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Multiphysics Modelling of the Behaviour of Cemented Tailings Backfill Materials

Liang Cui, Mamadou Fall
University of Ottawa, Department of Civil Engineering
161 Louis Pasteur, Ottawa, Ontario, Canada K1N 6N5
lcui090@uottawa.ca; mfall@uottawa.ca

Abstract– After the placement of cemented tailings backfill (CTB) into a stope (i.e., mined-out underground space), multiphysics interactions including thermal, hydraulic, mechanical and chemical processes, occur immediately within the mass of the backfill. The evolution of the material properties and performance of the CTB is dominated by these coupling processes. In order to quantitatively assess the influence of the coupled multiphysics phenomena on CTB behaviours, a fully coupled thermo-hydro-mechano-chemical (THMC) model is developed in this paper. For the chemical process, the THMC model fully considers the influence of binder hydration on the evolution of the CTB properties (e.g., cohesion, internal friction and dilation angles, thermal conductivity and coefficient of permeability). Hence, compared with common geomaterials (e.g., soil and rock), the material properties of CTB become functions of the degree of binder hydration. For the mechanical process, the chemical shrinkage induced by binder hydration and thermal expansion caused by the temperature gradient are taken into account. Moreover, an evolutive elasto-plastic model is incorporated into the strain analysis of the CTB structure. For the hydraulic process, the effective degree of saturation is utilized to define the hydraulic properties and capillary pressure. For the thermal process, the heat released by binder hydration is characterized as a heat source term in the energy balance equation. Laboratory and field case studies that concern the validation of the proposed THMC model are then presented and discussed in this study. There is good agreement between the modelling results and experimental data, which confirms the capability of the developed model to well capture the evolution of the CTB properties and behaviours of the CTB which are controlled by the fully coupled multiphysics phenomena that occur within a CTB structure.

***Keywords*:** Cemented tailings backfill, Multiphysics modelling, Coupling processes, THMC

1. Introduction

Backfilling with the use of cemented tailings is becoming a standard practice around the world (Fall and Nasir, 2009; Ghirian and Fall, 2014). Cemented tailings backfill (CTB) is an engineering mixture of total mill tailings, additives (e.g., Portland cement, blast furnace fly ash and slag), and water. After placement into a stope, the CTB not only provides support for the adjacent stopes, but also ensures high resource recovery as less ore is left behind in the pillars.

Once prepared and placed, the performance of a CTB structure is controlled by complex coupled multiphysics, including thermal (T), hydraulic (H), mechanical (M) and chemical (C) (THMC) processes. Specifically, as the binder hydration reaction proceeds, the pore water will be consumed by the binder hydration, which contributes to the dissipation of excess pore water pressure (PWP). Correspondingly, the porous medium will gradually change from a saturated to an unsaturated condition, which can result in increased effective stress in the CTB. In addition, the temperature of the surrounding rocks naturally increases with depth due to the influence of the geothermal gradient. The external temperature will directly affect the rate of binder hydration, and cause mechanical deformations through thermal expansion. Moreover, the CTB structure can also experience mechanical deformation under gravity, and shrinkage strain induced by the binder hydration. Hence, the performance of a CTB structure is controlled by complex coupled multiphysics, including THMC processes.

In order to quantitatively assess the influences of highly coupled THMC processes on CTB performance, a fully coupled THMC model needs to be developed. After a literature review, it is observed that previous studies (e.g. Fall et al., 2005; Nasir and Fall, 2008; Fall and Nasir, 2009; Fall et al., 2010; Thompson et al., 2012; Ghirian and Fall, 2013, 2014) have made tremendous progress in understanding the interaction between coupled processes in multiphysics phenomena with the use of both experimental analyses and field measurements. For the numerical modelling of the coupling process within the CTB mass, several partially coupled numerical models have been developed, such as the thermo-chemo-mechanical (TCM) model proposed by Fall and Nasir (2009), thermo-hydro-chemical (THC) model developed by Wu et al. (2014), and the hydro-chemo-mechanical (HCM) model established by Helinski et al. (2007). However, at the time of writing, no THMC model is available for CTB. Hence, the objective of the study is to develop a fully coupled multiphysics model to predict the THMC behaviour of CTB.

