

Thermo-Hydro-Mechanical Simulation of Unsaturated Bentonite Buffers under High Temperatures in COMSOL

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Abstract

Heating of unsaturated bentonite buffers involves coupled thermo-hydro-mechanical (THM) processes that influence the long-term behavior of geological repositories for nuclear waste storage. This study examines these processes using an axisymmetric COMSOL model of a heater surrounded by compacted MX80 bentonite. The model couples heat and water transport, vapor transport, and phase change with an elastic mechanical response, thermal expansion, and creep and suction strains. Heating produces outward heat propagation and drying near the heater. Farther away, water content initially increases before declining below its initial value. Local expansion and compression develop within the constrained bentonite, accompanied by spatially varying stress. The simulations characterize the coupled evolution of temperature, water state, and deformation during heating.

Keywords: unsaturated bentonite; heating; thermo-hydro-mechanical coupling; phase change; water transport; COMSOL Multiphysics

Introduction

Compacted bentonite is used as a buffer material in deep geological repositories, where coupled thermal, hydraulic, and mechanical processes influence the evolution of the engineered barrier. Earlier studies of coupled buffer behavior and fully coupled constitutive frameworks provide context for this problem [1], [2]. Under elevated temperatures, the local state is governed by heat transfer, liquid-water transport, vapor transport, and liquid-vapor phase change [3]. Constitutive models of expansive clays address thermal volume change [4] and interactions between microstructural and macrostructural deformation [5].

Vapor transfer is particularly relevant in unsaturated compacted bentonite and heated porous media, where temperature and water gradients can alter transport pathways near a heat source [6], [7]. Experimental studies have examined changes in temperature and water content in compacted MX80 bentonite during heating [8], [9]. High-temperature testing of compacted MX80 bentonite provides the immediate experimental motivation for the present work [10]. Pore-scale transport models also relate permeability to pore-size distribution and the area available for flow [11]. The present analysis evaluates temperature, water-state, and deformation-related variables in a two-dimensional axisymmetric heater-bentonite configuration. This study complements high-temperature experimental testing [10,12].

The COMSOL model combines Heat Transfer in Solids, Richards' Equation [13], Transport of Diluted Species in Porous Media, and Solid Mechanics. Soil-water retention and relative

hydraulic conductivity are represented by the van Genuchten and van Genuchten–Mualem models, respectively [14], [15]. Temperature-dependent water-retention models distinguish the contributions of adsorption and capillarity [16].

The model also accounts for thermal conductivity, vapor diffusion, and phase exchange at a finite rate. The mechanical response is represented by isotropic elasticity, thermal expansion, a temperature-dependent creep strain, and a suction-related strain. Experiments on compacted bentonite show instantaneous expansion after heating followed by time-dependent contraction during isothermal holding [17]. Volumetric strain updates porosity, which enters the water-content and permeability relations. The formulation, mechanical constraints, and deformation and stress results are presented below. The following sections present the balance equations, geometry, constitutive inputs, boundary conditions, and coupled response of the model.

Theory

Governing Equations

The energy balance is expressed using an effective volumetric heat capacity and conductive heat flux. Here T is temperature, λ is thermal conductivity, and Q_T denotes a volumetric heat source. A prescribed heater temperature supplies thermal loading.

$$(\rho C_p)_{\text{eff}} \frac{\partial T}{\partial t} + \nabla \cdot q_h = Q_T \quad (1)$$

$$q_h = -\lambda \nabla T \quad (2)$$

Equation (3) states liquid mass conservation in terms of volumetric water content θ . Equation (4) defines the Darcy flux with intrinsic permeability κ , relative permeability K_r , viscosity μ_w , pressure p ,

and gravitational acceleration g . The calculation uses a pressure-based Richards' formulation with linearized storage. The reported θ and S_e are constitutive water-state variables evaluated from the saved solution to the following equations:

$$\frac{\partial(\rho_w \theta)}{\partial t} + \nabla \cdot (\rho_w u_w) = Q_m \quad (3)$$

$$u_w = -\frac{\kappa K_r}{\mu_w} (\nabla p - \rho_w g) \quad (4)$$

For vapor transport, C_v denotes stored vapor moles per unit bulk volume, whereas c_v denotes vapor concentration in the gas phase. The vapor balance and diffusive flux are given below.

$$\frac{\partial C_v}{\partial t} + \nabla \cdot J_v = S_v \quad (5)$$

$$J_v = -D_{\text{eff},v} \nabla C_v \quad (6)$$

Finite-rate phase exchange is described by a vapor source S_v and its paired liquid mass source Q_m .

