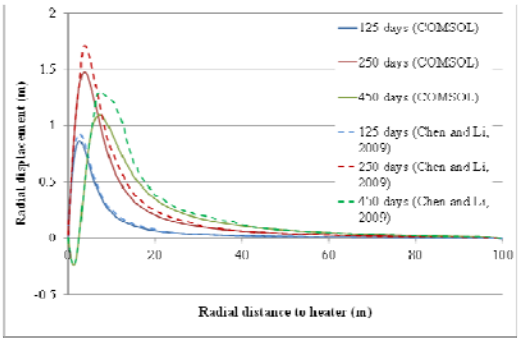

Figure 7. Radial displacements at the midplane of the heater after 125, 250 and 400 days.

4.3 Chemo-osmotic behaviour

The purpose of this exercise is to test the chemo-osmotic component of the model. This means only relevant terms of equation (5) and (8) are invoked. For this purpose, an experiment on semi-permeable behaviour of naturally occurring clay is considered (Bader and Kooi, 2005). The material was subjected to a salt gradient as shown in Figure 8. A buildup of pressure at one side of the membrane followed by an eventual decrease was seen in the experiment.

The model set up including initial conditions and boundary conditions are shown in Figure 8. Material parameters were obtained from Bader and Kooi (2005). Although this is a 1D problem, it is solved as a quasi 2D problem. The COMSOL model shows good correspondence with the measured pore water pressure at the left interface of porous stone and clay as shown in Figure 9. It shows an increase and subsequent decrease of pressure due to osmosis and diffusion. Note that the parameters used were

calibrated by Bader and Kooi (2005) and hence this is strictly not a validation.

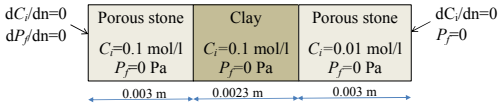

Figure 8. Modelling domain, initial and boundary conditions for Keijzer experiment (adapted from Bader and Kooi, 2005).

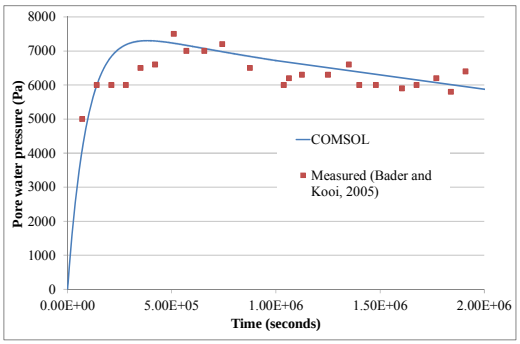

Figure 9. Comparison of measured and simulated pore water pressure at the interface.

4.4 Reactive transport

The purpose of this step is to verify reactive transport component (COMSOL-IPhreeqc) of the model. For this purpose, a well-known example of transport and ion exchange from Parkhurst et al. (2013) is considered, which nicely demonstrates chromatographic pattern between Na and K. Comparisons are made against an in-house code, HP1 (coupled HYDRUS-Phreeqc by Jacques and Šimůnek, 2005). Note that this verification is just one aspect of geochemical reactions and hence does not constitute a complete verification of the coupling.

Initially, a column (0.08 m) contains a Na-K-NO_3^{2-} solution in equilibrium with an exchanger. The column is flushed with three pore volumes (24 cm/day) of $CaCl_2$ solution. Ca, K, and Na react to equilibrium with the exchanger. Further details can be found in Parkhurst et al. (2013) (Example 11 therein).

Figure 11 shows comparisons of various ions between the COMSOL model and HP1 at the outlet of the domain (0.08 m). It is seen that there is good agreement between the two codes (including Phreeqc, results not shown). Chloride behaves as a conservative solute. The Na and K demonstrate expected chromatographic pattern. Ca reaches steady state concentration (equal to inlet concentration) after 2 pore volumes when there are no more exchangers left.

Further verifications have also been carried out at SCK•CEN on mineral precipitation/dissolution reactions, including complex cement chemistry using COMSOL-PHREEQC framework to solve decalcification of cracked concrete (not shown here).

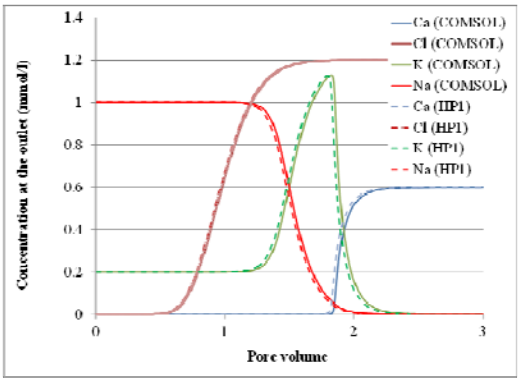

Figure 11. . Results of advective-dispersive transport simulations of the replacement of sodium and potassium on a cation exchanger by infilling calcium chloride solution.

7. Conclusions

This paper primarily discussed implementation aspects and verification of a coupled thermal-hydraulic-chemical-mechanical model in the context of porous media such as soil and concrete. The latest version of COMSOL provides a robust platform allowing the implementation of complex multiphysics formulations with great ease and thus serves as a powerful research tool. The maximum computational time was only required for benchmark 2 calculations (section 4.2) but even that took less than half hour. Constraints were faced primarily in the implementation of plasticity models which require more than one yield surface, typically seen in some state of the art mechanical models for soil and concrete.

8. References

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9. Acknowledgements

Scientific inputs from Dr. Chen Guangjing, EURIDICE, SCK•CEN, concerning benchmark problems is gratefully acknowledged.