2. Multiphysics modelling of CTB

2. 1. Conservation equations

The developed THMC model consists of four conservation equations, which are the (i) water mass balance, (ii) air mass balance, (iii) energy conservation, and (iv) momentum conservation (i.e., mechanical equilibrium) equations.

$$\phi S\frac{\partial \rho_w}{\partial t}+\phi\rho_w\frac{\partial S}{\partial t}+S\rho_w\left[\frac{\partial \varepsilon_v}{\partial t}+\frac{(1-\phi)}{\rho_s}\frac{\partial \rho_s}{\partial t}\right]-\phi S\dot{m}_{hydr}\left(\frac{\rho_w}{\rho_s}S-1\right)=-\nabla\cdot\left(\phi S\rho_w\mathbf{v}^{rw}\right) \tag{1}$$

$$\phi(1-S)\frac{\partial \rho_a}{\partial t}-\phi\rho_a\frac{\partial S}{\partial t}+(1-S)\rho_a\left[\frac{(1-\phi)}{\rho_s}\frac{\partial \rho_s}{\partial t}+\frac{\partial \varepsilon_v}{\partial t}-\frac{\phi S}{\rho_s}\dot{m}_{hydr}\right]=-\nabla\cdot\phi(1-S)\rho_a\mathbf{v}^{ra} \tag{2}$$

$$\left[(1-\phi)\rho_s C_s+\phi S\rho_w C_w+\phi(1-S)\rho_a C_a\right]\frac{\partial T}{\partial t}+Q_{cd}+Q_{ad}=Q_{hydr} \tag{3}$$

$$\nabla\cdot\left(\frac{\partial \boldsymbol{\sigma}}{\partial t}\right)+\frac{\partial\left[(1-\phi)\rho_s+\phi S\rho_w+\phi(1-S)\rho_a\right]}{\partial t}\mathbf{g}=0 \tag{4}$$

Where ρ_i is the density (i refers to air, water and solid) , ϕ is the porosity, S is the degree of saturation of the liquid phase, $\dot{m}_{hydr}$ refers to the mass source term induced by binder hydration, $\mathbf{v}^{ri}$ denotes the phase velocity with respect to the fixed spatial axes, Q_{cd} , Q_{ad} and Q_{hydr} respectively represent the heat gained by conduction, advection and heat generation by an exothermic chemical reaction (binder hydration), C_i is the specific heat capacity, $\boldsymbol{\sigma}$ is the (macroscopic) total stress tensor, and $\mathbf{g}$ is the acceleration of gravity.

2. 2. Constitutive relations

In order to solve the balance equations that govern the highly interactive multiphysics, the corresponding constitutive relations are required. It should be noted that, as mentioned in Section 1, binder hydration plays a critical role in terms of affecting both the CTB behaviours and properties. Therefore, a quantitative evaluation of the extent of the binder hydration ξ is a prerequisite to determining its influence. In the present study, the prediction model proposed by Schindler and Folliard (2003) is adopted:

$$\xi=\left(\frac{1.031\cdot w/c}{0.194+w/c}+0.5\cdot X_{FA}+0.30\cdot X_{slag}\right)\cdot\exp\left\{-\left\{\tau\Big/\left\{\int_0^t\exp\left[-\frac{E_a}{R}\left(\frac{1}{T_c}-\frac{1}{T_r}\right)\right]dt\right\}\right\}^{\beta}\right\} \tag{5}$$

Where τ is the hydration time parameter (hours), β represents the hydration shape parameter, t_e is the equivalent age at the reference temperature T_r, T_c is the temperature of the CTB, E_a is the activation energy (J/mol), R is a natural gas constant (8.314 J/mol/K), w/c is the water-cement ratio, X_{FA} and X_{slag} respectively represent the weight fraction of fly ash and blast furnace slag with respect to the total weight of the binder.