Here c_{eq} is the local equilibrium vapor concentration, k_{pc} is the phase-change coefficient, and M_w is water molar mass. The source terms represent interphase exchange between vapor and liquid water in the governing formulation.

$$S_v = k_{pc}(c_{eq} - c_v) \quad (7)$$

$$Q_m = -M_w S_v \quad (8)$$

Positive values of the vapor source represent evaporation and the corresponding liquid-water sink, negative values represent condensation and the corresponding liquid-water source.

Mechanical Balance and Elastic Response

Solid Mechanics is solved in the bentonite and aluminum domains. The transient calculation retains inertia and geometric nonlinearity. With displacement u , density ρ , and Cauchy stress σ , the mechanical balance without applied body forces is:

$$\rho \frac{\partial^2 u}{\partial t^2} = \nabla \cdot \sigma \quad (9)$$

The deformation gradient F maps reference coordinates X to the current configuration. The elastic part is obtained by removing the combined inelastic deformation gradient F_i :

$$F = I + \nabla_X u, \quad F_e = F F_i^{-1} \quad (10)$$

The elastic Green–Lagrange strain E_e and the isotropic elastic stress Σ_e in the intermediate configuration satisfy:

$$E_e = \frac{1}{2}(F_e^T F_e - I) \quad (11)$$

$$\Sigma_e = 2GE_e + \lambda_L \text{tr}(E_e)I \quad (12)$$

Here $G = E/[2(1 + \nu)]$ and $\lambda_L = E\nu/[(1 + \nu)(1 - 2\nu)]$, where E and ν are the Young's modulus and Poisson's ratio. The corresponding Cauchy stress is $\sigma = F_e \Sigma_e F_e^T / J_e$, with $J_e = \det F_e$. The inelastic deformation combines the thermal expansion and the two prescribed isotropic strain contributions defined below. Tensile normal strain is positive in these constitutive inputs; reported local volumetric strain is expressed as positive in compression.

Model Geometry

A two-dimensional axisymmetric heater-bentonite configuration represents the coupled heating response. The domain comprises a central heater, compacted bentonite, an aluminum side wall, a top cap, and a base. The symmetry axis is $r = 0$, and the heater surface is located at $r = 6.25$ mm.

The parameterized bentonite domain has a height of 21.05 cm and an outer radius of 27.725 cm. The central heater has a radius of 0.625 cm and an axial length of 10.20 cm. The geometry also includes a 5.72 cm top cap, a 2.00 cm base section, and a 1.65 cm aluminum-wall thickness. These dimensions define the two-dimensional axisymmetric configuration in Figure 1(a). Figure 1(b) combines the radial detail with the three-dimensional axial view, while Figures 2(a) and 2(b) show the global and local meshes.

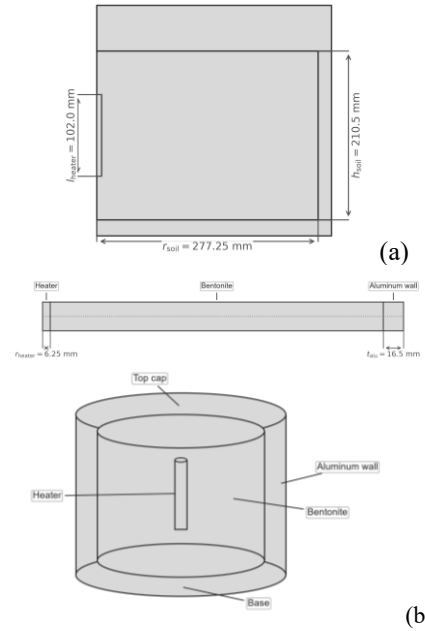


Figure 1. Axisymmetric model definition: (a) model geometry; (b) radial heater-bentonite-aluminum-wall detail and three-dimensional axial view

