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### Permalink

<https://escholarship.org/uc/item/8mv83359>

### Journal

Computers and Geotechnics, 190

### ISSN

0266-352X

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### Publication Date

2026-02-01

### DOI

10.1016/j.compgeo.2025.107736

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# Coupled THM modeling of bentonite heating and hydration in tank tests with a new temperature-dependent water retention model

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## ABSTRACT

This study presents a coupled thermo-hydro-mechanical (THM) model for simulating the heating and hydration behavior of bentonite, a buffer material in deep geological repositories (DGRs). The model incorporates a new temperature-dependent soil water retention curve which captures the thermal-induced shift in water retention behavior. It also distinguishes between liquid and gas permeability, modeling intrinsic gas permeability as a function of accessible porosity to improve vapor transport and desaturation predictions. The model was validated against two large-scale tank tests, demonstrating good agreement with measured temperature, relative humidity, and water inflow data. It revealed a complex porosity evolution driven by thermal expansion, vapor movement, vapor condensation, and hydration-induced swelling during heating and hydration processes. The simulation results also suggest that the permeability of the hydration layer plays a critical role in controlling water intake. Clogging of this layer can significantly reduce the volume of water inflow during the hydration phase. While the model effectively captures key THM behavior, further development of the mechanical constitutive law is required to account for possible thermo-elasto-plastic volume changes and microstructural effects. Overall, the model provides a robust tool for evaluating the evolution of bentonite-based barrier material in DGRs.

## 1. INTRODUCTION

Bentonite is widely used as a buffer material in deep geological repositories (DGRs) for high level radioactive waste (HLW) due to its favorable properties, including low permeability, high swelling capacity, radionuclide retention capability [1-5]. Throughout the operational lifespan of a DGR, the buffer material is subjected to heating from HLW and hydration from the surrounding host rock. These processes induce complex coupled thermo-hydro-mechanical (THM) interactions, involving water phase change, vapor advection and diffusion, and the swelling or shrinkage of bentonite. Additionally, chemical processes such as ion migration and exchange, mineral dissolution/precipitation, and phase transformations further influence the behavior of the buffer [6, 7]. While the effects of temperatures below 100°C have been extensively investigated in experimental and numerical studies, recent research has shifted focus to temperatures up to 200°C. Understanding the influence of elevated temperatures on the coupled THM processes is crucial for assessing the long-term performance of bentonite-based barriers. To this end, laboratory experiments, in situ tests, and numerical simulations have been conducted to strengthen the understanding of the coupled THM processes [8-13].

High temperatures significantly impact the hydraulic behavior of unsaturated, compacted bentonite. The phase transition from liquid water to vapor accelerates under high temperatures, leading to pronounced desaturation

around the heat source [14]. Vapor is transported away from the heater through advection and diffusion before condensing in cooler regions. As heating continues, the desaturation front expands outward until thermal equilibrium is reached. This desaturation process, in turn, reduces thermal conductivity, illustrating the two-way coupling between thermal and hydraulic processes. Tank tests conducted at the University of California, San Diego (UCSD) demonstrated that desaturation intensifies when the heater is enclosed in a large aluminum container, amplifying the thermal impact on the surrounding bentonite [8, 9].

The coupled thermo-hydraulic (TH) processes play a critical role in the mechanical behavior of compacted bentonite. Hydration leads to clay particle swelling and pore structure collapse, while heating induces material expansion and possibly thermally driven plastic contraction. Throughout the heating and hydration processes, bentonite density exhibits significant temporal and spatial variations. X-ray scan tests revealed that the wet density of bentonite increases as the hydration front approaches and decreases once the front passes [15]. As the hydration front advances toward the heater, the bentonite behind the front returns to its initial status. This phenomenon may be attributed to the highly dynamic interaction between local swelling and the resulting compressive stress [1]. Compared to the non-heated scenario, heating can lead to greater compression of the inner bentonite and more pronounced swelling around the heater [1].

Over the past decade, various coupled THM models have been developed to simulate bentonite behavior under heating and hydration conditions. These models typically incorporate key properties such as water retention, permeability, thermal conductivity, and mechanical constitutive behavior. The soil-water retention curve (SWRC) model developed by van Genuchten [16] (referred to here as the VG model) has been widely used to describe water retention in bentonite. However, the VG model assumes a fixed residual degree of saturation, does not explicitly distinguish between water retention by capillary and adsorptive mechanisms, and does not incorporate the effects of temperature on water retention. As a result, the vaporization of the "residual" water content is not accounted for in the coupled model, which is inconsistent with experimental findings showing that the degree of saturation can drop well below the residual value. Various advanced water retention models have been proposed to account for capillarity and absorptivity [17, 18]. Bosch, Qiao [19] adopted Dieudonne's model to describe the water retention behavior during the heating/hydration process. However, previous numerical studies have largely overlooked the temperature dependence of water retention behavior. For unsaturated compacted bentonite, the initial gas permeability is several orders of magnitude larger than the liquid permeability because of the dual pore structure [14]. However, this important difference has often been neglected in many previous studies. Consequently, vapor transfer and the desaturation process of the bentonite near the heater may not have been accurately simulated.

To address these limitations, this study implements a temperature-dependent water retention model [10], hereafter referred to as LM model, and a novel thermal conductivity function [11] into the TOUGH3 simulator [20]. The intrinsic gas permeability is modeled as a power function of accessible porosity to capture its evolution with changing porosity and degree of saturation. Various mechanical constitutive models, such as the Barcelona Expansive Model (BExM) [21], the modified Cam Clay model [19], the linear swelling model [22], and the state surface model [1], have been employed in previous studies. Given the focus of this investigation on the coupled TH processes, the state surface model has been adopted for the current numerical study.

This paper presents the implementation of these models within the TOUGH3-FLAC multiphysics simulator. A parametric analysis is conducted to evaluate the influence of key parameters on coupled THM behavior. Additionally, the numerical model is applied to simulate large-scale tank tests conducted in UCSD and the key findings are analyzed to improve the predictive capability of THM models for bentonite-based barriers in DGRs.

## 2. COUPLED THM MODEL FOR HEATING AND HYDRATION OF BENTONITE

### 2.1. Governing Equations

An integral finite difference method is used in TOUGH3 to solve mass and energy balance equations which are written in the following unified form [20]:

$$\frac{d}{dt} \int_{V_n} M^k dV_n = \int_{\Gamma_n} \mathbf{F}^k \cdot \mathbf{n} d\Gamma_n + \int_{V_n} q^k dV_n \quad (1)$$

where  $M^k$  is the accumulation term for component  $\kappa$  or energy ( $\kappa = h$ ) per volume,  $\mathbf{F}^k$  is the mass or heat flux,  $q^k$  denotes sinks or sources,  $\mathbf{n}$  is a normal vector on the surface element  $d\Gamma_n$ , pointing inward an arbitrary subdomain  $V_n$ .

The general form for the mass accumulation term is written as

$$M^k = \phi \sum_{\beta} S_{\beta} \rho_{\beta} X_{\beta}^k \quad (2)$$

where  $\phi$  is the porosity,  $S_{\beta}$  is the saturation of phase  $\beta$ ,  $\rho_{\beta}$  is the density of phase  $\beta$ ,  $X_{\beta}^k$  is the mass fraction of component  $\kappa$  (air or water) in phase  $\beta$  (gas or liquid).

The energy accumulation term is written as

$$M^h = (1 - \phi) \rho_s C_s T + \phi \sum_{\beta} S_{\beta} \rho_{\beta} u_{\beta} \quad (3)$$

where  $C_s$  is the specific heat of the solid grains,  $T$  is the temperature, and  $u_{\beta}$  is the specific internal energy of phase  $\beta$ .

The momentum balance equation is written as

$$\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{g} = 0 \quad (4)$$

where  $\boldsymbol{\sigma}$  is the total stress tensor and  $\mathbf{g}$  is the gravitational acceleration.

### 2.2. Hydraulic Constitutive Models

The mass flux term in Eq. (1) consists of the advection part,  $\mathbf{F}_{adv}^k$ , and the diffusion part,  $\mathbf{F}_{diff}^k$ :

$$\mathbf{F}^k = \mathbf{F}_{adv}^k + \mathbf{F}_{diff}^k \quad (5)$$

#### 2.2.1. Advection Flux

The advection mass flux is expressed as

$$\mathbf{F}_{adv}^k = \sum_{\beta} X_{\beta}^k \mathbf{F}_{\beta} \quad (6)$$

where the flux for phase  $\beta$  is calculated by a generalized Darcy's law:

$$\mathbf{F}_\beta = \rho_\beta \mathbf{u}_\beta = -\frac{k_\beta k_{r\beta} \rho_\beta}{\mu_\beta} (\nabla P_\beta - \rho_\beta \mathbf{g}) \quad (7)$$

111 where  $\mathbf{u}_\beta$  is the Darcy's velocity,  $k_\beta$  is the intrinsic permeability of phase  $\beta$ ,  $k_{r\beta}$  is the relative permeability  
 112 of phase  $\beta$ ,  $\mu_\beta$  is dynamic viscosity,  $P_\beta$  is the pressure of phase  $\beta$  and  $\mathbf{g}$  is the gravitational acceleration.

113 The effect of suction on the vapor pressure is considered via Kelvin's equation [23]:

$$P_v(T, S_l) = P_{sat}(T) \exp \left[ \frac{-M_w \psi(T, S_l)}{\rho_l R(T + 273.15)} \right] \quad (8)$$

114 where  $P_{sat}$  is the saturated vapor pressure of bulk aqueous phase,  $\psi$  is the suction,  $M_w$  is the molecular mass  
 115 of water, and  $R$  is the universal gas constant (8.31432 J/mol/K).

116 The gas pressure,  $P_g$ , is the sum of air pressure,  $p_a$  and vapor pressure,  $p_v$ . According to Henry's law, air  
 117 pressure is expressed as a function of the mass fraction of air in liquid:

$$p_a = X_l^a / H_c \quad (9)$$

118 where  $H_c = 10^{-10} Pa^{-1}$  is Henry's constant for air dissolution in water. It should be noted that Henry's  
 119 constant is inherently temperature dependent and can be represented as a quadratic function of temperature  
 120 [24-26]. This temperature effect is not considered in the current study but will be addressed in future work.

121 Assuming the air pressure is an ideal gas, the air density is then expressed as:

$$\rho_a = \frac{M_a}{RT} p_a \quad (10)$$

122 where  $M_a$  is the molecular mass of air.

123 All thermodynamic properties of water, including density, specific enthalpy, internal energy, and viscosity in  
 124 both liquid and vapor phases, are calculated using the steam table equations established by International  
 125 Formulation Committee [27]. The viscosity of the air-vapor mixture is determined based on the formulation  
 126 provided by Hirschfelder, Curtiss [28].

## 127 **2.2.2. Diffusion Flux**

128 The diffusion flux of component  $\kappa$  is written as

$$\mathbf{F}_{diff}^\kappa = -\sum_\beta D_\beta^\kappa \nabla X_\beta^\kappa \quad (11)$$

129 where  $D_\beta^\kappa$  is the effective diffusion coefficient of component  $\kappa$  in phase  $\beta$ , which is written as [29]

$$D_\beta^\kappa = \phi^{4/3} S_\beta^{10/3} \rho_\beta d_\beta^\kappa \quad (12)$$

130 where  $d_\beta^\kappa$  is the molecular diffusion coefficient for component  $\kappa$  in phase  $\beta$ . For the gas phase,  $d_\beta^\kappa$  is pressure  
 131 and temperature dependent via [30]

$$d_g^\kappa(P_g, T) = d_g^\kappa(P_{g0}, T_0) \frac{P_{g0}}{P_g} \left[ \frac{T + 273.15}{273.15} \right]^\xi \quad (13)$$

where  $d_g^k(P_{g0}, T_0) = 2.13 \times 10^{-5} \text{ m}^2/\text{s}$ ,  $P_{g0} = 1 \text{ atm}$  and  $\xi = 2.0$  is an empirical constant. It should be noted that Eq. (13) accounts only for molecular diffusion, whereas in compacted bentonite with nano-scale pores, Knudsen diffusion may also contribute significantly to the overall gas transport [31]. In the present study, this effect is not explicitly included, but future extensions may adopt a Bosanquet-type formulation that combines molecular and Knudsen diffusion to more accurately capture gas diffusion under such conditions [32].

### 2.2.3. Temperature-dependent soil water retention curve

Lu and McCartney [10] extended the SWRC of Lu [18] to account for temperature effects. The total volumetric water content of the model consists of an adsorption part,  $\theta_a$ , and a capillary part,  $\theta_c$ :

$$\theta = \theta_a + \theta_c \quad (14)$$

$$\theta_a = \theta_{a,\max}(T) \left\{ 1 - \left[ \exp\left(\frac{\psi - \psi_{\max}(T)}{\psi}\right) \right]^m \right\} \quad (15)$$

$$\theta_c = \frac{\theta_s - \theta_a}{2} \left\{ 1 - \operatorname{erf}\left[\sqrt{2} \frac{\psi}{\psi_c} \left(\frac{\eta + T}{\eta_r + T_r}\right) - \sqrt{2}\right] \right\} \cdot \left\{ 1 + \left[ \alpha \psi \left(\frac{\eta + T}{\eta_r + T_r}\right) \right]^n \right\}^{\frac{1}{n}-1} \quad (16)$$

where  $\theta_{a,\max}$  is the adsorption capacity,  $\psi_{\max}$  is the maximum matrix suction,  $m$  is the adsorption strength,  $\theta_s$  is the saturated volumetric water content,  $\psi_c$  is the mean cavitation suction,  $\alpha$  is the inverse of air entry value,  $n$  is a capillary pore-size distribution parameter,  $\eta$  is a correction factor on suction at capillary regime,  $\eta_r$  is a correction factor on suction at reference temperature,  $T_r$ ,  $T$  is the temperature,  $\psi$  is the suction. Models for  $\psi_{\max}$ ,  $\theta_{a,\max}$  and  $\psi_c$  are detailed in Appendix A.

The capillary pressure varies as the permeability and porosity changes, which is described by the Leverett law:

$$\psi = \psi \left( \frac{k_{w0} \phi}{\phi_0 k_w} \right)^{0.5} \quad (17)$$

Implementing the new SWRC in TOUGH3 differs from other water retention models, where capillary pressure can be analytically expressed as a function of degree of saturation or volumetric water content. In the Ning Lu (NL) model, capillary pressure must be determined numerically using the Newton-Raphson method. To achieve this, the derivative of the volumetric water content with respect to suction is first derived, followed by applying Newton-Raphson iterations to compute the capillary pressure. Notably, when the volumetric water content approaches the saturated value (99%), a bisection method is employed instead of Newton-Raphson. This adjustment is necessary to avoid convergence issues caused by the extremely small derivative values in such cases.

### 2.2.4. van Genuchten SWRC

The VG model was employed to represent the water retention behavior of auxiliary materials, such as the hydration layer and the hydration channel, which are not geomaterials. The temperature effect on these materials was assumed to be negligible with respect to the overall heating and hydration process in bentonite. Furthermore, the VG model provides superior numerical stability at high degrees of saturation, as suction can be expressed analytically as a function of saturation. For these reasons, the VG model was adopted for auxiliary materials. The capillary pressure of the unsaturated porous media reads [16]:

$$\psi = \psi_{ent} \left[ S_e^{-\frac{1}{\lambda}} - 1 \right]^{1-\lambda}, \psi \leq \psi_{cmax} \quad (18)$$

162 where  $\psi_{ent}$  is the air entry value,  $\psi_{cmax}$  is the maximum value for suction,  $\lambda$  is a shape factor for the curve  
 163 and  $S_e = (S - S_r)/(1 - S_r)$ ,  $S_r$  is the residual degree of saturation.