To characterize the chemical and plastic strains in terms of the mechanical process, which govern the hardening/softening behaviour of CTB, an evolutive mechanical model proposed by the authors (2015b) is adopted in this study. The yield and corresponding plastic potential functions are written as:

$$F(I_1,\sqrt{J_2},\xi,\kappa)=\alpha(\xi,\kappa)\left[I_1+C(\xi)\right]+\sqrt{J_2}=0 \tag{6}$$

$$G=\frac{2\sin\psi(\xi)}{\sqrt{3}\left[3+\sin\psi(\xi)\right]}I_1+\sqrt{J_2} \tag{7}$$

Where I_1 and $\sqrt{J_2}$ represent the first stress invariant and equivalent deviatoric stress, respectively, $\alpha(\xi,\kappa)$ and $C(\xi)$ are the material parameters and control the chemo-plastic strain hardening/softening behaviour, κ is the effective plastic strain and ψ is the dilation angle. For detailed information on determining the mechanical properties, such as cohesion, internal friction angle, elastic modulus and dilation angle, see Cui and Fall (2015b).

Apart from pure mechanical elastic and plastic strain components, thermal expansion and chemical shrinkage are also taken into consideration in this study. The key parameters which determine the thermal expansion and chemical shrinkage are the coefficient of thermal expansion (CTE), α_T, and chemical shrinkage coefficient (CSC), α_{ch}. The CSC α_{ch} and CTE α_T can be derived based on previous work by Powers and Brownyard (1946) and Neville and Brooks (1987).

$$\alpha_{ch}=\frac{\left(2v_w-v_n-v_{ab-w}\right)R_{n-w/hc}}{(w/c)v_w+v_c+\left(1/C_m-1\right)v_{tailings}} \tag{8}$$

$$a_T=a_p-\frac{2v_t\left(1/C_m-1\right)\left(a_p-a_t\right)}{2v_t\left(1/C_m-1\right)+\left[(w/c)v_w+v_c\right]\left\{1+\left[L_1\cdot(1-\phi_h)^{L_2}\right]/E_t\right\}} \tag{9}$$

Where $R_{n-w/hc}$ is the mass ratio of chemically consumed water and hydrated cement, v is the specific volume, C_m is the binder content, ϕ_h is the porosity, a_t and a_p are the CTE of the tailings and CTB paste, and E_t is the elasticity of the tailings. Details on the derivation of the relevant parameters listed above is presented in Cui and Fall (2015a).

For the hydraulic process, Darcy's law is utilized to describe the fluid flow within the CTB medium. The key parameter required to calculate the fluid velocity is the saturated hydraulic conductivity. Based on the experimental data reported by Ghirian and Fall (2013), the coefficient of permeability can be expressed as:

$$K = K_T \exp\left(C_1 \xi^{C_2}\right) \tag{10}$$

Where K_T is the coefficient of the permeability of the tailings, and C_1 and C_2 are the fitting parameters.

The relation between water content and pore-water pressure is usually presented with a water retention curve (WRC). In this study, the van Genuchten model (1980) is used to characterize the WRC of the CTB:

$$\theta = \theta_r + \left(\theta_s - \theta_r\right) \Big/ \left[1 + \left(\alpha P_c\right)^n\right]^m \tag{11}$$

Where α, m and n are the fitting parameters and can be related to the degree of binder hydration by using the WRC data of the CTB.