Material Relations

Figure 3 shows reference temperature-dependent water-retention curves. Effective saturation follows the van Genuchten form [15], with temperature-dependent coefficients defined below:

$$S_e = [1 + (\alpha_T \psi_{eff})^n]^{-m} \quad (13)$$

$$\alpha_T = \alpha \exp[\eta(1 - \frac{T_0}{T})] \quad (14)$$

$$\psi_{eff} = \psi_s \frac{T + \chi}{T + T_0} \quad (15)$$

The reference curves use $\alpha = 8 \times 10^{-8} \text{ Pa}^{-1}$, $n = 1.60$, $m = 1 - 1/n = 0.375$, $\eta = 1$, $T_0 = 293.15 \text{ K}$, and $\chi = 300 \text{ K}$. Here ψ_s is the suction coordinate plotted in Figure 3. Effective saturation provides a common variable for comparing retention, relative hydraulic conductivity, and the water-state results.

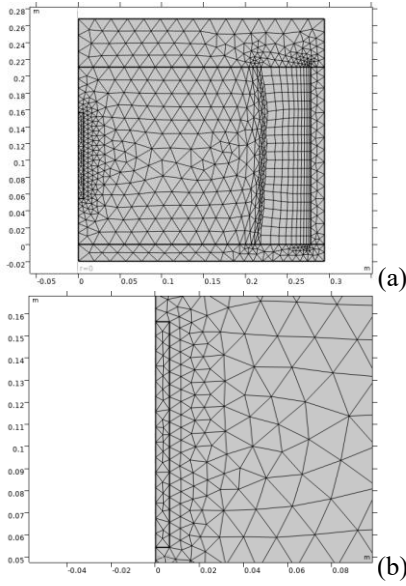


Figure 2. Axisymmetric mesh definition: (a) global mesh; and (b) local heater-region mesh.

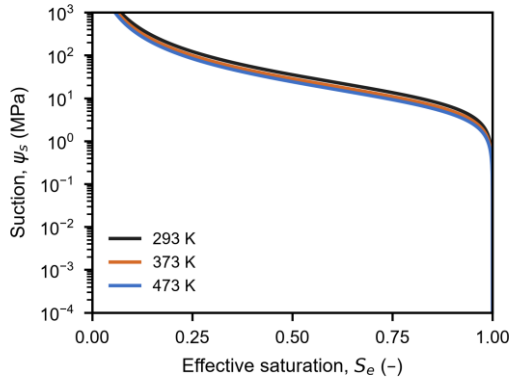


Figure 3. Reference temperature-dependent water-retention curves: suction versus effective saturation at 293, 373, and 473 K, evaluated with $\chi = 300$ K.

Constitutive Transport Functions

Figure 4 shows the saturation-dependent thermal conductivity function (TCF) and the normalized van Genuchten–Mualem relative hydraulic conductivity function [14], [15], [18].

For the TCF, following the adopted thermal-conductivity relation [18], the degree of saturation is $S = \theta/\theta_s$ and the thermal conductivity is evaluated from the following normalized relation:

$$\frac{\lambda - \lambda_{dry}}{\lambda_{sat} - \lambda_{dry}} = \left[1 - \frac{1 - S^{\eta_{TCF}}}{1 + (\frac{S}{S_c})^{\eta_{TCF}}} \right]^{1 - \frac{1}{\eta_{TCF}}} \quad (16)$$

The thermal-conductivity parameters are $\lambda_{dry} = 0.340$ W/(m K), $\lambda_{sat} = 0.935$ W/(m K), $S_c = 0.600$, and $\eta_{TCF} = 3.30$. The reference saturated water content is $\theta_s = 0.41$.