## 164 2.2.5. Permeability model

165 In traditional porous media, intrinsic permeability is generally assumed to be the same for both gas and liquid  
 166 phases. However, this assumption no longer holds for unsaturated compacted bentonite. It is well known that  
 167 two distinct pore structures coexist in unsaturated compacted bentonite: macroscopic pores and microscopic  
 168 pores. In contrast, saturated bentonite exhibits a unimodal pore size distribution. As a result, the intrinsic  
 169 permeability measured in the saturated state is not applicable to the unsaturated condition. Experimental results  
 170 have demonstrated that the intrinsic gas permeability for unsaturated bentonite can be several orders of  
 171 magnitude higher than the intrinsic water permeability [14, 33-35]. As the degree of saturation increases, the  
 172 size of accessible pores for gas flow decreases, resulting in a reduction of intrinsic gas permeability. To capture  
 173 the evolution of intrinsic gas permeability, a simple empirical model defined with respect to the accessible  
 174 porosity was employed in this study [34, 35]:

$$k_{gas} = k_{gas0}[\phi(1 - S)]^{n_k} \quad (19)$$

175 where  $k_{gas0}$  and  $n_k$  are calibration parameters.

176 When the mean free path of gas molecules becomes comparable to the pore size of the porous media, the gas  
 177 molecules can “slip” along the walls of the pores rather than fully interacting with them as they would at higher  
 178 pressures. This “slip flow” causes the gas to experience less resistance, leading to an increase in the measured  
 179 permeability. This phenomenon is referred to as the Klinkenberg effect. Given the extremely small pore sizes  
 180 in compacted bentonite, the Klinkenberg effect is considered in evaluating the evolution of gas permeability  
 181 through:

$$k_g = k_{gas}(1 + \frac{b}{p_g}) \quad (20)$$

182 where  $k_g$  is the corrected gas permeability employed in Darcy’s law,  $b$  is the Klinkenberg gas slippage factor  
 183 and  $p_g$  is the pore gas pressure. The Klinkenberg gas slippage factor is approximated as follows [36]:

$$b = 0.12k_{gas}^{-0.39} \quad (21)$$

184 The initial gas permeability used in the following simulations, is around  $1.0 \times 10^{-16} m^2$ , which approximates  
 185  $b$  as  $2.09 \times 10^5$  Pa.

186 Horseman and Harrington [37] proposed an empirical model for MX80 bentonite based on experimental data.  
 187 This model was subsequently employed in [38] to simulate gas migration in MX80 bentonite. The formulation  
 188 of the empirical model is written as:

$$k_w = 3.45 \times 10^{-20} \left( \frac{\phi}{1 - \phi} \right)^{4.28} \quad (22)$$

189 The initial porosities of the bentonite samples in Tank Test 1 and Tank Test 2 are 0.508 and 0.51, respectively,  
 190 corresponding to intrinsic permeabilities of  $3.69 \times 10^{-20} m^2$  and  $4.1 \times 10^{-20} m^2$ . More advanced permeability  
 191 models for bentonite have been developed, which incorporate the effects of montmorillonite content and  
 192 temperature [9, 39]. These will be considered in future work to further refine the analysis.

193 The relative permeability for liquid phase and gas phase read

$$k_{rw} = S_e^4 \quad (23)$$

$$k_{rg} = (1 - S_e)^2(1 - S_e^2) \quad (24)$$

where  $S_e = (\theta - \theta_a)/(\theta_s - \theta_a)$  is the effective degree of saturation. It is worth noting that the adsorptive water content here is no longer a constant, but a variable changing with suction, as modeled by Eq. (15).

### 2.3. Thermal Constitutive Model

Heat flux in TOUGH3 consists of conductive, convective, and radiative components [20]:

$$\mathbf{F}^h = -\lambda_{th}\nabla T + \sum_{\beta} h_{\beta}\mathbf{F}_{\beta} + f_{\sigma}\sigma_0\nabla T^4 \quad (25)$$

where  $\lambda_{th}$  is the thermal conductivity,  $h_{\beta}$  is the specific enthalpy in phase  $\beta$ ,  $f_{\sigma}$  is the radiant emittance factor, and  $\sigma_0$  is the Stefan-Boltzmann constant. A novel thermal conductivity function for the unsaturated MX80 bentonite developed by Lu and McCartney [11] is used in this study:

$$\frac{\lambda_{th} - \lambda_{dry}}{\lambda_{sat} - \lambda_{dry}} = \left[ 1 - \frac{1 - S_l^{\chi}}{1 + \left(\frac{S_l}{S_c}\right)^{\chi}} \right]^{1 - \frac{1}{\chi}} \quad (26)$$

where  $\lambda_{th}$ ,  $\lambda_{dry}$  and  $\lambda_{sat}$  are thermal conductivity at unsaturated, dry and saturated state,  $S_l$  is the degree of saturation,  $S_c$  is the degree of saturation at the onset of the capillary water retention regime,  $\chi$  is the model parameter. The advantage of this model over previous thermal conductivity models is that it is linked to the nonlinear shape of the SWRC and converges to the thermal conductivity at dry and saturated states with  $S_l$  approaches 0 or 1, respectively.

### 2.4. Mechanical Constitutive Model

State-surface approach adopts two stress state variables (net normal stress and suction) to construct the mechanical constitutive model. Total strain consists of elastic component,  $d\epsilon_{ij}^e$ , thermal component,  $d\epsilon_{ij}^T$ , and hydraulic component,  $d\epsilon_{ij}^H$ , (due to suction change):

$$d\epsilon_{ij}^t = d\epsilon_{ij}^e + d\epsilon_{ij}^T + d\epsilon_{ij}^H \quad (27)$$

Assuming the temperature and suction contribute only to the normal strain, then the constitutive model is written as

$$d\sigma'_{ij} = 2G_M d\epsilon_{ij}^t + \left(K_M - \frac{2}{3}G_M\right) d\epsilon_{kk}^t - 3K_M\alpha_T dT\delta_{ij} - \frac{K_M}{K_H} d\psi\delta_{ij} \quad (28)$$

where  $\sigma'_{ij} = \sigma_{ij} + P_g\delta_{ij}$  is the net normal stress,  $\alpha_T$  is the linear thermal expansion coefficient,  $K_M$  is the mechanical bulk modulus,  $G_M$  is the shear modulus and  $K_H$  is the hydraulic bulk modulus. These moduli are suction dependent and determined using the state-surface model.

The state-surface model is used to describe the mechanical behavior of unsaturated bentonite [40]. The void ratio is expressed as

$$e = A + B\ln(-\sigma'_m) + C\ln(\psi + p^a) + D\ln(-\sigma'_m)\ln(\psi + p^a) \quad (29)$$

where  $e$  is the void ratio,  $\sigma'_m$  is the mean net normal stress,  $p^a$  is the atmosphere pressure,  $A, B, C$  and  $D$  are empirical constants.

219 Based on the Eq. (29), the increment of volumetric strain,  $d\epsilon_v$ , is defined as:

$$d\epsilon_v = \frac{de}{1+e} = \frac{1}{1+e} \left( \frac{\partial e}{\partial \sigma'_m} d\sigma'_m + \frac{\partial e}{\partial \psi} d\psi \right) \quad (30)$$

220 Then, the mechanical and hydraulic bulk modulus are determined as

$$K_M = \frac{(1+e)\sigma'_m}{B + D \ln(\psi + p^a)} \quad (31)$$

$$K_H = \frac{(1+e)(\psi + p^a)}{C + D \ln(-\sigma'_m)} \quad (32)$$

$$G_M = \frac{3K_M(1-2\nu)}{2(1+\nu)} \quad (33)$$

221 where  $\nu$  is Poisson's ratio.

## 222 2.5. Coupling between TOUGH3 and FLAC3D

223 The coupling between TOUGH3 and FLAC3D is briefly introduced in this section. More details about the  
 224 coupling strategies of TOUGH-FLAC3D are referenced in the TOUGH3 manual and previous publications  
 225 [41, 42]. TOUGH4-FLAC3D is a two-way sequential coupling simulator. The coupling between the codes is  
 226 achieved by iteratively writing/reading the binary files generated by each code during the simulation process.  
 227 At the beginning of each time step, the porosity is updated based on the increments of volumetric strain, pore  
 228 pressure and temperature in the previous time step. Then, the updated porosity is further corrected by the  
 229 increment of the pressure and the temperature during the iteration process at the current time step. This  
 230 coupling strategy corresponds to a special case of the “fixed-stress” split sequential scheme, which has been  
 231 demonstrated to be unconditionally stable and free of oscillations with respect to time [43, 44]. The coupling  
 232 time step is governed by the adaptive time-stepping algorithm in TOUGH3, which automatically adjusts the  
 233 step size within prescribed minimum and maximum limits to satisfy the specified convergence criterion [20].  
 234 A relative convergence criterion of  $1.0 \times 10^{-6}$  and a minimum time step of 0.01 s were employed in this study.  
 235 To evaluate the effect of the maximum allowable time step on computational efficiency and accuracy, four  
 236 values (1000 s, 5000 s, 10,000 s, and  $5.0 \times 10^5$  s) were tested. The numerical results across these cases showed  
 237 excellent agreement, with only minor discrepancies observed in the vertical stress component, as illustrated by  
 238 Figure 23 in Appendix B. This indicates that the adaptive time-stepping algorithm produced sufficiently small-  
 239 time steps (generally less than 30,000s in the subsequent tank test simulations) to ensure accuracy. Based on  
 240 this assessment, a larger maximum time step of  $5.0 \times 10^5$  s was adopted in the simulations to comply with the  
 241 convergence-based time step and reduce computational effort.

242 Mathematically, the porosity is updated at each time step as [43, 45]

$$\phi^{i+1} - \phi^i = \frac{(\alpha_B^i)^2 + (\alpha_B^i - \phi^i)(1 - \alpha_B^i)}{K_{dr}^i} \sum_{\beta} [S_{\beta}(P_{\beta}^{i+1} - P_{\beta}^i)] + 3\phi^i \alpha_T (T^{i+1} - T^i) - \Delta\phi_c \quad (34)$$

$$\Delta\phi_c = \frac{(\alpha_B^i)^2}{K_{dr}^i} \sum_{\beta} [S_{\beta}(P_{\beta}^i - P_{\beta}^{i-1})] + 3\alpha_B^i \alpha_T (T^i - T^{i-1}) - \alpha_B^i (\epsilon_v^i - \epsilon_v^{i-1}) \quad (35)$$

243 where  $\alpha_B$  is the Biot's coefficient, and  $K_{dr}$  is the drained bulk modulus.

244 Once the coupled TH process reaches equilibrium, the equivalent pore pressure is calculated and then  
 245 transferred to FLAC3D. The coupling discussed above is the direct coupling between the TH process and the

mechanical process. In addition, some indirect couplings, such as changes in permeability and capillary pressure, have been implemented in the coupling code.

### 3. MODEL VALIDATIONS AND PARAMETER ANALYSIS

#### 3.1. Comparison between LM and VG SWRC

This section evaluates the impact of two SWRCs, i.e., the temperature-dependent LM model and the classical VG model, on hydraulic behavior during the heating process for a hypothetical case. In this subsection, the temperature-dependent features are deactivated to facilitate comparison. To simplify the analysis, mechanical effects are neglected, and a one-dimensional (1D) geometry, as illustrated in Figure 1, is employed for the simulations in Section 3. For the LM model, the parameters used are:  $M = 0.12$ ,  $n = 1.15$ ,  $\alpha^{-1} = 3.3 \times 10^6 \text{ MPa}$ ,  $CEC_{max} = 0.8 \text{ meq/g}$ ,  $SSA = 750 \text{ m}^2/\text{g}$ . The VG model uses a shape factor of 1.5 and the same gas entry value as the LM model. The intrinsic gas permeability is defined by parameters:  $k_{gas0} = 4.1 \times 10^{-15} \text{ m}^2$ ,  $n_k = 2.0$ . The diffusion coefficient of vapor in the gas phase at the initial pressure and temperature is  $d_g^k(P_{g0}, T_0) = 2.13 \times 10^{-5} \text{ m}^2/\text{s}$ . The temperature of the heater (“HEATS” domain in Figure 1) was kept at 200 °C. Additional key parameters employed in the simulations are listed in Table 1. The following numerical analysis is conducted for the monitoring point (as marked in Figure 1).

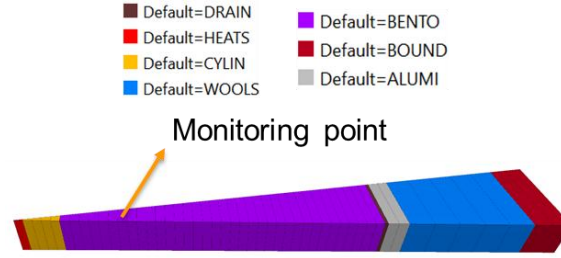


Figure 1 1D axisymmetric geometry for the column test (“HEATS”: Heater, “CYLIN”: Aluminum cylinder encasing the heater, “BENTO”: Bentonite, “SANDS”: Hydration layer, “ALUMI”: Aluminum container, “WOOLS”: Thermal insulation material, “BOUND”: Atmosphere)

Table 1 Model parameters for the key components in the TH analysis

| Parameter                                                            | Heater | Aluminum | Bentonite             | Wools |
|----------------------------------------------------------------------|--------|----------|-----------------------|-------|
| Solid (grain) density [ $\text{kg}/\text{m}^3$ ]                     | 7800   | 2700     | 2660                  | 500   |
| Initial porosity                                                     | 0.1    | 0.1      | 0.51                  | 0.1   |
| Grain specific heat capacity [ $\text{J}/(\text{kg}\cdot\text{K})$ ] | 1.0e50 | 887      | 880                   | 700   |
| Thermal conductivity (wet) [ $\text{W}/(\text{m}\cdot\text{K})$ ]    | 20.0   | 237.0    | 0.93                  | 0.46  |
| Thermal expansion coefficient<br>$\times 10^{-5} [\text{K}^{-1}]$    | 0      | 0        | 6.6                   | 0     |
| Initial liquid permeability [ $\text{m}^2$ ]                         | 0      | 0        | $4.1 \times 10^{-20}$ | 0     |

Figure 2 presents a comparison of numerical time series results for the domain shown in Figure 1 with all boundary conditions the same except for using different SWRC models. The coupled TH model incorporating the temperature-dependent LM SWRC accurately captures both hydration (driven by vapor condensation) and dehydration induced by elevated temperatures. In contrast, the predictive performance of the VG model is highly sensitive to the prescribed residual degree of saturation. As the residual saturation increases, the magnitudes of both hydration and dehydration effects diminish. When the residual saturation reaches 0.25, the influence of heating on the evolution of the degree of saturation becomes negligible.

This discrepancy arises because the VG model treats adsorbed water as immobile through the definition of residual saturation, thereby preventing the residual water from evaporating and participating in vapor-phase transport. Consequently, when residual saturation is high, the hydration and dehydration processes are significantly suppressed. Furthermore, the reduction in saturation leads to a decrease in the thermal conductivity of bentonite, resulting in a slower temperature rise, as illustrated in Figure 2(a). This behavior is consistent with observations from the tank tests, as will be discussed in Section 4. In summary, the LM model provides a realistic representation of both hydration and dehydration processes during heating.