Moreover, there is a sink term, $\dot{m}_{hydr}$, in the water mass balance equation and a heat source term, Q_{hydr}, in the energy balance equation. Based on previous research by Schindler and Folliard (2003) and Powers and Brownyard (1946), the water sink and heat source terms caused by binder hydration can be derived with:

$$\begin{aligned} \dot{m}_{hydr} &= 2m_{hc-initial}\left(0.187x_{C_3S} + 0.158x_{C_2S} + 0.665x_{C_3A} + 0.2130x_{C_4AF}\right) \\ &\times \left\{\left(\frac{\tau}{t_e}\right)^{\beta}\left(\frac{\beta}{t_e}\right)\xi \exp\left[\frac{E}{R}\left(\frac{1}{273+T_r} - \frac{1}{273+T}\right)\right]\right\} \end{aligned} \tag{12}$$

$$\begin{aligned} Q_{hydr} &= \left(H_{cem} \cdot X_{cem} + 461 \cdot X_{slag} + 1800 \cdot x_{CaO/FA} \cdot X_{FA}\right)C_b \\ &\times \left(\frac{\tau}{t_e}\right)^{\beta} \cdot \left(\frac{\beta}{t_e}\right) \cdot \xi\left(t_e\right) \cdot \exp\left[\frac{E}{R}\left(\frac{1}{273+T_r} - \frac{1}{273+T}\right)\right] \end{aligned} \tag{13}$$

Where $m_{hc-initial}$ is the initial cement mass, T_c is the temperature of the cement-based materials, H_{cem} is total heat of the hydration of the cement, C_b is the apparent binder density with respect to the total volume of the CTB mixture, and X_i is the weight ratio of the corresponding minerals in terms of total binder content.

3. Multiphysics modelling of CTB

The developed coupled multiphysics model is implemented into a commercial finite element method code, Comsol Multiphysics. A comprehensive experimental program (high column experiments, 150 cm in height) on the coupling of the THMC processes in CTB performed by Ghirian and Fall (2013, 2014) is chosen as a case study. In the experiments, the experimental data (e.g. temperature, PWP and vertical settlement) were measured at different positions of a high column. Among the measured data, the middle

(75 cm from the bottom of the column) of the high column is selected in this study as a reference observation point. Detailed information on the experiments can be found in Ghirian and Fall (2013, 2014).