For liquid flow, the van Genuchten–Mualem HCF [14], [15] is expressed in terms of effective saturation S_e , which is retained as the water-state

variable in the van Genuchten relation and is distinct from S used in the TCF:

$$K_r = S_e^\ell \left[1 - (1 - S_e^{\frac{1}{m}})^m \right]^2 \quad (17)$$

$$K = K_s K_r, \quad K_s = \frac{\kappa \rho_w g}{\mu_w} \quad (18)$$

The reference hydraulic parameters are $\theta_r = 0.05$, $\theta_s = 0.41$, $\alpha = 8 \times 10^{-8}$ Pa⁻¹, $n = 1.60$, $m = 0.375$, and $\ell = 0.50$. Evaluated water content follows $\theta = \theta_r + S_e(n_{por} - \theta_r)$, using evolving porosity n_{por} . Intrinsic permeability follows $\kappa = \kappa_0(n_{por}/0.41)^3$. Figure 4(b) shows only $K_r(S_e)$; absolute conductivity additionally depends on κ , liquid density, and viscosity.

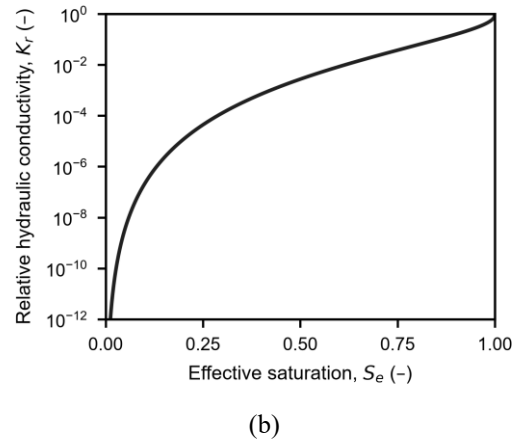
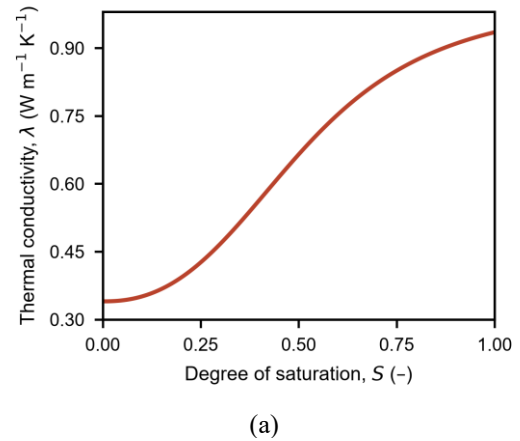


Figure 4. Constitutive transport functions used as material inputs: (a) saturation-dependent thermal conductivity $\lambda(S)$, with $S = \theta/\theta_s$; (b) van Genuchten–Mualem relative hydraulic conductivity $K_r(S_e)$. Absolute liquid conductivity follows $K = K_s K_r$.

The vapor-diffusion variable is defined as $D_{v,air} n_{por}(1 - S_e)$, with $D_{v,air} = 2 \times 10^{-4}$ m²/s. This saturation-dependent scaling is evaluated with the model effective-saturation state, while residual water is retained separately in the water-content relation. The factor $n_{por}(1 - S_e)$ is distinct from the gas volume fraction $n_{por} - \theta$.

The bentonite inputs include density 1700 kg/m³, specific heat capacity 800 J/(kg K), and reference porosity 0.41. The reference intrinsic permeability is $\kappa_0 = 1 \times 10^{-16}$ m². The adopted free-air vapor diffusivity is $D_{v,air} = 2 \times 10^{-4}$ m²/s.

Mechanical Constitutive Relations

The bentonite has $E = 80$ MPa and $\nu = 0.30$, while the aluminum has $E = 70$ GPa and $\nu = 0.33$.

Thermal expansion is coupled to the temperature field in the bentonite using a constant secant coefficient $\alpha_\ell = 2.667 \times 10^{-5}$ K⁻¹ and reference temperature $T_0 = 293.15$ K. Its isotropic thermal stretch is:

$$F_T = [1 + \alpha_\ell(T - T_0)]I. \quad (19)$$

The thermal-creep contribution is prescribed as an isotropic normal strain e_c . A temperature-dependent amplitude $a(T)$ and an exposure time measured from t_s define the implemented relation:

$$e_c = -\frac{1}{3} a(T) \max(t - t_s, 0), \quad (20)$$

$$a(T) = A_{ref} g(T) \exp\{B[T_c - T_{ref}]\}, \quad (21)$$

$$g(T) = \frac{1}{1 + \exp[-(T - T_a)/\Delta T]}. \quad (22)$$

Here $T_c = \min(T, T_{cap})$. The adopted parameters are $A_{ref} = 3.4722 \times 10^{-9}$ s⁻¹, $B = 0.0224$ K⁻¹, $T_a = 353.15$ K, $\Delta T = 5$ K, $T_{ref} = 393.15$ K, $T_{cap} = 413.15$ K, and $t_s = 3600$ s. Equation (20) evaluates the prescribed strain from the current local temperature and elapsed exposure time. A second isotropic normal strain e_s represents the suction contribution:

$$e_s = \frac{\beta(\psi - \psi_0)}{3K_\psi}. \quad (23)$$

The coefficient β is 0.25, the prescribed modulus K_ψ is 50 GPa, and ψ is the Kelvin-based suction evaluated from vapor concentration and temperature. The reference ψ_0 is 14.266 MPa, corresponding to the initial relative humidity of 0.90 at 293.15 K. Both e_c and e_s are supplied as isotropic external strains in the bentonite. Their signed inputs, together with thermal expansion and the displacement constraints, determine the calculated mechanical response.

The compression-positive volumetric strain updates the porosity through the linearized volume relation

$$n_{raw} = n_0 - (1 - n_0)\epsilon_v^c, \quad n_0 = 0.41. \quad (24)$$

The implementation confines porosity to 0.05–0.80. These limits are inactive in the plotted samples. The resulting porosity enters the water-content and permeability relations, completing the deformation-to-transport connection.

Initial and Boundary Conditions

Thermal Loading

The model is initialized at 293.15 K. The prescribed heater boundary temperature increases linearly to 473.15 K during the first hour and remains constant thereafter. In Figure 5(a), "0 mm" labels this

boundary input; the heater surface is physically located at $r = 6.25$ mm. The other labels denote soil radii measured from the symmetry axis. The aluminum side wall exchanges heat with an ambient environment at 295.75 K through a heat-transfer coefficient of 15 W/(m² K).

Liquid-Water and Vapor Transport Conditions

The transport configuration has no liquid inflow and includes a prescribed vapor-concentration boundary. The initial relative humidity is 0.90. The phase-change coefficient is $k_{pc} = 1 \times 10^{-5}$ s⁻¹. At the initial sampled state, S_v is approximately -1.49×10^{-6} mol/(m³ s), indicating a condensation tendency before the heating transient develops. Initial liquid-vapor disequilibrium may also contribute to the early water redistribution.

Mechanical Conditions

Radial displacement is prescribed as zero along the outer bentonite boundary at $r = 277.25$ mm.

Vertical displacement is prescribed as zero at the lower and upper bentonite boundaries, $z = 0$ and 210.5 mm. The remaining displacement components on these boundaries are unconstrained. Axial symmetry is applied on the exposed $r = 0$ segments. The other unconstrained mechanical boundaries are traction free. The mechanical calculation includes bentonite and aluminum; the cap, base, and heater enter through the thermal geometry and the stated bentonite constraints. Initial displacement and velocity are zero.

COMSOL Implementation

The calculation was performed with COMSOL Multiphysics 6.2 using a time-dependent study over 0–1000 h. The Solid Mechanics interface uses isotropic elasticity and the Thermal Expansion coupling, with the two prescribed external strain contributions applied to bentonite. Time histories were evaluated at $r = 50, 100, 150$, and 200 mm and $z = 105.25$ mm. Radial profiles use evaluations from $r = 50$ to 250 mm at the same elevation. The mechanical plots use the same saved solution as the heat and water results. Local volumetric strain is reported with compression positive, and von Mises stress is calculated from the Cauchy stress.

The domain-wide volume-change measure is the volume-weighted mean volumetric strain, evaluated over the full bentonite domain with axisymmetric weighting:

$$\overline{\epsilon_v} = -\frac{\int_\Omega \epsilon_v^c 2\pi r \, dA}{\int_\Omega 2\pi r \, dA} \quad (25)$$

Here Ω is the bentonite domain in the meridional plane and $2\pi r$ is the axisymmetric volume weight. The mean strain is positive in expansion, whereas the local strain ϵ_v^c is positive in compression.

