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Modeling the thermo-hydro-chemical behavior of cemented coal gangue-fly ash backfill

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HIGHLIGHTS

- We develop a THC model to analyze the coupled thermo-hydro-chemical behavior of CGFB.
- We design a test apparatus to investigate the thermal and hydraulic properties of hydrating CGFB.
- Increasing the binder hydration rate contributes to the temperature and suction developments in CGFB.
- Increasing the initial CGFB temperature and the environment temperature can both lead to the suction development in CGFB.

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ABSTRACT

Cemented coal gangue-fly ash backfill (CGFB), which is a mixture of coal gangue, fly ash, cement and water, is being extensively utilized in underground coal mines of China for subsidence control and waste management. One of the most significant evaluation criteria for CGFB is its mechanical performance, which is affected by the thermal (T, e.g., temperature evolution), hydraulic (H, e.g., suction development) and chemical (C, e.g., binder hydration) factors and thus subjected to the coupled THC effects. Modeling the coupled THC behavior of CGFB is crucial for effectively estimating the mechanical performance of CGFB. Therefore, a numerical model is developed to analyze and predict the coupled THC behavior of CGFB and its evolution versus time. The analysis and prediction results of the developed THC model are compared with laboratory investigations conducted on CGFB. There is a good agreement between the modeling results and experimental data, validating the capability of the developed model to simulate the coupled THC responses in CGFB.

1. Introduction

In China, coal mining is a primarily basic industry, especially underground coal mining, which accounts for approximately 95% of the total coal production [1]. The underground coal mining produces substantial financial revenues, but at the same time, it also causes serious social and environmental consequences such as ground surface subsidence and solid waste (coal gangue) discharge. Recently, cemented coal gangue-fly ash backfill (CGFB) mixtures are designed and introduced in underground coal mining operations for both strata control and waste management [2–4]. CGFBs, which are prepared by mixing cement, coal gangue, fly ash and water [2–4], are utilized to fill underground openings. This solution can not only help to control subsidence, but also reduce surface hazardous waste (e.g., coal gangue and fly ash) discharge and thus to some extent, solve the associated problems (e.g., spontaneous combustion of coal gangue piles and dust pollution of fly ash).

Because of the composition of CGFB, the binder (cement and fly ash) used will chemically react with water. This chemical reaction, which is also called binder hydration, generates hydration products, consumes water and releases heat. The generation of hydration products results in the hardening and strength gain of the CGFB, and the consumption of water leads to the decrease of pore water pressure or the suction development within the CGFB, while the generation of heat contributes to the temperature increment of the CGFB.

In addition to the utilization of CGFBs in disposing mine waste, another significant application of them is to fill mined-out areas for supporting the overlying strata and thus relieve subsidence. This

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requires the CGFBs to possess enough mechanical performance, which is affected by their chemical (e.g., binder hydration), thermal (e.g., self-heating, heat exchange with surroundings) and hydraulic (e.g., suction development) factors. The interaction of these three factors is stated as follows:

- Chemical (C)–Thermal (T) interaction. Binder hydration releases heat to increase the CGFB temperature, while the temperatures of the CGFB and its surroundings affect the rate of binder hydration.
- Chemical (C)–Hydraulic (H) interaction. Binder hydration consumes water to contribute to the suction development in the CGFB. However, it should be pointed out that the suction development has insignificant impact on the binder hydration process.
- Thermal (T)–Hydraulic (H) interaction. Temperature variation affects the suction evolution of the CGFB. The suction development has insignificant impact on the thermal factor.

As discussed above, the CGFB, which is a type of cement-based geo-materials, is subjected to the coupled thermal (T), hydraulic (H) and chemical (C) (THC) factors. These factors influence each other, together exerting THC coupled effects on the mechanical properties of CGFB.