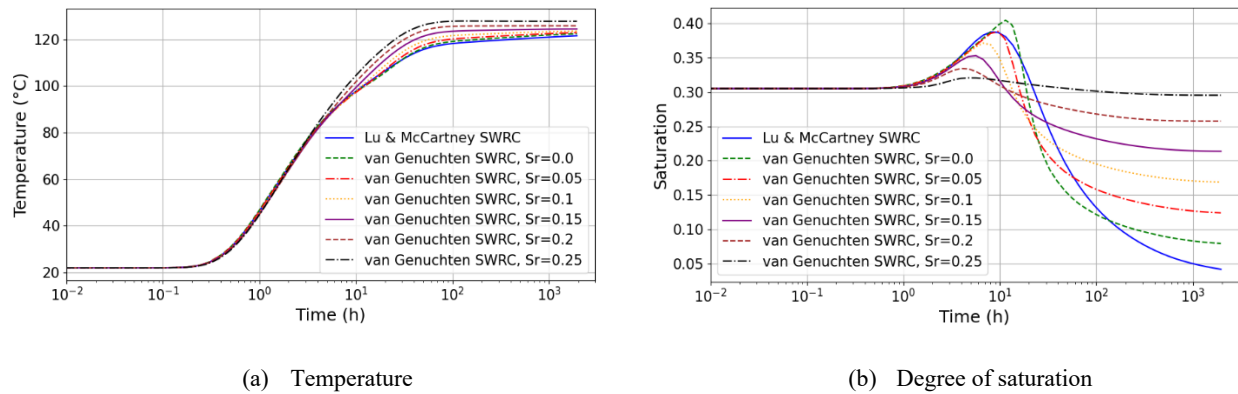
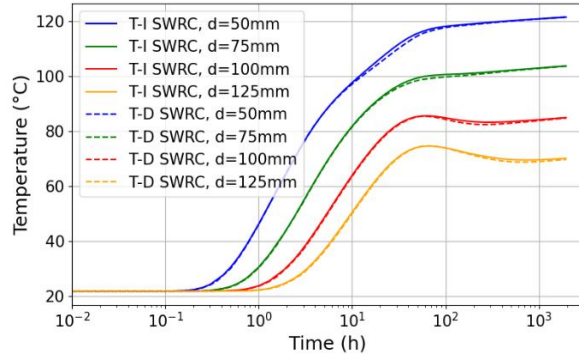


Figure 2 Evolution of temperature and degree of saturation with different SWRCs

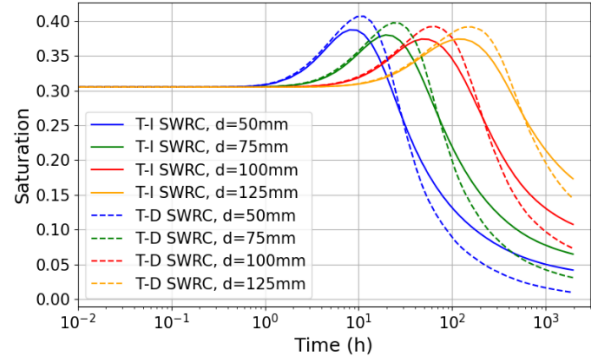
### 3.2. Effect of Temperature Dependency of SWRC

This section examines the influence of the temperature dependency of the SWRC on coupled thermal and hydraulic processes. The LM SWRC is adopted for the simulations. Figure 3(a) shows that the temperature dependency of the SWRC has a negligible effect on the thermal response, with the temperature evolution predicted by the temperature-independent (T-I) SWRC being only slightly higher than predicted by the temperature-dependent (T-D) one. In contrast, Figure 3(b) highlights the significant impact of temperature dependency on the hydraulic response. Incorporating the temperature effect into the SWRC leads to enhanced hydration and dehydration processes. Specifically, the T-D SWRC predicts a higher peak saturation due to vapor condensation and a lower residual saturation during dehydration compared to the T-I case. This reduction in water retention is attributed to elevated temperatures, which reduces the capacity of bentonite to retain water.

As illustrated in Figure 4, the temperature-dependent SWRC successfully captures the curve shift behavior induced by thermal variations. Compared to the T-I SWRC, the T-D curve shifts leftward, reflecting a decrease in water retention capacity at elevated temperatures. Additionally, SWRCs vary spatially, with lower water retention observed closer to the heat source due to higher temperatures. In contrast, the T-I SWRC produces consistent results regardless of location, as it does not account for temperature effects. A minor hysteresis observed at the beginning of the heating phase may be attributed to changes in porosity. In summary, the T-D SWRC provides a more realistic representation of thermo-hydraulic coupling by effectively capturing the thermally induced shift in water retention behaviors.



(a) Temperature



(b) Degree of saturation

Figure 3 Evolution of temperature and degree of saturation based on temperature-dependent (T-D) SWRC and temperature-independent (T-I) SWRC

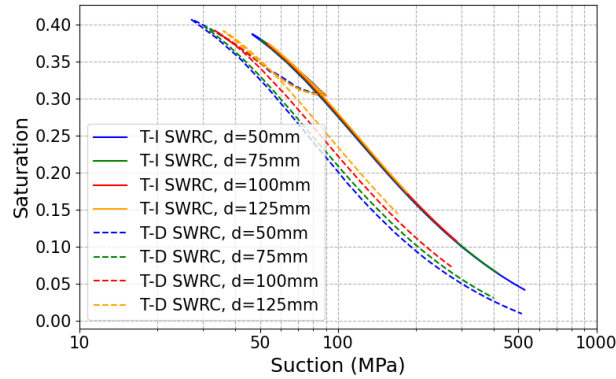


Figure 4 Comparison of temperature-dependent (T-D) SWRC and temperature-independent (T-I) SWRC

### 3.3. Intrinsic Gas Permeability and Diffusion Coefficients

This section analyzes the influence of intrinsic gas permeability and the diffusion coefficient of vapor in the gas phase on coupled TH behavior. The intrinsic gas permeability is controlled through the parameter  $k_{gas0}$  in Eq. (19), while the diffusion coefficient is adjusted via  $d_{g0}^v$ . For a fixed value of  $k_{gas0}$ , a lower vapor diffusion coefficient results in a delayed peak in the degree of saturation. Moreover, the peak saturation associated with the lowest diffusion coefficient (indicated by the solid blue line in Figure 5) is significantly higher than those in the three other cases with larger diffusion coefficients (represented by dashed lines). As the intrinsic permeability increases, the peak saturation increases across all four cases, whereas the timing of the peak remains relatively unchanged. Notably, the case with the lowest diffusion coefficient shows a pronounced rise in peak saturation. These results indicate that the vapor diffusion coefficient plays a critical role in both the timing and magnitude of the saturation peak. However, its influence diminishes as the diffusion coefficient increases. In parallel, higher intrinsic permeability consistently enhances the peak degree of saturation within the considered range.

322 **3.3.1. Coupled TH simulations**

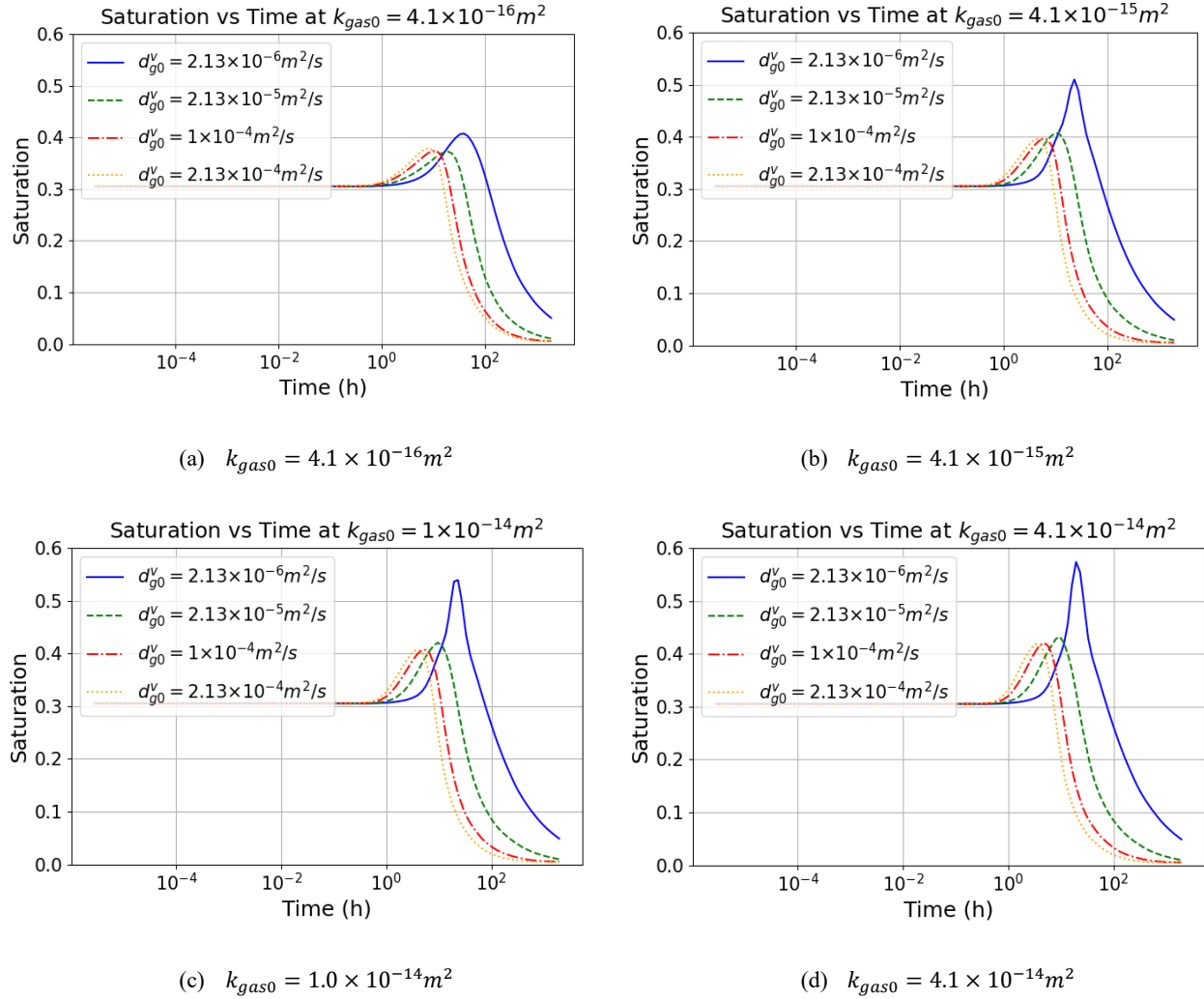
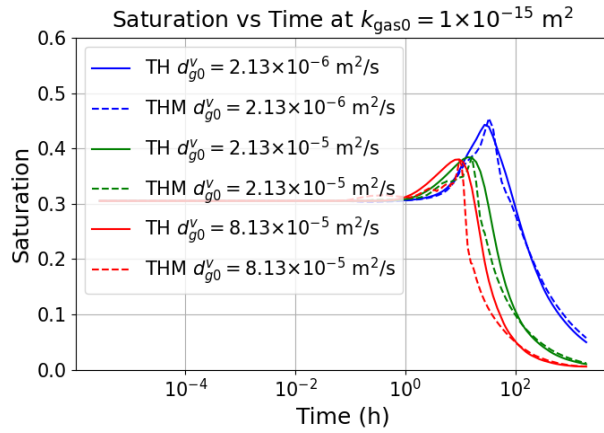


Figure 5 Effect of intrinsic gas permeability and vapor diffusion coefficient on the evolution of degree of saturation

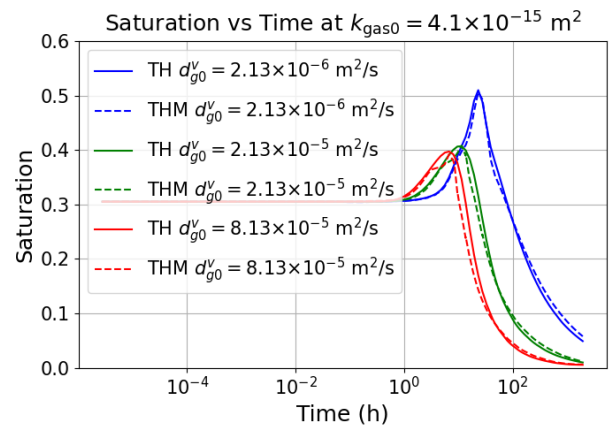
325 **3.3.2. Coupled THM simulations**

326 This section examines the mechanical effect on the evolution of the degree of saturation at the  
 327 monitoring point in Figure 1. A roller boundary condition is applied to all boundaries of the 1D  
 328 axisymmetric geometry to enforce the constant volume condition. The mechanical properties and  
 329 parameters are the same as those given in Section 4.2.2, while the hydro-mechanical properties are  
 330 given in Table 1.

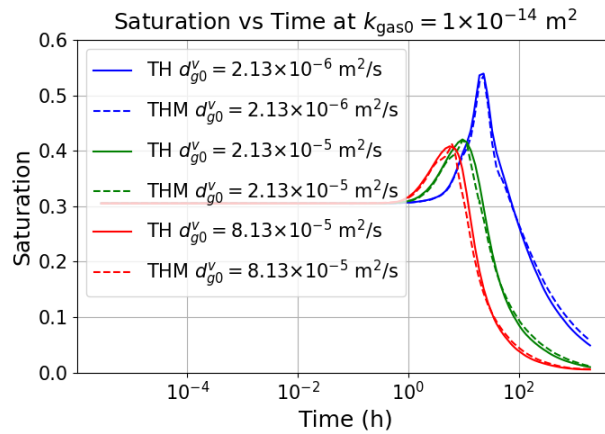
331 The comparison between TH and THM simulations in Figure 6 highlights the influence of mechanical  
 332 coupling on saturation evolution. In all cases, the THM model predicts slightly lower peak saturations  
 333 compared to the TH model. However, as the intrinsic gas permeability increases, the differences  
 334 between TH and THM results become less pronounced, indicating that vapor transport dominates  
 335 over mechanical effects under higher permeability conditions. Overall, the mechanical effect on  
 336 saturation evolution is minimal in the 1D axisymmetric simulations.



(a)  $k_{gas0} = 1.0 \times 10^{-15} m^2$



(b)  $k_{gas0} = 4.1 \times 10^{-15} m^2$



(c)  $k_{gas0} = 1.0 \times 10^{-14} m^2$

Figure 6 Effect of intrinsic gas permeability on the evolution of temperature and degree of saturation

## 4. NUMERICAL SIMULATION OF TANK TESTS AND ANALYSIS

Two tank tests investigating the heating and hydration behavior of bentonite were conducted at UCSD [8, 9, 46]. Detailed descriptions of the experimental procedures for Tank Test 1 and Tank Test 2 can be found in [9, 46]. In Tank Test 1, bentonite was subjected to a constant vertical stress on the top boundary during the heating phase, followed by a constant volume condition during hydration. In contrast, the Tank Test 2 maintained a constant volume condition throughout the entire experiment. Additionally, in Tank Test 2, a cylindrical aluminum sleeve was wrapped around the heater to simulate the presence of a canister, resulting in a larger heating area compared to the first test that resulted in higher bentonite temperatures.

### 4.1. Simulation Results of Tank Test 1

#### 4.1.1. Geometry, Boundary and Initial Conditions

Figure 7 presents the key dimensions of Tank Test 1 and locations of sensors. To realistically simulate the heat transfer and hydration process, all the necessary components (including the aluminum tank, the insulation wool, the atmosphere, the channel to the water source and the water source) have been explicitly included in the grid for TOUGH3, as seen in Figure 8(a). In contrast, only internal materials (including the heater, the

bentonite, the hydration layer and the concrete cap) that may involve the critical mechanical process are considered in the grid for FLAC, as seen in Figure 8(b). This meshing strategy makes the whole simulation more stable and efficient. To further reduce the computational effort, Tank Test 1 is assumed to be axis-symmetric, and therefore, only one element is used along the circumferential direction. The azimuthal angle is set as 10 degrees.