Results and Discussion

Heat Transfer and Water Flow Response

Figure 5 compares the prescribed heater temperature with the bentonite temperature response and shows the accompanying changes in water content and effective saturation. Among the soil locations, temperature rises earliest and most strongly at 50 mm and remains below the heater temperature. At 100, 150, and 200 mm, water content and effective saturation initially increase before falling below their initial values. At 50 mm, both variables are at or below their initial values.

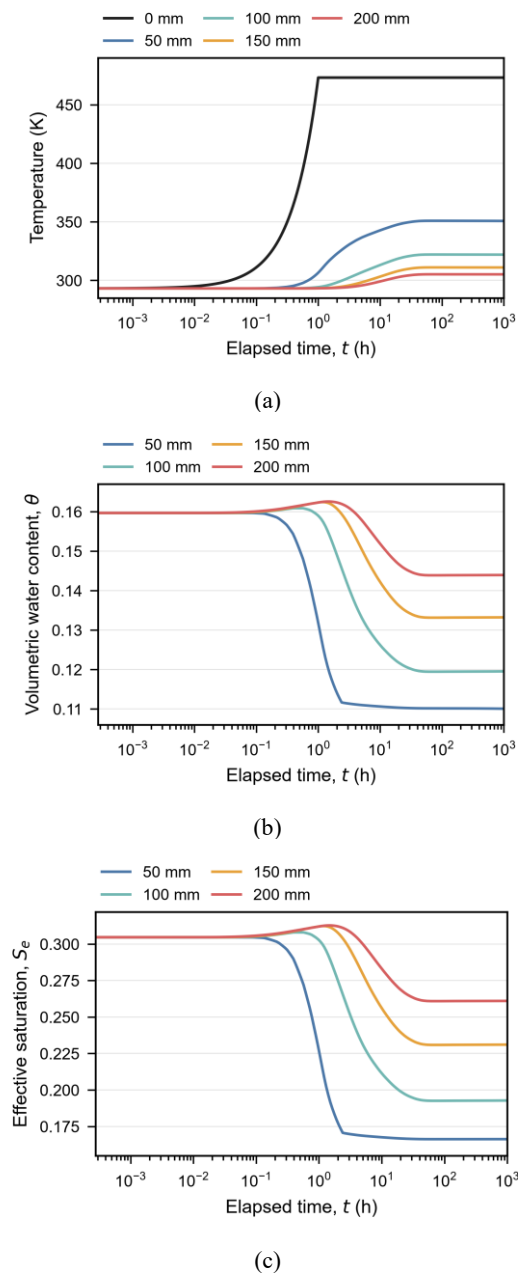


Figure 5. Heating histories at $r = 50, 100, 150$, and 200 mm and $z = 105.25$ mm: (a) temperature; (b) volumetric water content; (c) effective saturation.

Figure 6 shows radial temperature and effective-saturation profiles at 0, 1, 10, 100, and 1000 h. In the profiles at 10–1000 h, temperature decreases outward, while effective saturation is lower near the heater and higher at larger radii.