In recent years, multi-filed coupled model has become a popular research topic in natural (e.g., rock, soil) and artificial geo-materials (e.g., concrete, cemented tailings backfill (CTB or CPB)). Hudson et al. [5] have proposed a numerical model to assess the performance of high radioactive waste repositories responding to thermo-hydro-mechanical (THM) coupled processes. Nasir et al. [6] have numerically investigated and described the thermo-hydro-mechanical-chemical (THMC) coupled processes resulting from long term past climate changes and glaciation cycles in the sedimentary rocks of southern Ontario. Similar studies of multi-field coupled modeling on rocks or soils can be found in the references (e.g., [7–10]). With regard to concrete, Ulm and Coussy [11] have conducted a numerical simulation study to investigate the thermo-chemo-mechanical (TCM) coupling behavior of concrete at early ages. Luzio et al. [12] have analyzed self-heating and self-desiccation of early-age high performance concrete. In addition, a variety of multi-field coupling models for concrete have been presented in some other researches (e.g., [13–15]). As to CTB or CPB, Wu et al. [16] have proposed a mathematical model for predicting and assessing the evolution of the rheological properties of fresh CPB under the coupled effects of temperature and progress of binder hydration. Nasir and Fall [17] have built a numerical model to predict the strength development of undrained CPB under the coupled effects of temperature and degree of hydration. Helinski et al. [18] have proposed a model to discuss the behavior of CTB in response to coupled hydro-chemo-mechanical (HCM) effects. In addition, Wu et al. [19] have developed a thermo-hydro-chemical (THC) coupled model to describe the coupled thermal and hydraulic processes within CPB. Cui and Fall [20] have presented a coupled thermo-hydro-mechanical-chemical (THMC) model for underground CTB. However, the knowledge on the multi-field coupled effect in CTB/CPB is still limited.

Although CGFB is similar to concrete and CTB/CPB in some properties such as cementation and consolidation, they are still different from each other in some other aspects like aggregate used, mix proportion and operating conditions. To date, no studies have been conducted on the development of a multi-field coupling model to investigate the behavior of CGFB in response to coupled thermal-hydraulic-chemical (THC) effects. Therefore, the objective of this study is to develop a numerical model to analyze and predict the THC behavior of CGFB. The numerical simulation results of the model are compared with the data from an experimental study.

2. Development of the THC model

2.1. Thermal equations

CGFB mixture is a type of self-heating composites, due to the fact that the binder used to prepare the CGFB reacts with the mixed water to release heat. Within the CGFB, heat convection due to fluid flow and heat radiation are insignificant, hence these two ways of thermal transfer are not considered in the present study. In consideration of self-heating and thermal conduction between the CGFB and its surroundings, the following equation can be obtained [21]:

$$(\rho C)_{\mathrm{eq}} \frac{\partial T}{\partial t} - \nabla \cdot (k_{\mathrm{eq}} \nabla T) = Q_H \tag{1}$$

where, $(\rho C)_{\mathrm{eq}}$ is the equivalent volumetric heat capacity of the CGFB (a solid-fluid composite) at constant pressure; T is the temperature; t is the time; k_{eq} is the equivalent thermal conductivity of the CGFB; and Q_H is the term representing heat generation, which can be expressed as follows:

$$Q_H = C_B \cdot q_h \tag{2}$$

where, C_B is content of the binder used for preparing the CGFB (kg/m^3); q_h is the heat generated by binder hydration per unit time and mass (W/kg), which can be presented as below [22]:

$$q_h = q_{\mathrm{m}} \cdot c \cdot \left[\sin(\pi \cdot \alpha)^a\right] \cdot \exp(-b \cdot \alpha) \cdot \exp\left[\frac{E_A}{R}\left(\frac{1}{T_r} - \frac{1}{T_c}\right)\right] \tag{3}$$

where, q_{m} is the maximum heat generation rate at the temperature of 20 °C; α is the degree of binder hydration; a, b, and c are experimentally determined constants; T_r is the reference temperature (i.e., 20 °C); T_c is the temperature of the CGFB; and E_A is the apparent activation energy, which is related with T_c [23]: if $T_c \geqslant 20$ °C, E_A = 33500 J/mol; while if $T_c \leqslant 20$ °C, $E_A = 33500 + 1470 \times (293 - T_c)$.

2.2. Hydraulic equations

The hydraulic properties of a CGFB structure mainly includes hydraulic conductivity, suction, and (positive) pore water pressure. In the present study, we only focus on the suction development, which is induced by the binder hydration (i.e., the binder chemically reacts with water) within the CGFB. The suction of CGFB can be calculated by using the following formula which is derived from the Kelvin equation [24]:

$$\psi = -\frac{RT}{v_{wo} w_v} \ln h_C \tag{4}$$

where, ψ is the total suction (kPa) of the CGFB, R is the universal (molar) gas constant [8.31432 J/(mol K)], v_{wo} is the specific volume of water [$(1/\rho_w)$ (m^3/kg)], w_v is the molecular mass of water vapour (18.016 g/mol), and h_C is the relative humidity of the CGFB.

CGFB is a cement-based material as similar as concrete, therefore the expression developed to calculate the relative humidity of concrete is applied to CGFB [25]:

$$h_C = 100 + X \cdot \exp(Y \cdot S) \tag{5}$$

where, X and Y are fitting parameters; and S is the CGFB saturation, which can be expressed as follows [26]:

$$S = \frac{V_{cw} + V_{gw}}{V_{cw} + V_{gw} + V_{cs}} \tag{6}$$