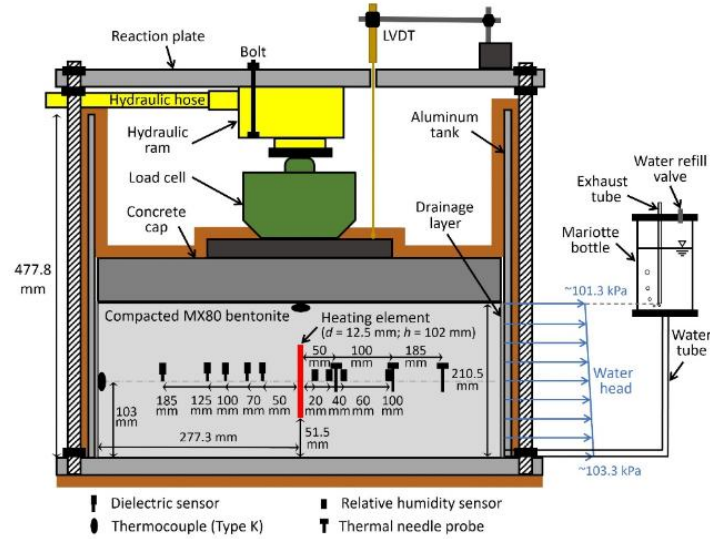


Figure 7 Schematic diagram of Tank Test 1 and locations of sensors [9]

Roller boundary conditions are applied to all external boundaries of the FLAC grid, except for the top boundary, which is initially subjected to a constant vertical stress of 1.98 kPa from a concrete cap. This top boundary condition is switched to a roller constraint just prior to the onset of hydration. Gravity is neglected in simulations. In the TOUGH3 model, the atmosphere is explicitly represented by the “BOUND” domain, and non-flux boundary conditions are applied to all external boundaries for both thermal and hydraulic processes.

In the bentonite domain, the initial conditions are set as follows: gas pressure of 0.1 MPa, degree of saturation of 0.323, and temperature of 22.0 °C. An initial isotropic stress of  $-0.10198$  MPa is imposed. The heating process is simulated by applying a constant temperature boundary (200 °C) at the heater. Hydration is modeled by switching the permeability of domains CHAN1, CHAN2, and SOURS from zero to a high value of  $1.6 \times 10^{-13} \text{ m}^2$  at 2543 hours after the start of heating. The total simulation period is 6747 hours. It is important to note that the thermal-hydraulic properties of the hydration layer (HYDRA domain) are identical to those of bentonite, except for its intrinsic water permeability, which is several orders of magnitude higher than that of the bentonite sample. Our results indicate that the intrinsic permeability of the hydration layer plays a critical role in controlling water inflow and the evolution of swelling pressure.

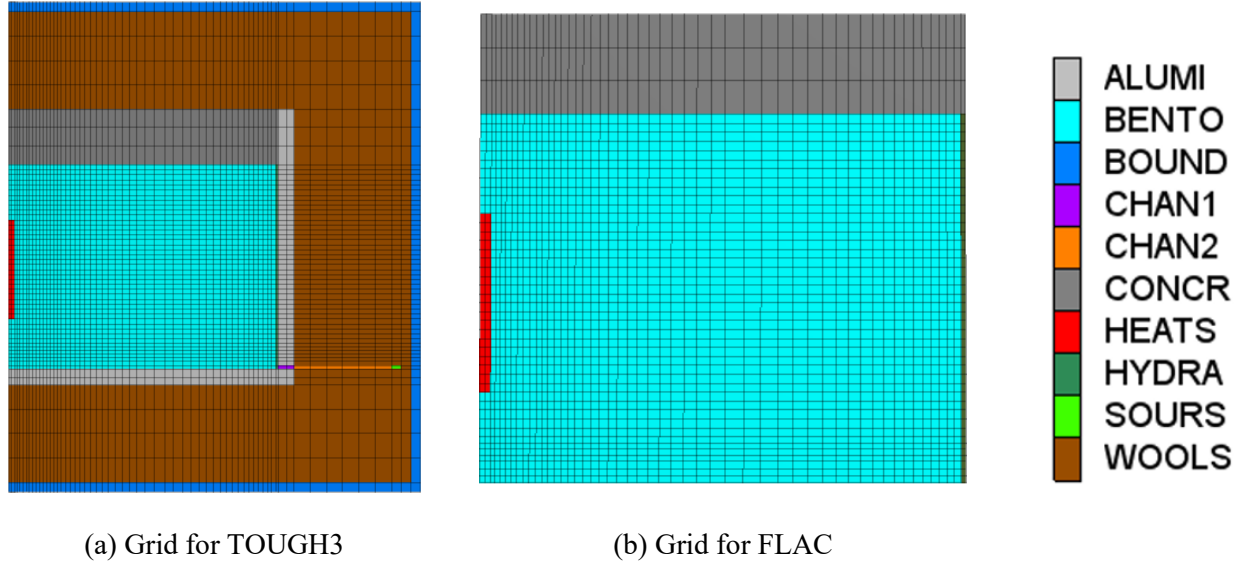


Figure 8 Grids for Tank Test 1 simulation (ALUMI: Aluminum container; BENTO: Bentonite sample; BOUND: Atmospheric boundary; CHAN1, 2: Conductive Channel 1 and 2; CONCR: Concrete loading plate; HEATS: Heater; HYDRA: Hydration layer; SOURS: Water source; WOOLS: Thermal insulation material)

#### 4.1.2. Material Properties

The material properties used for the key components in the tank-scale test are summarized in Table 2. Parameters for the state surface model are:  $A=1.001268$ ,  $B=-0.0552446$ ,  $C=-0.0406413$ ,  $D=0.00479977$ . The latter three parameters were adopted from [40] and the first parameter  $A$  is calculated based on these values, the initial suction and the initial porosity. Additional experimental work is needed to refine these values. For the temperature-dependent soil-water retention model, the parameters are:  $M = 0.12$ ,  $n = 1.15$ ,  $\alpha^{-1} = 3.3e6 \text{ MPa}$ ,  $CEC_{max} = 0.8 \text{ meq/g}$ ,  $SSA = 750 \text{ m}^2/\text{g}$ . The intrinsic gas permeability is characterized by:  $k_{gas0}=4.1 \times 10^{-15} \text{ m}^2$ ,  $n_k=2.0$ . The diffusion coefficient in Eq. (11) is scaled by a factor 3.817 for calibration purposes. For the thermal conductivity model, the parameters are:  $S_c = 0.58$ ,  $\chi = 3.8$ . As will be discussed in Section 4.2, our experiments demonstrated that the hydration layer can become clogged by swollen bentonite, leading to a reduction in its intrinsic permeability. To account for this effect, an evolutionary model for intrinsic permeability is proposed here as:

$$k_{in}^{hy} = \begin{cases} k_0^{hy}, & \text{if } t < t_{start} \\ 10^{[1-w(t)] \log_{10} k_0^{hy} + w(t) \log_{10} k_f^{hy}}, & \text{if } t_{start} \leq t \leq t_{end} \\ k_f^{hy}, & \text{if } t > t_{end} \end{cases} \quad (36)$$

where  $w(t) = \frac{t-t_{start}}{t_{end}-t_{start}}$  is the weight for permeability transition,  $k_0^{hy}$  is the intrinsic permeability before permeability transition at  $t_{start}$ ,  $k_f^{hy}$  is the intrinsic permeability after the end of permeability transition. Unless otherwise stated, the parameters for simulating Tank Test 1 are  $k_0^{hy} = 3.0 \times 10^{-15} \text{ m}^2$ ,  $k_f^{hy} = 3.0 \times 10^{-17} \text{ m}^2$ ,  $t_{start} = 3098.56 \text{ h}$ , and  $t_{end} = 4487.44 \text{ h}$ .

Table 2 Model parameters for the key components in the THM analysis

| Parameter                                                             | Heater | Aluminum | Bentonite                | Concrete | Wools |
|-----------------------------------------------------------------------|--------|----------|--------------------------|----------|-------|
| Solid grain density [kg/m <sup>3</sup> ]                              | 7800   | 6700     | 2660                     | 3200     | 500   |
| Initial porosity                                                      | 0      | 0        | 0.508                    | 0.1      | 0.1   |
| Young's modulus [GPa]                                                 | 120    | 70       | -                        | 30       | -     |
| Poisson's ratio                                                       | 0.3    | 0.33     | 0.3                      | 0.25     | -     |
| Grain specific heat capacity [J/(kg*K)]                               | 1.0e50 | 887.0    | 880                      | 880      | 700   |
| Thermal conductivity (Wet) [W/(m*K)]                                  | 20.0   | 237.0    | 0.93                     | 0.94     | 0.46  |
| Thermal expansion coefficient<br>×10 <sup>-5</sup> [K <sup>-1</sup> ] | 0      | 2.0      | 6.6                      | 1.2      | 0     |
| Initial liquid permeability [m <sup>2</sup> ]                         | 0      | 0        | 3.96 × 10 <sup>-20</sup> | 0        | 0     |

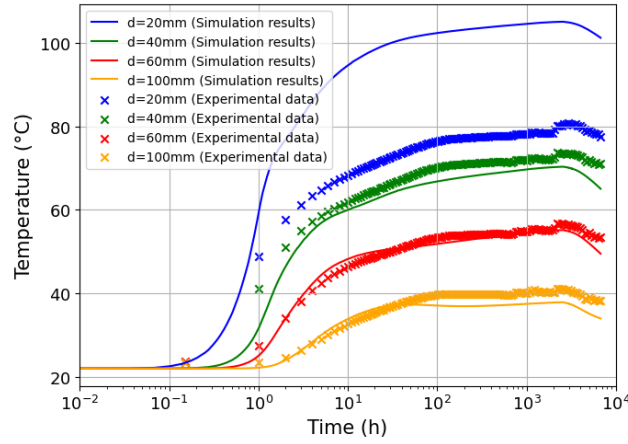
396

### 397 4.1.3. Evolution of Temperature, RH and Volumetric Water Content

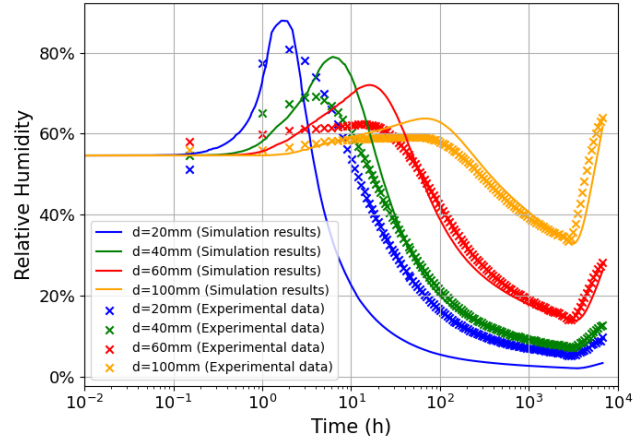
398 Figure 9 presents a comparison between the simulated and measured evolution of temperature and relative  
399 humidity (RH) at various radial distances from the heater, as recorded by RH sensors. Overall, the numerical  
400 results show good agreement with the experimental data for both temperature and RH. During the heating  
401 phase, the relative humidity initially increases due to vapor transfer and condensation near cooler regions,  
402 followed by a decline driven by the drying effect of elevated temperatures. After hydration is initiated, RH  
403 exhibits a sharp increase, with the rate of increase diminishing as the distance from the hydration boundary  
404 grows.

405 A notable discrepancy arises at the sensor location nominally placed 20 mm from the heater. The simulated  
406 temperature at this point is significantly higher than the measured values. Moreover, the experimental data  
407 reveal that the temperature gradient between 20 mm and 40 mm is unexpectedly small compared to the gradient  
408 between 40 mm and 60 mm. For a homogeneous medium, a steeper temperature gradient is typically expected  
409 closer to the heat source. This observation suggests that the RH sensor labeled as being 20 mm from the heater  
410 may have shifted slightly during the test, resulting in its actual position being farther from the heater than  
411 recorded. Even a small spatial offset could significantly influence the measured temperature due to the steep  
412 thermal gradient near the heat source. Furthermore, local heterogeneities in dry density around the heater may  
413 have contributed to the discrepancy by altering the thermal conductivity and, consequently, the heat transfer  
414 behavior in that region.

415



(a) Temperature



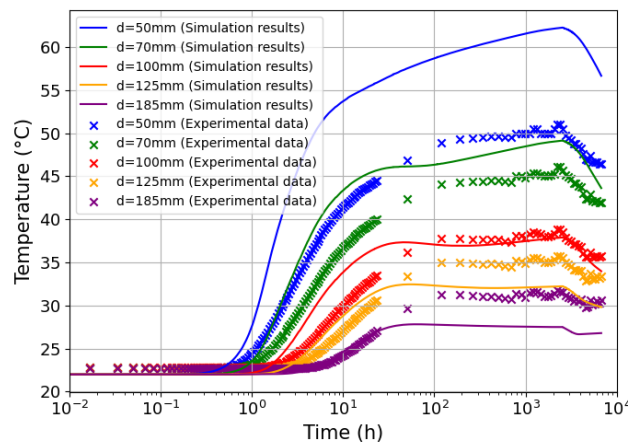
(b) Relative humidity

Figure 9 Comparisons with temperature and RH obtained from RH sensors

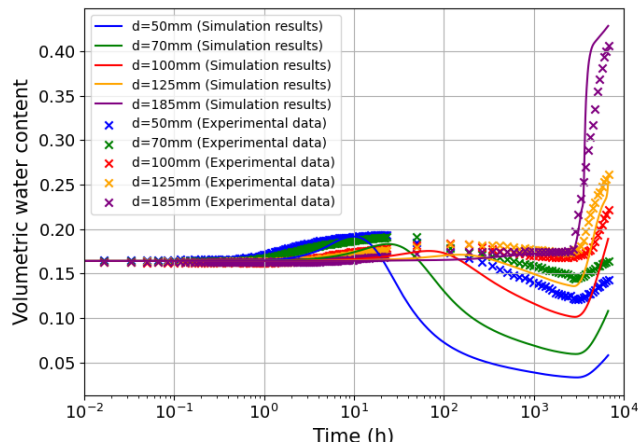
Figure 10 compares the evolution of temperature and volumetric water content obtained from numerical simulations and experimental measurements using dielectric sensors. Compared to the results shown in Figure 9, notable discrepancies are observed for both temperature and water content. These differences may be attributed to heterogeneities in the dry density or initial moisture content of the bentonite, as well as potential limitations in the accuracy of the dielectric sensors.

Anomalous behavior is particularly evident in Figure 9(a) and Figure 10(a), where the temperature at  $d=60$  mm (red crosses in Figure 9(a)) exceeds that at  $d=50$  mm (blue crosses in Figure 10(a)), contrary to the expected thermal gradient near the heat source. In terms of moisture behavior, simulated volumetric water contents are generally lower than those measured, except at locations close to the hydration boundary during the hydration stage, such as  $d=125$  mm and at  $d=185$  mm (purple and yellow lines in Figure 10(b)), where good agreement is observed. Furthermore, a notable inconsistency arises between the RH and dielectric sensor readings at  $d=100$  mm: the RH sensor indicates a substantial drop in relative humidity prior to hydration (Figure 9(b), yellow crosses), while the dielectric sensor shows a slight increase in volumetric water content at the same location (Figure 10(b), red crosses). This discrepancy may result from potential limitations in the accuracy of the dielectric sensors, or from the heterogeneous distribution of dry density and water content.

Despite these differences, the overall trends in both temperature and volumetric water content are well reproduced by the coupled THM model.