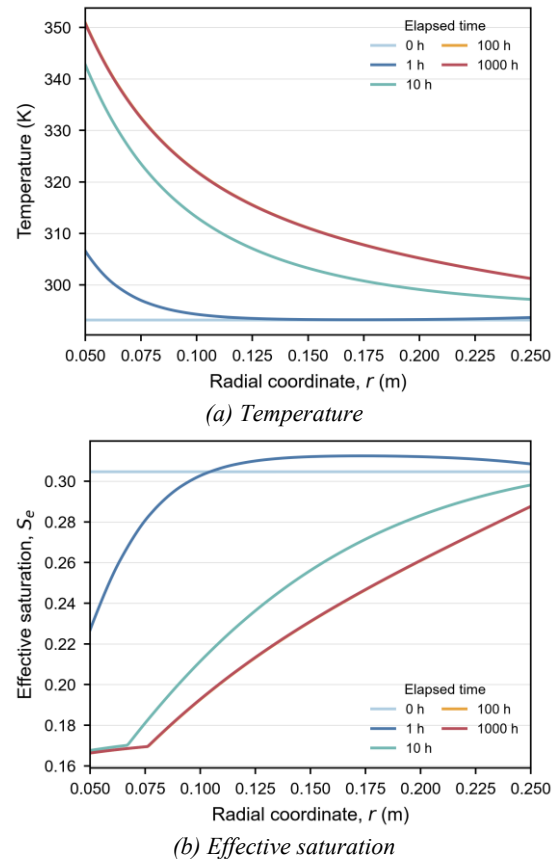
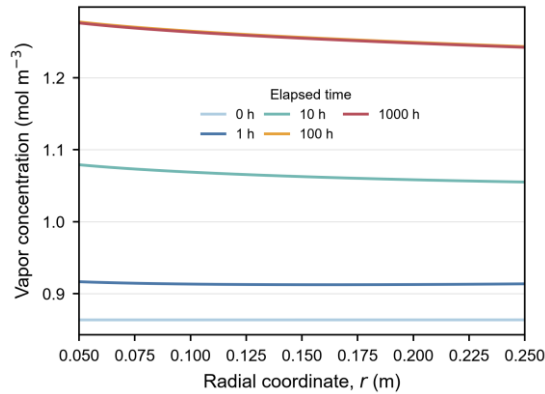


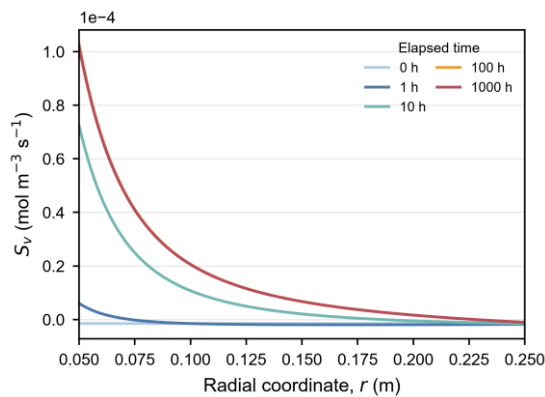
Figure 6. Radial profiles at 0, 1, 10, 100, and 1000 h: (a) temperature; (b) effective saturation.

Vapor Transport and Phase Change

Figure 7 compares actual vapor concentration with the vapor phase-change source at the same elevation and selected times. The actual vapor concentration varies modestly across the sampled radius, while the later phase-change source is strongest near the heater. The phase-change source identifies the local direction and rate of vapor-liquid exchange under the adopted definition. The initial phase-change source is negative at the sampled locations, consistent with vapor concentration exceeding its equilibrium value. The subsequent response reflects both the initial liquid-vapor state and evolving thermal and hydraulic conditions. Figure 8 shows Kelvin-based suction derived from actual vapor concentration. At 100, 150, and 200 mm, suction initially decreases and subsequently increases, accompanying the early water-state changes in Figure 5. The 50 mm response rises earlier and more strongly. The plotted quantity is calculated from vapor concentration and temperature using the Kelvin relation.



(a)



(b)

Figure 7. Radial vapor response at 0, 1, 10, 100, and 1000 h: (a) actual vapor concentration; (b) vapor phase-change source.

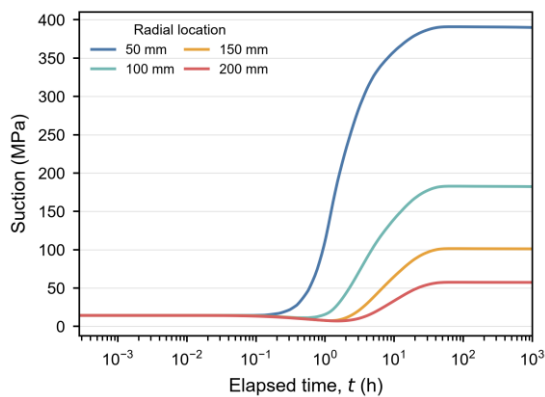


Figure 8. Kelvin-based suction histories at $r = 50, 100, 150,$ and 200 mm, with $z = 105.25$ mm.