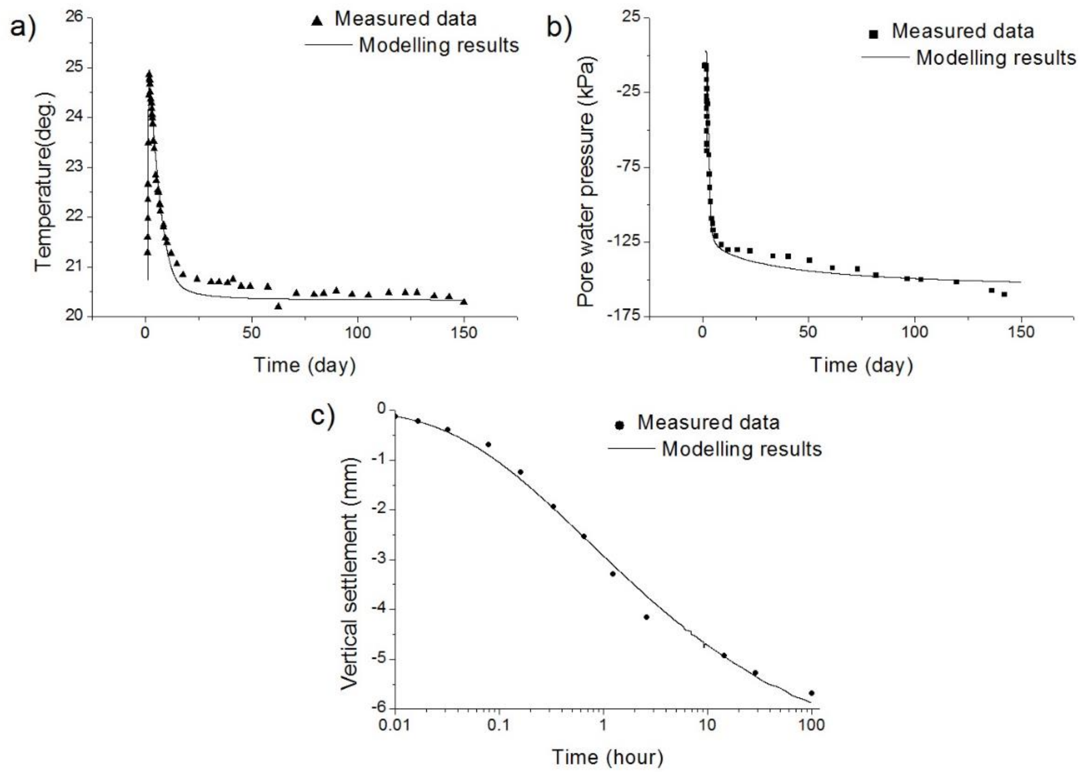

Fig. 1. Comparison of simulation results and experimental data: a) evolution of temperature; b) evolution of pore water pressure; c) vertical settlement

The multiphysics modelling results of the high column experiments on CTB are presented in Fig. 1. As shown in this figure, both the experimental data and simulation results show that the major changes in temperature, PWP and vertical settlement occur during at very early ages of CTB curing, which can be attributed to the influence of the rapid rate of binder hydration in the early ages. As mentioned in Section 1, with the advancement of binder hydration, the exothermal chemical reaction causes a variation in the temperature within the CTB. The water consumption by binder hydration induces the evolution of the PWP. Moreover, chemical shrinkage plays a critical role in the development of vertical settlement. The modelling results show good agreement with the measured data in terms of both evolution trends and peak values.

Moreover, the simulation results of the evolution of the material properties, including thermal conductivity and saturated hydraulic conductivity, are compared against the experimental data as presented in Fig. 2. As expected, the agreement between the predicted results and experimental data is fairly good.

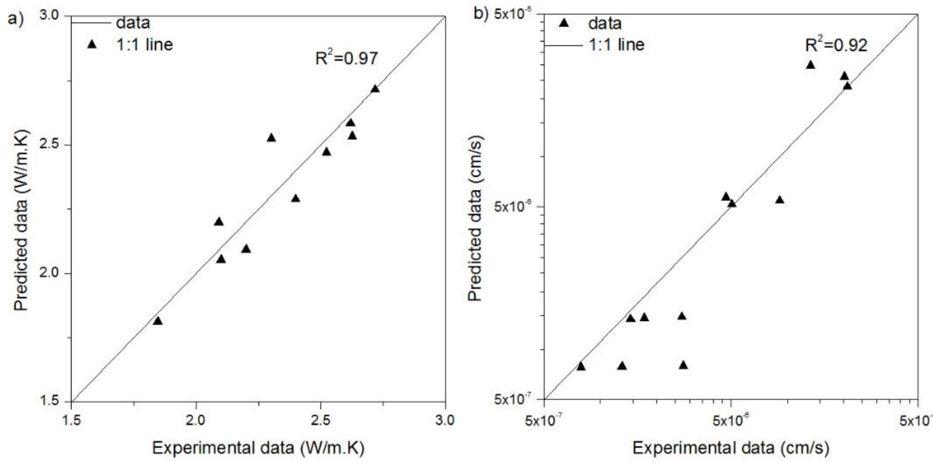

Fig. 2. Comparison of predicted results against measured data of material properties: a) evolution of thermal conductivity, b) evolution of saturated hydraulic conductivity

4. Conclusion

The highly interactive multiphysics phenomena within CTB dominate the evolution of the CTB behaviour and properties. A fully coupled model is proposed to characterize the CTB performance. Good agreement between the simulation results and experimental data is obtained. Both the modelling results and measured data show that a significant evolution of the temperature, PWP, vertical settlement as well as material properties (i.e., thermal conductivity and saturated hydraulic conductivity) occurs within the CTB, which not only confirms the predictive capability of the developed model, but also proves the necessity of the development of a coupled multiphysics model.

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