(a) Temperature



(b) Volumetric water content

#### 4.1.4. Evolution of Water Inlet and Swelling Pressure

Figure 11 (a) presents a comparison between the simulated and measured cumulative water inlet volume. The intrinsic permeability of hydration layer varies across the three simulations cases. Simulation case 1 corresponds to the baseline case analyzed in the previous subsection. In simulation case 2, the start and the end times of the permeability transition are  $t_{start} = 3654.11h$ , and  $t_{end} = 5043h$ , respectively, while all other parameters remain the same as in case 1. In simulation case 3, the initial intrinsic permeability is set to  $k_0^{hy} = 1.0 \times 10^{-15} m^2$ , with all other parameters again matching those of case 1. Since the permeability transition from a higher to a lower value occurs later in case 2 than in case 1, a greater volume of water enters the bentonite sample in case 2, as evidenced by the dashed versus solid lines in Figure 11(a). Consequently, the swelling pressure in case 2 reaches a higher value, as shown in Figure 11(b). In case 3, the smaller initial intrinsic permeability leads to reduced water intake and a correspondingly lower swelling pressure during hydration. These simulation results highlight that both the volume of water inlet and the resulting swelling pressure are highly sensitive to the evolution of the intrinsic permeability of the hydration layer. Therefore, it is essential to design laboratory-scale hydration systems that can realistically replicate field hydration processes in order to reliably assess bentonite performance.

Moreover, while the cumulative water inlet predicted by case 1 aligns well with the experimental data, the swelling pressure is underestimated, as seen from the solid lines in Figure 11. Additionally, the evolution of the simulated swelling pressure differs from the experimental trend. In the simulations, the swelling pressure continues to increase linearly after the permeability transition, failing to reproduce the plateau behavior observed experimentally. This discrepancy may stem from limitations of the current state-surface constitutive model, particularly in its ability to capture complex mechanical phenomena such as pore structure collapse and thermo-plastic behavior. To better represent these mechanisms, more advanced mechanical models will be required in future work.

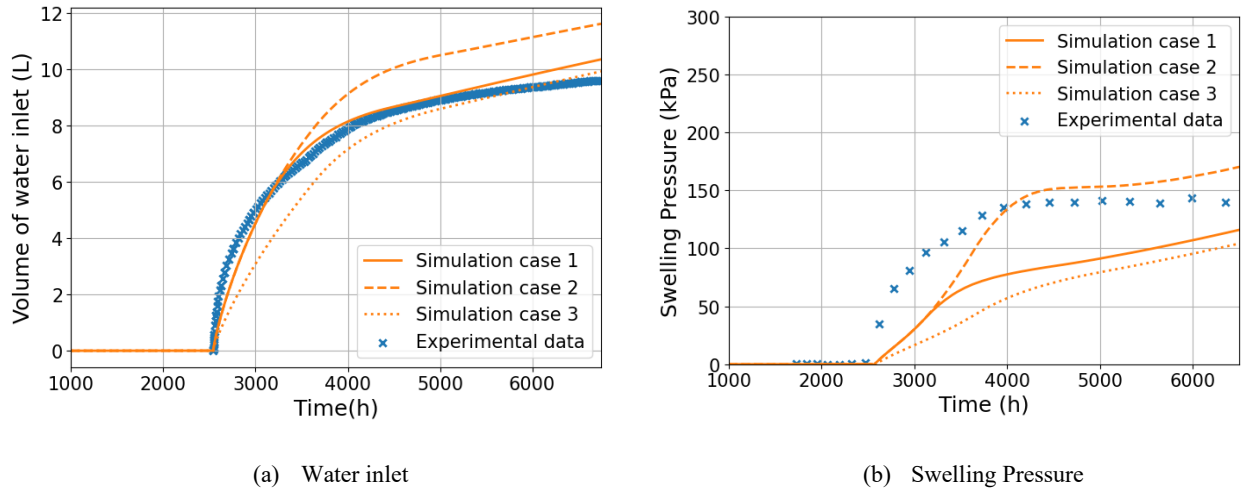


Figure 11 Comparison of volume of water inlet and swelling pressure between numerical and experimental results (Simulation case 1:  $k_0^{hy} = 3.0 \times 10^{-15} m^2$ ,  $t_{start} = 3098.56h$ ,  $t_{end} = 4487.44h$ ; Simulation case 2:  $k_0^{hy} = 3.0 \times 10^{-15} m^2$ ,  $t_{start} = 3654.11h$ ,  $t_{end} = 5043h$ ; Simulation case 3:  $k_0^{hy} = 1.0 \times 10^{-15} m^2$ ,  $t_{start} = 3098.56h$ ,  $t_{end} = 4487.44h$ )

#### 4.1.5. Horizontal Profiles During Heating

The profiles for temperature, porosity, degree of saturation, and stress are constructed along a horizontal monitoring line, positioned at the same vertical level as the RH sensors. Figure 12 illustrates these profiles at six selected time points during the heating phase, prior to the onset of hydration.

As shown in Figure 12 (a), the temperature near the heater rises rapidly and stabilizes within approximately 10 hours after heating begins. In the early stages, porosity near the heater increases significantly (Figure 12 (b)), primarily due to thermal expansion and localized hydration driven by vapor condensation. However, as heating continues, porosity decreases and eventually falls below its initial value. This reduction is attributed to shrinkage caused by drying and mechanical compression from adjacent swelling zones formed due to vapor condensation. Figure 12 (c) demonstrates that vapor condensation-induced hydration gradually propagates radially outward from the heater, leading to the formation of distinct dehydrated and hydrated zones. This zonation becomes increasingly pronounced at later times, as shown by the saturation profiles at 41.683 days and 105.324 days. As shown in Figure 12 (d), the vertical stress along the top boundary of the soil column increases slightly relative to the initial condition at the early stages, as shown by the red line. This increase is likely driven by both thermal expansion and swelling resulting from vapor condensation. At later stages, the vertical stress near the heater is lower than that near the hydration boundary, reflecting the more intense drying-induced shrinkage occurring in the hotter, inner region of the bentonite.

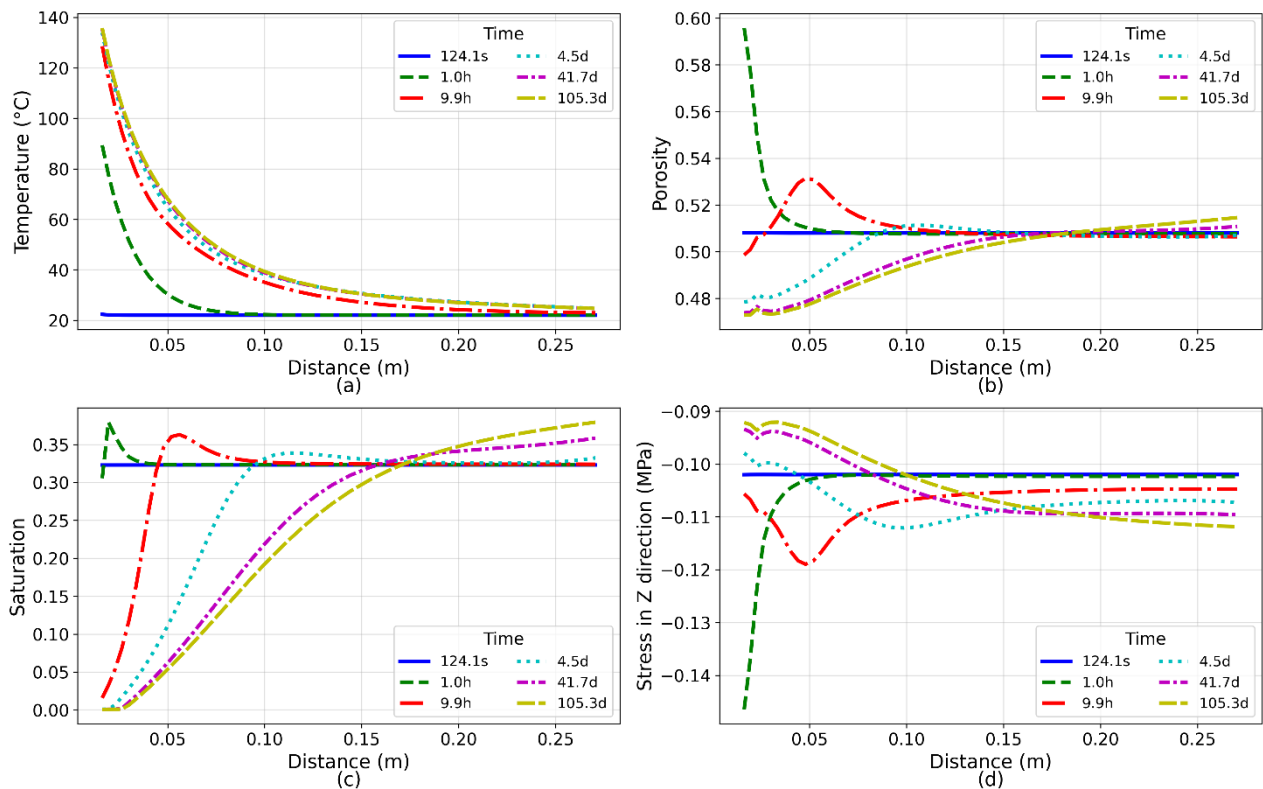


Figure 12 Profiles of temperature, porosity, saturation and stress along radial direction during heating

#### 4.1.6. Horizontal Profiles During Hydration

Figure 13 shows the evolution of temperature, porosity, water saturation, and vertical stress along the radial direction at six different time points following the onset of hydration.

As shown in Figure 13 (a), the hydration process has a minimal effect on the temperature distribution, which slightly decreases after the hydration started. In contrast, porosity undergoes significant changes as hydration

progresses. During the early phase of hydration, swelling occurs primarily near the hydration boundary, resulting in a local increase in porosity, as illustrated by the red curve in Figure 13 (b). As the hydration front propagates toward the heater, bentonite in the central region becomes increasingly saturated and begins to swell, as evidenced in Figure 13 (c) and (d). This central swelling exerts compressive forces on the adjacent zones near both the heater and the hydration boundary. Consequently, porosity in these regions decreases over time, as observed in the profiles at 174.506 days, 204.598 days, and 281.125 days in Figure 13 (b). Interestingly, in certain regions (e.g., within the distance range [0.1, 0.15] m at 281.125 days), the degree of saturation exceeds its initial value, while the porosity remains below the initial value. This suggests that the deformation of bentonite in this zone is primarily driven by compressive forces from the hydration side. Consequently, swelling on the hydration side can strongly compress the bentonite in the inner regions. A slight increase in porosity is observed near the heater, which can be attributed to thermal expansion in this high-temperature region. The continuous uptake of water and associated swelling lead to the development of swelling pressure within the bentonite. This is reflected in the progressive increase in compressive vertical stress shown in Figure 13 (d). Vertical stress becomes more negative (i.e., more compressive) over time, particularly in the later stages of hydration.

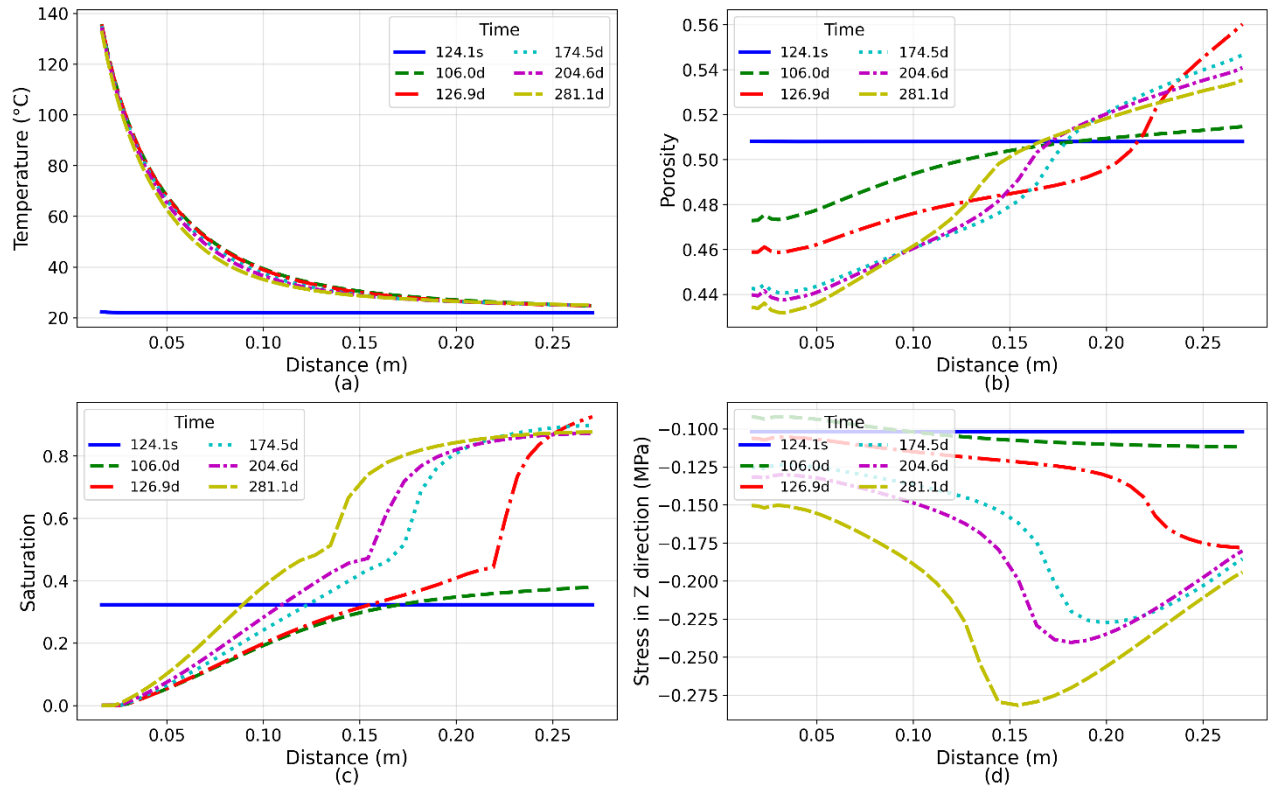


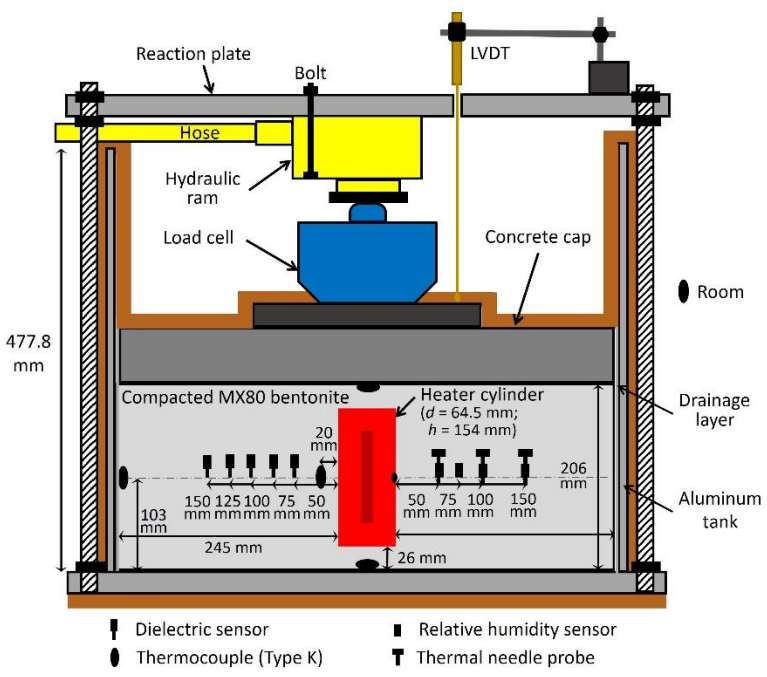
Figure 13 Profiles of temperature, porosity, saturation and stress along radial direction during hydration