Mechanical Response

Figure 9 shows that the volume-weighted mean volumetric strain over the full bentonite domain remains small throughout heating. It reaches a maximum of 2.24×10^{-6} and is 1.27×10^{-6} at 1000 h. These values describe the domain-wide average, which reflects the offsetting contributions of local expansion and compression. Figure 10(a) shows the local volumetric-strain histories. Negative local strain denotes expansion and positive strain denotes compression. At 50 mm, expansion reaches

approximately 0.30% before partially recovering. The 100 and 150 mm histories pass through small compressive stages before becoming expansive, whereas the 200 mm history remains predominantly compressive. The radial profiles in Figure 10(b) and 10(c) show coexisting expansion and compression. At 1000 h, compression-positive volumetric strain ranges from -0.224% to 0.0484% along the sampled line. The corresponding von Mises stress ranges from 0.0236 to 0.135 MPa. The later stress profiles develop a strong spatial variation near the inner end of the sampled radius. These results show redistribution of deformation and stress as the temperature, suction, and prescribed creep strain evolve under the mechanical constraints.

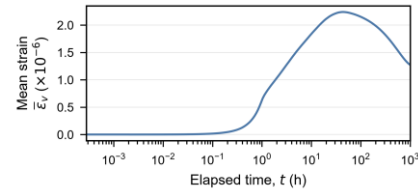


Figure 9: Volume-weighted mean volumetric strain over the bentonite domain

Discussion

At 1000 h, effective saturation at every sampled location is below its initial value. From 927.296 to 1000 h, the largest absolute changes across the four sampled locations are 0.0105 K in temperature and 1.18×10^{-5} in effective saturation, indicating that the sampled thermal and hydraulic histories have reached their final equilibrium response. The mechanical response combines a small volume-weighted domain mean with spatially nonuniform strain and stress. Local expansion and compression largely offset over the constrained bentonite domain. At 50 mm, expansion partly recovers while the thermal and hydraulic histories approach their plateaus, showing continued local deformation.

Conclusion

A two-dimensional axisymmetric COMSOL model was used to examine the coupled thermal, hydraulic, and mechanical response of compacted bentonite during heating. The simulations show outward heat propagation and drying near the heater, while locations farther away exhibit an initial increase in water content followed by drying. Local expansion and compression coexist under the imposed displacement constraints, accompanied by redistribution of stress. Their volume-weighted mean over the bentonite domain remains close to zero. Volumetric deformation modifies porosity and thereby links the mechanical response to water content and permeability. Together, these results describe moisture redistribution and spatially nonuniform deformation within a constrained bentonite buffer during heating.

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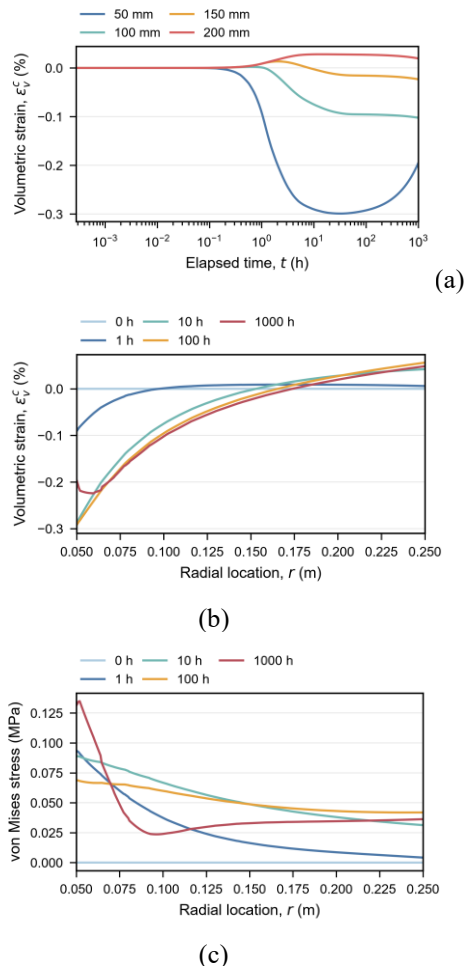


Figure 10. Mechanical response during heating: (a) local strain histories; (b) radial strain profiles; (c) radial von Mises stress profiles.

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