## 4.2. Simulation Results of Tank Test 2

### 4.2.1. Geometry, Boundary and Initial Conditions

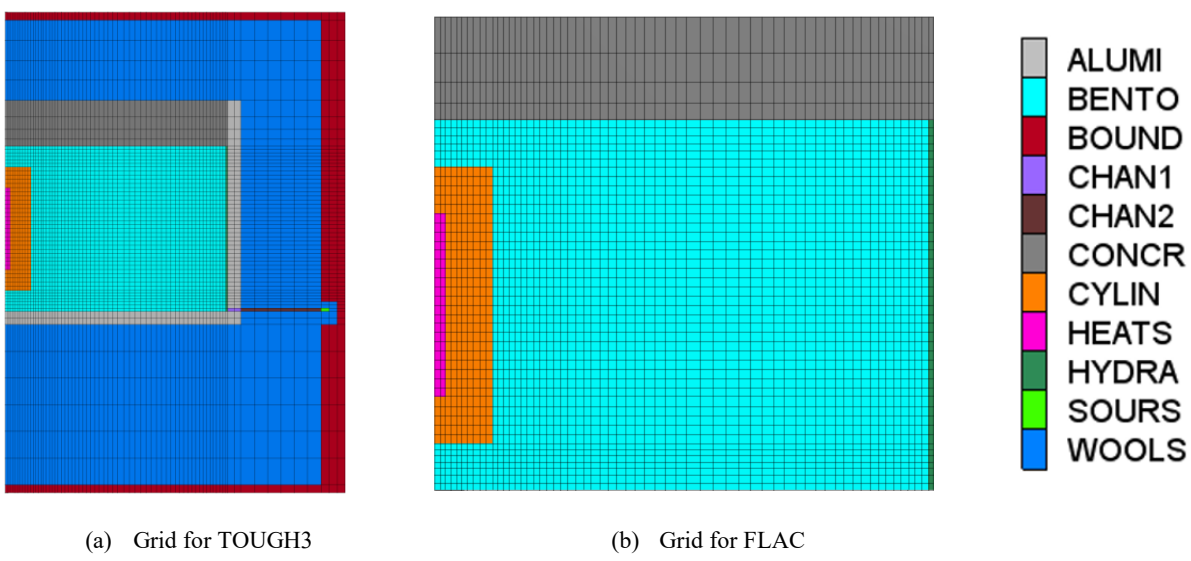
Figure 14 presents the key dimensions of Tank Test 2 and the locations of the sensors [46]. The test is similar to Tank Test 1 but a large aluminum cylinder was added around the heater to mimic the effects of the canister. The computational grids for TOUGH3 and FLAC are shown in Figure 15. The meshing strategy follows a

511 similar approach to that of Tank Test 1, with the addition of a CYLIN domain to represent the aluminum  
 512 cylinder.



513  
 514 Figure 14 Schematic diagram of Tank Test 2 and locations of sensors [46].

515 Roller boundaries are applied to all external boundaries to enforce the constant volume condition. No flux  
 516 boundaries are specified on all external boundaries for both thermal and hydraulic process. In the bentonite  
 517 domain, the initial gas pressure, degree of saturation and temperature are set to 0.1MPa, 0.305 and 22.0 C,  
 518 respectively. The initial isotropic stress state is -0.10198 MPa. A time-dependent temperature boundary is  
 519 applied at the heater to simulate the heating process. Hydration is modeled by switching the intrinsic  
 520 permeability for domain CHAN1, CHAN2 and SOURS from 0 to 1.6e-13 m<sup>2</sup> at 1950h after the start of heating.  
 521 The total simulation time is 8888.9h.



522 Figure 15 Grids for Tank Test 2 simulation (ALUMI: Aluminum container; BENTO: Bentonite sample;  
 523 BOUND: Atmospheric boundary; CHAN1, 2: Conductive Channel 1 and 2; CONCR: Concrete loading

plate; CYLIN: Aluminum cylinder; HEATS: Heater; HYDRA: Hydration layer; SOURS: Water source;  
WOOLS: Thermal insulation material)

#### 4.2.2. Material Properties

The material properties for the key components in the Tank Test 2 are listed in Table 3. The parameters for state surface model are:  $A=1.015$ ,  $B=-0.0552446$ ,  $C=-0.0406413$ ,  $D=0.00479977$ . The parameters for the water retention model are identical to those for Tank Test 1. The intrinsic gas permeability is characterized by:  $k_{gas0}=4.1 \times 10^{-15} m^2$ ,  $n_k=2.0$ . The diffusion coefficient in Eq. (11) is scaled by a factor 3.817 for calibration purposes. For the thermal conductivity model, the parameters are:  $S_c = 0.58$ ,  $\chi = 3.8$ . The intrinsic permeability of the hydration layer is calculated by Eq. (36). In this section, we performed two simulation cases with varying permeability of hydration layer. In Case 1, the parameters for the evolutionary permeability model were set as:  $k_0^{hy} = 4.1 \times 10^{-17} m^2$ ,  $k_f^{hy} = 5.4 \times 10^{-20} m^2$ ,  $t_{start} = 1950h$ , and  $t_{end} = 2220.1h$ . These parameters are determined through calibration of the simulated water inlet volume against experimental data, as discussed in subsection 4.2.4. In Case 2,  $k_f^{hy} = 4.1 \times 10^{-17} m^2$  and all other parameters remained identical to those in Case 1.

Table 3 Model parameters for the key components in the THM analysis

| Parameter                                                  | Heater | Aluminum | Bentonite             | Concrete | Wools |
|------------------------------------------------------------|--------|----------|-----------------------|----------|-------|
| Solid (grain) density [kg/m <sup>3</sup> ]                 | 7800   | 6700     | 2700                  | 3200     | 500   |
| Initial porosity                                           | 0      | 0        | 0.51                  | 0.1      | 0.1   |
| Young's modulus [GPa]                                      | 120    | 70       | -                     | 30       | -     |
| Poisson's ratio                                            | 0.3    | 0.33     | 0.3                   | 0.25     | -     |
| Grain specific heat capacity [J/(kg*K)]                    | 1.0e50 | 887.0    | 880                   | 880      | 700   |
| Thermal conductivity (Wet) [W/(m*K)]                       | 20.0   | 237.0    | 0.93                  | 0.94     | 0.46  |
| Thermal expansion coefficient<br>$\times 10^{-5} [K^{-1}]$ | 0      | 2.0      | 6.6                   | 1.2      | 0     |
| Initial liquid permeability [m <sup>2</sup> ]              | 0      | 0        | $4.1 \times 10^{-20}$ | 0        | 0     |

#### 4.2.3. Evolution of Temperature, RH and Volumetric Water Content

Figure 16 presents the comparison of temperature and RH between numerical results from the two simulation cases and experimental data. Despite some deviations observed, the numerical results for both temperature and relative humidity (solid lines) are in good agreement with the experimental data before hydration. The transient hydration caused by vapor condensation and the dehydration due to the high temperature are well described by the proposed model.

However, once hydration begins, the measured RH increases at a much smaller rate than that in Tank Test 1. One possible explanation for this phenomenon is clogging of the hydration layer, potentially caused by the intrusion of clay particles. To investigate the influence of this clogging on the hydration process, the initial intrinsic permeability in Case 1 was reduced from  $4.1 \times 10^{-17} m^2$  to  $5.4 \times 10^{-20} m^2$ , whereas in Case 2, the permeability was kept constant throughout the hydration phase. As illustrated in Figure 16, the intrinsic permeability of hydration layer plays a critical role in governing the evolution of both temperature and RH during hydration. In Case 1, the temperature exhibits only a slight decrease, while in Case 2, a more pronounced temperature drop is observed. This difference may be attributed to enhanced heat transfer resulting from increased water infiltration. Similarly, the increase of RH in Case 1 is considerably slower than in Case 2.

When the intrinsic permeability approaches that of the bentonite matrix, the effective hydration boundary is restricted to the region in direct contact with the hydration channel. This is evident in Figure 17, where the hydration boundary is confined to the right corner of the domain under low permeability conditions. Consequently, the overall hydration rate is substantially reduced due to clogging of the hydration layer.

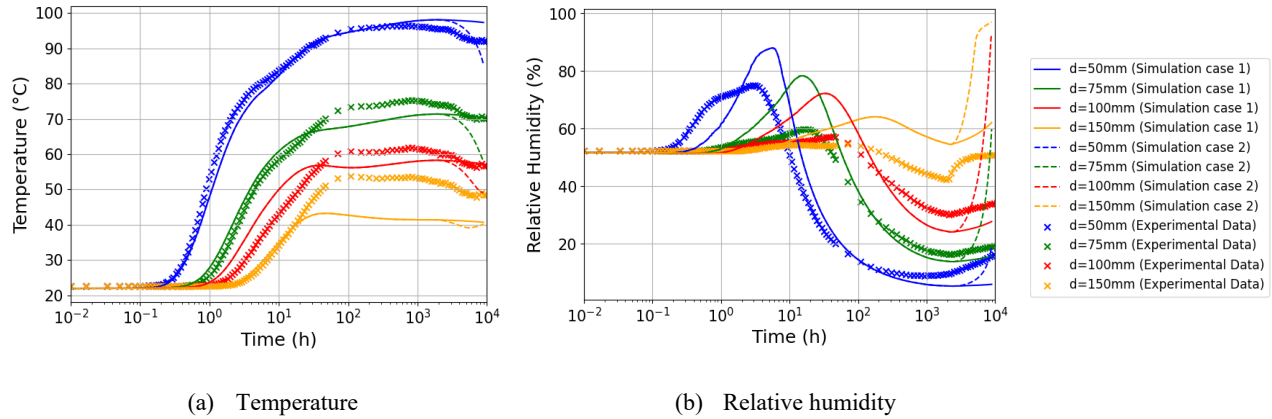


Figure 16 Evolution of temperature and RH in Tank Test 2 (Simulation case 1:  $k_f^{hy} = 5.4 \times 10^{-20} m^2$ ; Simulation case 2:  $k_f^{hy} = 4.1 \times 10^{-17} m^2$  )

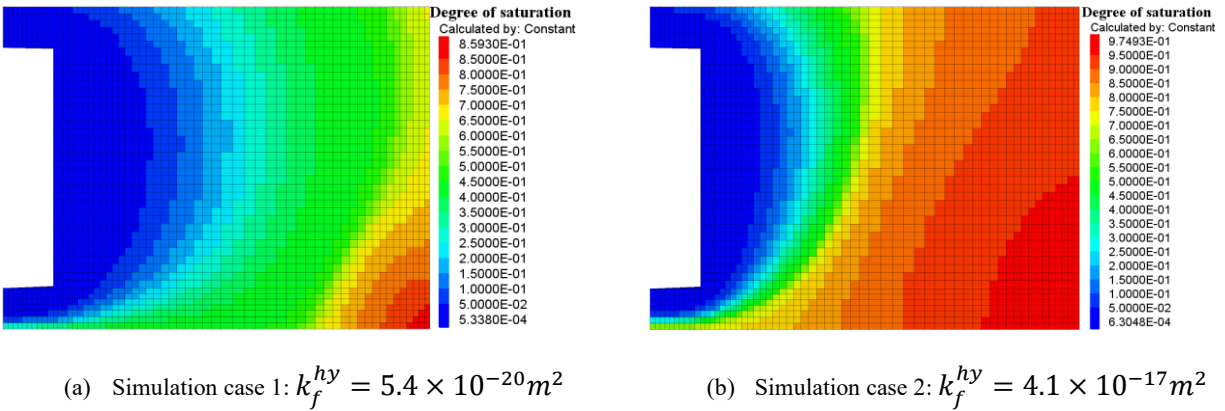


Figure 17 Distribution of degree of saturation at the end of simulation for the two cases

This clogging hypothesis is supported by observations of the bentonite condition following dismantling of the test setup [46]. Gravimetric water content sampling of the bentonite surrounding the water inlets revealed that the highly saturated zone was confined to the vicinity of the inlets, while regions farther from the inlets had lower degrees of saturation. While hydration still occurred in the tank tests at a slower than expected rate, possible clogging of the hydration layer by the hydrated bentonite likely did not lead to a uniform distribution of water inflow over the height of the soil layer.

Figure 18 compares the simulated evolution of temperature and volumetric water content with experimental measurements obtained from dielectric sensors in Tank Test 2. Similar to the results for Tank Test 1 (Figure 10), noticeable discrepancies are observed between the simulations and the experimental data for both temperature and volumetric water content. These differences may arise from heterogeneities in the dry density or initial moisture content of the bentonite, as well as potential limitations in the accuracy of the dielectric sensors.

During the heat phase, a notable inconsistency is evident at  $d=100$  mm between the RH and dielectric sensor readings. Specifically, the RH sensor indicates a pronounced drop in RH prior to vaporization (Figure 16(b), yellow crosses), whereas the dielectric sensor shows a slight increase in volumetric water content at the same location (Figure 18(b), red crosses). This discrepancy may be attributed to sensor limitations or to local heterogeneities in dry density and moisture distribution. During the hydration phase, simulations assuming a high permeability in the hydration layer (Simulation Case 2) significantly overpredict the water infiltration compared to experimental data. In contrast, when the clogging effect is represented by reducing the hydration layer permeability (Simulation Case 1), the simulated trends for both temperature and volumetric water content show much improved agreement with the experimental observations.

Overall, despite some discrepancies, the coupled THM model successfully captures the key trends in both temperature and volumetric water content during Tank Test 2.

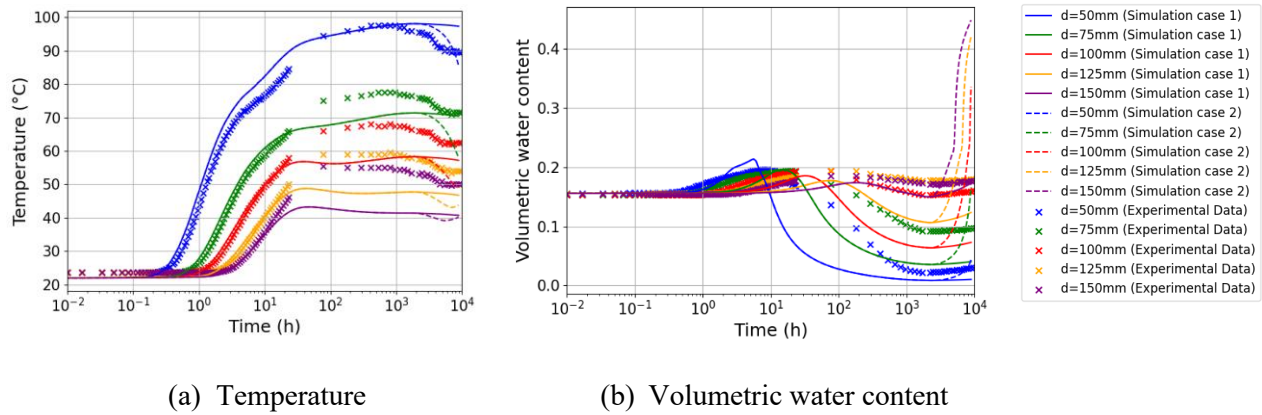
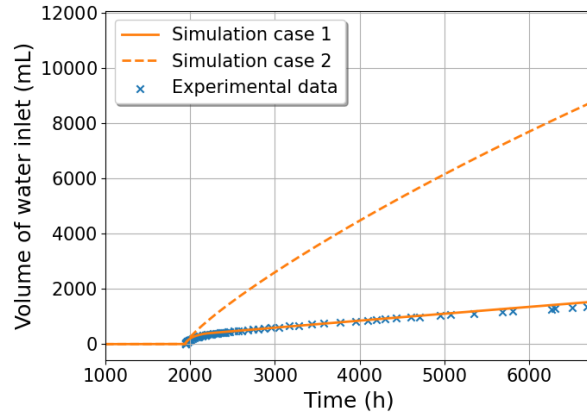


Figure 18 Evolution of temperature and volumetric water content in Tank Test 2 (Simulation case 1:  $k_f^{hy} = 5.4 \times 10^{-20} m^2$ ; Simulation case 2:  $k_f^{hy} = 4.1 \times 10^{-17} m^2$ )

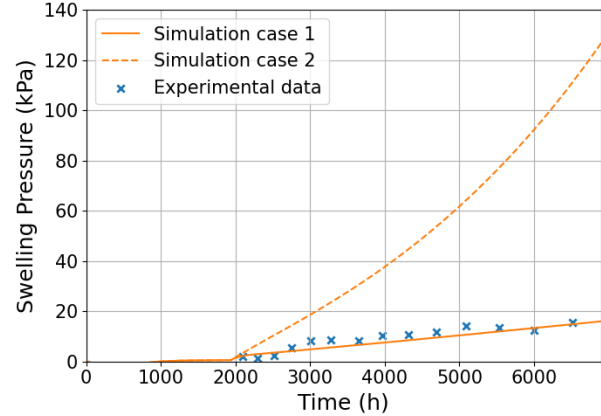
#### 4.2.4. Evolution of Water Inlet and Swelling Pressure

Figure 19(a) compares the simulated and experimental evolution of the water inlet volume. The parameters used in Simulation Case 1 were calibrated to match the experimental measurements of water inlet volume, resulting in good agreement with the observed data. Notably, the model also reproduces the swelling pressure trends at the top of the bentonite with reasonable accuracy, as shown in Figure 19(b), indicating that the state-surface performed well in this simulation case.

In contrast, Simulation Case 2, where the clogging effect is not considered and the hydration layer permeability remains high, predicts significantly larger water inflow and swelling pressure compared to both Case 1 and the experimental observations. These results further highlight that the permeability of the hydration layer plays a critical role in controlling the hydration rate and the development of swelling pressure in the system.



(a) Volume of water inlet



(b) Swelling pressure

Figure 19 Evolution of volume of water inlet and swelling pressure (Simulation case 1:  $k_f^{hy} = 5.4 \times 10^{-20} m^2$ ; Simulation case 2:  $k_f^{hy} = 4.1 \times 10^{-17} m^2$ )

#### 4.2.5. Horizontal Profiles During Heating

Figure 20 presents the evolution of temperature, porosity, water saturation, and vertical stress at six different time points during the heating phase, prior to hydration. The temperature profile (Figure 20(a)) stabilizes after approximately 12 hours of heating, consistent with the trends observed in Tank Test 1. The saturation profiles (Figure 20(c)) clearly capture the vapor condensation-induced hydration and temperature-driven dehydration. As heating progresses, the bentonite was gradually partitioned into a hydrated zone and a dehydrated zone along the radial direction, similar to the behavior observed in Tank Test 1.

In contrast, the distribution of porosity along the monitoring line differs from that observed in Tank Test 1. In Tank Test 1, porosity near the heater decreased significantly below the initial value (see curves at 4.494 d, 41.683 d, and 105.324 d in Figure 12). However, in Tank Test 2, porosity near the aluminum cylinder remains either slightly above or just below the initial value (see curves at 4.554 d, 42.587 d, and 80.660 d in Figure 20(b)). This difference can be attributed to the larger heating surface area introduced by the aluminum cylinder, which enhances thermal expansion effects. The stronger thermal expansion in Tank Test 2 effectively offsets the shrinkage induced by drying near the aluminum cylinder at later stages of heating.

Interestingly, both the porosity and vertical stress profiles exhibit distinct peaks near 0.05m at early times (e.g., at  $t=1h$ ), as seen in Figure 20(b) and (d). This behavior suggests a complex interplay between thermal expansion and drying-induced shrinkage in the region surrounding the aluminum cylinder during the initial stages of heating. Additionally, the vertical stress profile (Figure 20 (d)) evolves dynamically over time, influenced by vapor transport and condensation, as well as by thermal expansion of the bentonite matrix.

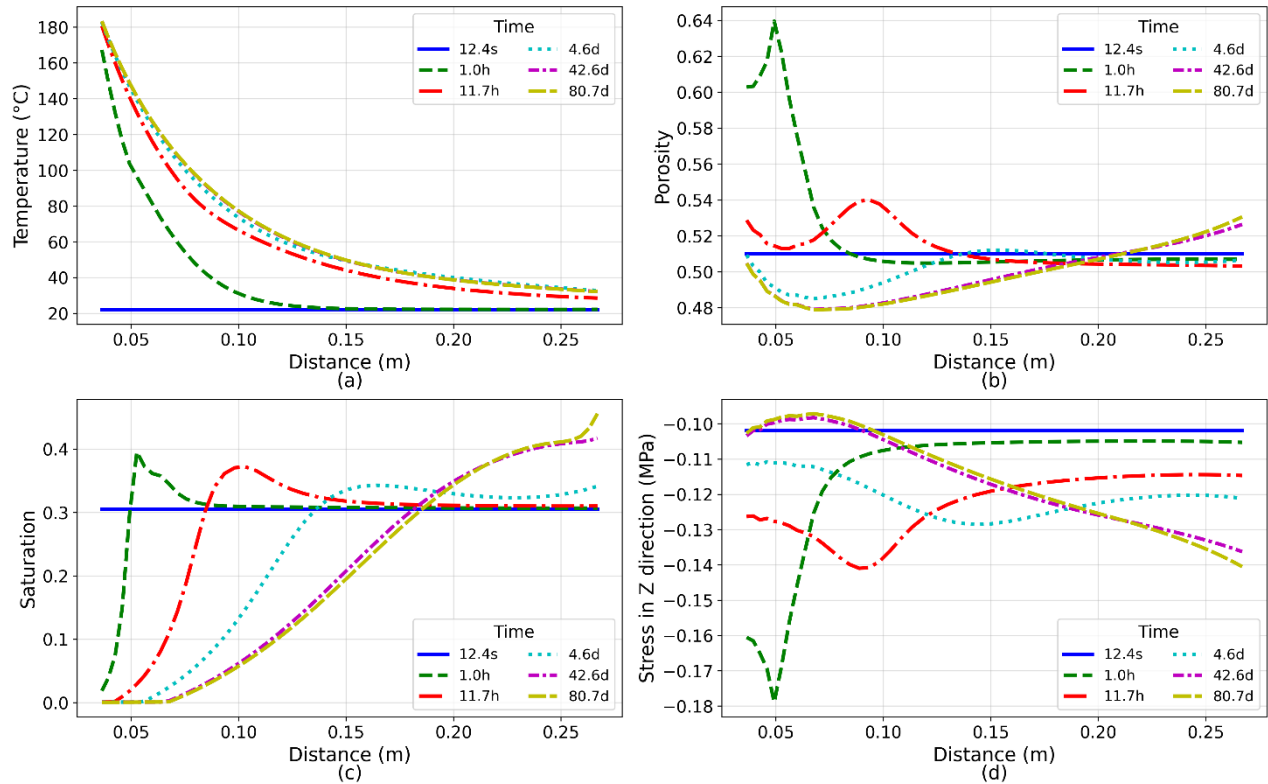


Figure 20 Profiles of temperature, porosity, saturation and stress along z direction during heating

#### 4.2.6. Horizontal Profiles During Hydration

Figure 21 presents the profiles of temperature, porosity, water saturation, and vertical stress at six different time points during the hydration phase, for Simulation Case 2 where the clogging effect of the hydration layer is not considered. The hydration process leads to a decrease in temperature along the profiles, primarily due to the enhanced thermal conductivity associated with increased water content in the bentonite, as shown in Figure 21 (a).

As the hydration front advances toward the heater, porosity exhibits notable dynamic variations (Figure 21 (b)). In the early stages of hydration, significant swelling of bentonite occurs near the hydration boundary, resulting in an increase in porosity (green curve). As hydration progresses further toward the heater, swelling of the central bentonite induces compression in regions near both the heater and the hydration boundary, causing a reduction in porosity in these areas. However, in the regions adjacent to the aluminum cylinder, porosity remains relatively elevated due to the dominant influence of thermal expansion.

Throughout the hydration process, vertical stress increases progressively across the profile (Figure 21 (d)). The evolution of the stress front closely follows that of the hydration front, as reflected by the corresponding trends in saturation (Figure 21 (c)) and stress profiles. This indicates that the mechanical response of the bentonite is strongly coupled to the advancing hydration front.

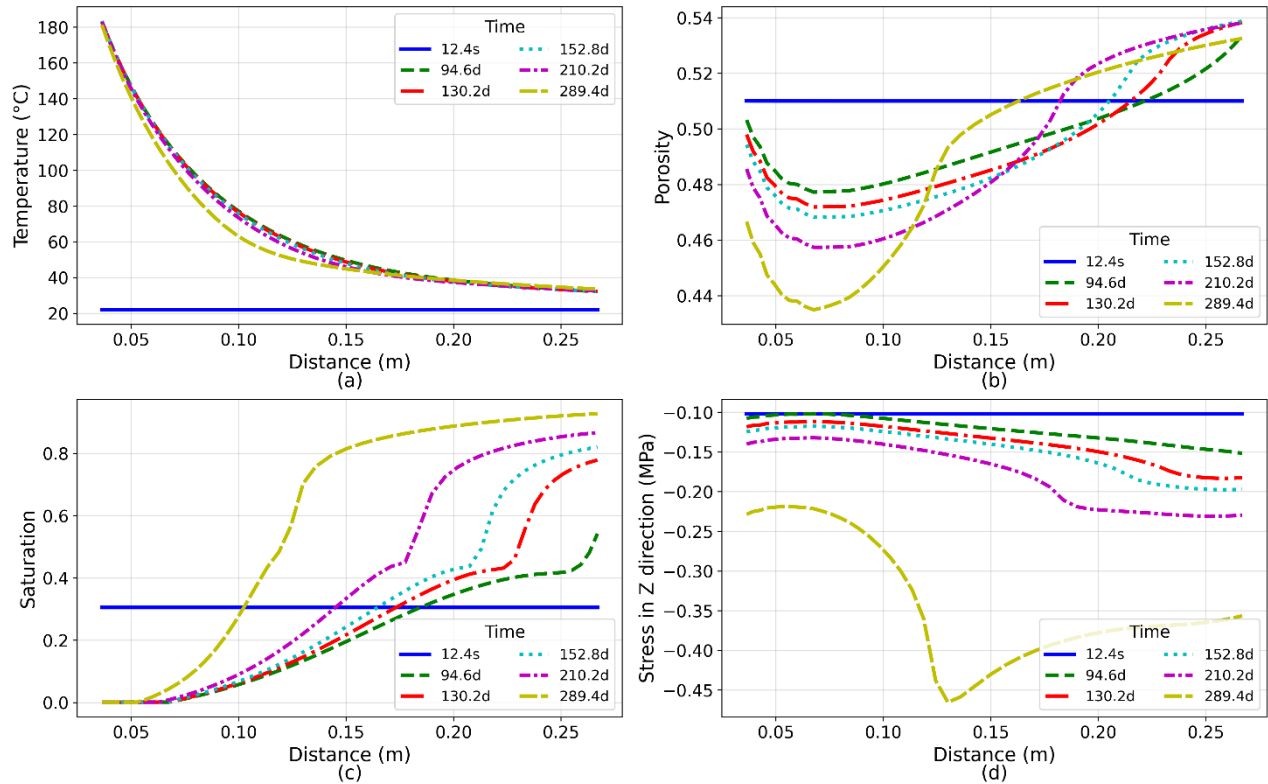


Figure 21 Profiles of temperature, porosity, saturation and stress along z direction during hydration without considering the clogging effect of hydration layer (Simulation case 2)

Figure 22 illustrates the profiles of temperature, porosity, water saturation, and vertical stress at six time points during the hydration phase, for Simulation Case 1, which accounts for the clogging effect of the hydration layer. The temperature profiles (Figure 22 (a)) remain largely unchanged throughout the hydration process, reflecting the limited amount of water infiltration into the bentonite. As shown in Figure 22 (b) and Figure 22 (c), the hydration front is confined to the region near the hydration boundary, with minimal progression toward the heater. This localized hydration results in only moderate changes in porosity and saturation near the boundary, while the remainder of the bentonite remains largely unaffected. Correspondingly, the evolution of vertical stress (Figure 22 (d)) is much less pronounced compared to the scenario without clogging (Simulation Case 2, Figure 21), with relatively low stress gradients developing across the profile.

These results clearly demonstrate that clogging of the hydration layer significantly alters the coupled THM behavior of the system, severely limiting the extent of hydration and the associated mechanical response in the bentonite.

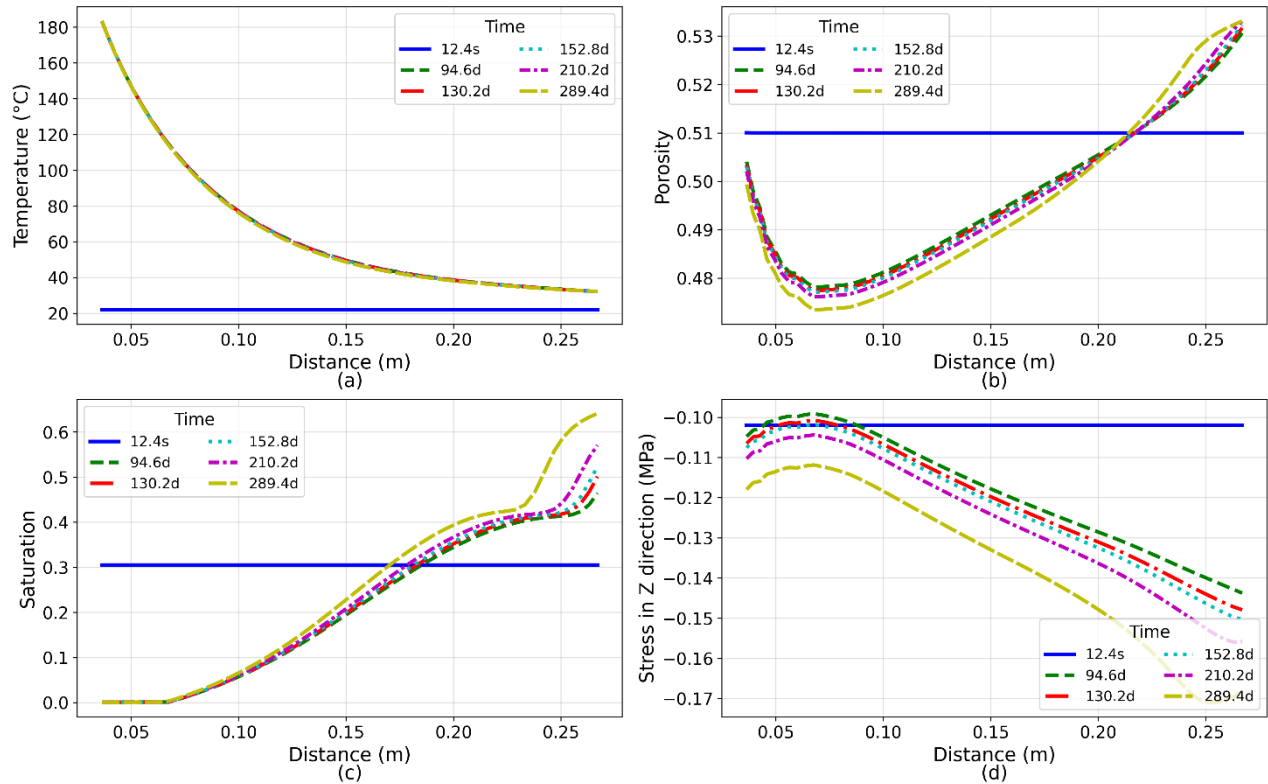


Figure 22 Profiles of temperature, porosity, saturation and stress along z direction during hydration with considering the clogging effect of hydration layer (Simulation case 1)

## 5. DISCUSSION

The numerical simulations of Tank Test 1 and Tank Test 2 demonstrate that the developed model is capable of reliably capturing the coupled THM behavior of bentonite during heating and hydration processes. During the heating phase, bentonite near the heater undergoes a short transient moisture redistribution phase due to vapor condensation, followed by dehydration resulting from vaporization and vapor transport. The vaporized water subsequently condenses in the region close to the hydration boundary, leading to the formation of a distinct dehydrated zone adjacent to the heater and a hydrated zone near the hydration boundary. The bentonite adjacent to the heater or the aluminum cylinder is subject to a complex interplay between thermal expansion, drying-induced shrinkage, and mechanical compression exerted by the swelling zone near the hydration boundary. In Tank Test 1, the porosity in the vicinity of the heater approaches the minimum value observed in the profile. In contrast, in Tank Test 2, the porosity adjacent to the aluminum cylinder remains substantially higher than the minimum porosity, due to the enhanced thermal expansion effect induced by the larger heating surface of the aluminum cylinder. Concurrently, vertical stress increases slightly, which can be attributed to thermal expansion and the swelling of hydrated bentonite.

During the subsequent hydration phase, porosity evolves both spatially and temporally in a highly dynamic manner. Upon the onset of hydration, bentonite near the hydration boundary begins to swell, leading to a localized increase in porosity. As the hydration front advances toward the heater, swelling in the central region of the bentonite generates compressive stresses on the material near both the heater and the hydration boundary, resulting in a corresponding reduction in porosity in these zones. In addition, due to pronounced thermal expansion, the porosity in the region adjacent to the heater or aluminum cylinder remains higher than that in regions located slightly farther away. This effect is more prominent in Tank Test 2, owing to the enhanced thermal expansion associated with the larger heating surface of the aluminum cylinder. The lowest porosity is observed in the middle zone between the thermally expanded region and the advancing hydration front, where

the bentonite is subjected to compressive forces from both directions. During this phase, the swelling pressure increases progressively across the bentonite profile. The evolution of the stress front closely tracks the movement of the hydration front, highlighting the strong coupling between hydraulic and mechanical processes in the system.

Analysis of the simulation results from Tank Test 1 and Tank Test 2 demonstrates that both the volume of water infiltrating the bentonite and the resulting swelling pressure are highly sensitive to the intrinsic permeability of the hydration layer. The limited water intake observed in Tank Test 2 is attributed to clogging of the hydration layer, which is supported by both post-test inspection of the bentonite sample and the numerical simulations. These findings suggest that further refinement of the hydration layer design could help enhance its reliability and support more uniform hydration in future tests.

Despite the model's effectiveness in capturing key THM responses, certain discrepancies remain between simulation results and experimental observations. Notably, temperature and water content-related variables (e.g., relative humidity and volumetric water content) from the numerical simulations show better agreement with measurements obtained from relative humidity sensors than those from dielectric sensors. Further investigation revealed inconsistencies between these two sensor datasets across both tank tests. For example, at a given distance from the heater (100mm in Tank Test 1, and 100mm, 150mm in Tank Test 2), relative humidity measurements indicated a decreasing trend, whereas dielectric sensors recorded volumetric water content values near or exceeding the initial condition. These contradictions likely stem from heterogeneities in dry density or initial moisture distribution in the bentonite, as well as differences in the accuracy or sensitivity of the two types of sensors. As a result, it is not feasible to achieve simultaneous agreement with both experimental datasets.

Additionally, a discrepancy in swelling pressure was observed in Tank Test 1. While the numerical model predicted a continuous increase in swelling pressure, the experimental data exhibited a plateau. This mismatch suggests limitations in the current state-surface constitutive model, particularly in its ability to capture complex mechanical processes such as macrostructural collapse and thermal-induced plasticity. To improve predictive accuracy, future developments should focus on incorporating more advanced constitutive models that account for these mechanisms.

## 6. CONCLUSIONS

A fully coupled THM model has been developed to simulate the complex behavior of bentonite during heating and hydration processes in tank tests. The model incorporates a novel temperature-dependent soil water retention model and thermal conductivity model proposed by Lu and McCartney [10], Lu and McCartney [11], respectively. By accounting for temperature effects, the water retention model captures the thermally induced shift in the retention curve and enables spatial variability in retention behavior resulting from radial temperature gradients. Additionally, the model differentiates between intrinsic liquid and gas permeability, with intrinsic gas permeability defined as a power function of accessible porosity (the product of porosity and gas saturation). This differentiation enables the THM model to accurately predict hydration and dehydration during heating.

The simulation results effectively captured key experimental trends, particularly the evolution of temperature and relative humidity throughout the heating and hydration processes. The predicted relative humidity profiles indicate that bentonite adjacent to the heater undergoes a transient hydration phase due to vapor condensation, followed by dehydration driven by vaporization and vapor transport. In parallel, the numerical results revealed a complex, time-dependent evolution of porosity. During the heating phase, the bentonite adjacent to the heater undergoes complex coupled THM coupled processes, including thermal expansion, drying-induced shrinkage, and mechanical compression from the swelling region. As a result, the porosity in these regions exhibits significant variations throughout the heating process in both tank tests. During the hydration phase, bentonite near the hydration boundary becomes saturated first, leading to swelling and an increase in porosity. As the hydration front advances toward the heater, swelling occurs progressively in the central region. This expansion compresses the bentonite near both the heater and the hydration boundary, resulting in a reduction in porosity in those regions. The lowest porosity is observed in the intermediate zone between the thermal expansion

region and the advancing hydration front, where material is simultaneously compressed from both directions. These results underscore the model's capability to capture the coupled THM interactions that govern porosity evolution in unsaturated expansive clays.

While the model demonstrates strong predictive capability, some discrepancies remain when compared to experimental data, particularly with respect to swelling pressure behavior and water content measurements. These deviations may stem from spatial heterogeneities in the initial dry density of the bentonite, sensor limitations, or simplifications in the current constitutive model. In particular, the inability to capture phenomena such as thermal-induced plasticity and microstructural evolution may contribute to the mismatch between simulated and measured swelling pressures in Tank Test 1. These findings highlight the necessity of further advancing the mechanical modeling framework to better represent irreversible deformation mechanism. Despite these limitations, the study establishes a robust and flexible framework for simulating coupled THM processes in engineered barrier systems. The insights gained contribute to a deeper understanding of bentonite behavior under repository-relevant conditions and support the design and long-term safety assessment of deep geological repositories for radioactive waste.

## APPENDIX A

In the adsorption regime, the temperature-dependent parameters are [10]

$$\psi_{\max} = \frac{RT}{3v_w} \exp\left(\frac{E_1 - E_L}{RT}\right) \quad (37)$$

$$\theta_{a,\max} = (1 - \theta_s) \left[ \frac{CEC}{\bar{\xi}_s} + \frac{b_w}{b} \right] \quad (38)$$

$$CEC = \frac{1}{2} CEC_{\max} \left[ \cos\left(A\pi \frac{BT - T_a}{T_b - T_a}\right) + 1 \right] \quad (39)$$

where  $v_w$  is the molar volume of water ( $1.8 \times 10^{-5} \text{ m}^3/\text{mol}$ ),  $E_1$  is the heat of adsorption for the first layer,  $E_L$  is the heat of adsorption for the second and higher layers and is equal to the heat of liquefaction,  $\bar{\xi}_s$  is a parameter related to the slope of sorption curve,  $CEC$  is the cation exchange capacity,  $CEC_{\max}$  is the maximum value of  $CEC$ ,  $A$  and  $B$  are model parameters,  $T_a$  and  $T_b$  are temperatures associated with  $CEC_{\max}$  and  $CEC_{\min}$ ,  $b_w$  is the excess mass of water per gram of dry soil,  $b = 1$  a model parameter.

In the capillary regime, the temperature dependent parameters are:

$$\psi_c = \frac{A_H}{6\pi H^3} \quad (40)$$

$$A_H = \frac{3}{4} k_B T \left( \frac{\varepsilon_s - \varepsilon_w}{\varepsilon_s + \varepsilon_w} \right)^2 + \frac{3h_p v_e (n_s^2 - n_w^2)^2}{16\sqrt{2} (n_s^2 + n_w^2)^{3/2}} \quad (41)$$

$$\varepsilon_w = 10 \left[ 0.7017 + \frac{642.0}{T} - \frac{1.167 \times 10^5}{T^2} + \frac{9.190 \times 10^6}{T^3} + \left( 1.667 - \frac{11.41}{T} - \frac{3.526 \times 10^4}{T^2} \right) \lg \rho_w \right] + 1 \quad (42)$$

$$H = \theta_{a,\max} / (\rho_d \cdot SSA) \quad (43)$$

$$\eta = -\frac{\Delta h}{C_1} \quad (44)$$

$$\Delta h = \Delta h_{T_r} \left( \frac{1 - T_r}{1 - T} \right)^{0.38} \quad (45)$$

$$\alpha = \frac{\alpha_0}{\exp \left( \eta_\alpha \left( \frac{T_r}{T} - 1 \right) \right)} \quad (46)$$

where  $A_H$  is the Hamaker constant,  $k_B$  is the Boltzmann constant ( $1.3806505 \times 10^{-23}$  J/K),  $h_p$  is the Planck constant ( $6.626068 \times 10^{-23}$  Js),  $\nu_e$  is the main electronic adsorption frequency in ultraviolet light (2.45 GHz),  $\epsilon_s$  is the dielectric constant of soil particle,  $\epsilon_w$  is the dielectric constant of water,  $n_s$  is the refractive index of soil particle,  $n_w$  is the refractive index of water,  $H$  is the equilibrium film thickness,  $\omega$  is the gravimetric water content,  $\rho_d$  is the dry density,  $\rho_w$  is the density of water,  $SSA$  is the specific surface area,  $\Delta h$  is the enthalpy of immersion per unit area,  $C_1$  is a constant and  $\eta_\alpha$  is a material parameter.

Parameters used in the temperature-dependent SWRC are given below.

Table 4 Parameters for adsorptive water content

| $v_w$ [m <sup>3</sup> /mol] | $E_1 - E_L$ [J/mol] | $\bar{\xi}_s$ [meq/g] | $b_w$ [g/g] | $CEC_{max}$ [meq/g] |
|-----------------------------|---------------------|-----------------------|-------------|---------------------|
| $1.8 \times 10^{-5}$        | 7534                | 2.8                   | 0.18        | 0.776               |
| $A$                         | $B$                 | $T_a$ [K]             | $T_b$ [K]   | $m$                 |
| 0.92                        | 0.9                 | 373.15                | 1273.15     | 0.12                |

Table 5 Parameters for capillary water content

| $SSA$ [m <sup>2</sup> /kg] | $A_H$ [kPa] | $\Delta H$ [J/m <sup>2</sup> ] | $\epsilon_s$ | $n_s$ | $n_w$ | $\alpha_0^{-1}$ [MPa] |
|----------------------------|-------------|--------------------------------|--------------|-------|-------|-----------------------|
| $7.0 \times 10^5$          | 10213       | -0.516                         | 3.5          | 1.55  | 1.33  | 3.3                   |
| $\eta_\alpha$              | $C_1$       | $n$                            |              |       |       |                       |
| 5.0                        | -0.00151    | 1.15                           |              |       |       |                       |

## APPENDIX B

Figure 23 presents the comparison of numerical results (temperature, porosity, saturation and  $\sigma_{zz}$ ) for Tank Test 1 under different maximum time-step sizes ( $5.0 \times 10^5$  s,  $5.0 \times 10^4$  s,  $1.0 \times 10^4$  s and  $1.0 \times 10^3$  s). The numerical results from these cases showed excellent agreement, with only minor discrepancies observed in the vertical stress component (Figure 23 (d)). This confirms that the adaptive time-stepping algorithm can produce sufficiently small-time steps (generally less than 30,000 s) to ensure accuracy.

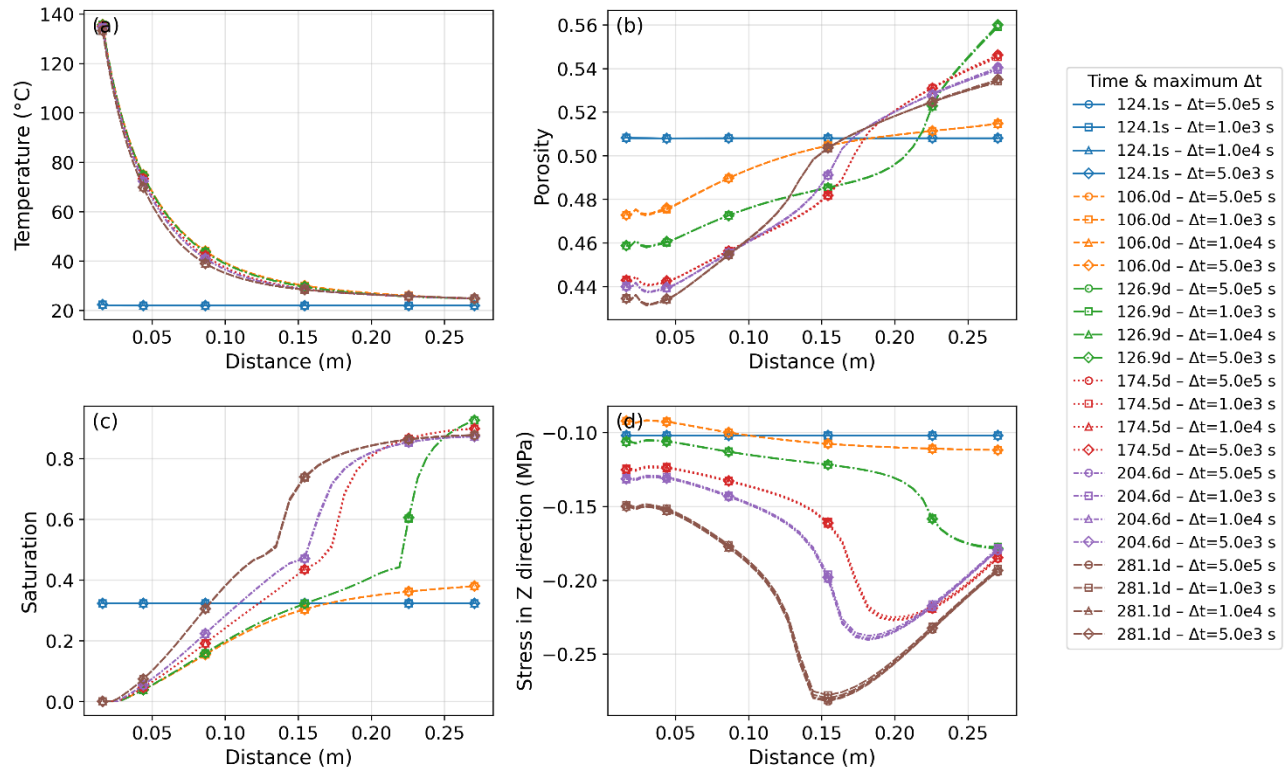


Figure 23 Comparison of numerical results for Tank Test 1 under different maximum time-step sizes

## ACKNOWLEDGMENT

The authors gratefully acknowledge Dr. Radhavi Samarakoon and Dr. Hafssa Tounsi for their insightful discussions and technical assistance with the TOUGH3-FLAC coupling framework during the initial phase of this work. The authors appreciate support from the U.S. Department of Energy award AWD00007822.

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