



A homogenization-based model for the effective thermal conductivity of bentonite–sand-based buffer material☆



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ABSTRACT

A homogenization-based effective thermal conductivity model was proposed for unsaturated compacted bentonite–sand-based buffer materials. The microstructure of the mixture was approximated with pores and sand particles of spheroidal shape and random orientation embedded in the homogeneous bentonite matrix. By virtue of the analytical solution to the inhomogeneous inclusion problem in heat conduction, the model was developed using homogenization techniques such as the Mori–Tanaka (MT) and interaction direct derivative (IDD) schemes for different consideration of the interactions between pores, sand particles, and the bentonite matrix. The proposed estimates are dependent on the thermal conductivities of the bentonite matrix, the liquid and gas phases and sand, porosity, the degree of saturation, sand content, and the aspect ratios of pores and sand particles. The proposed model was validated against four sets of laboratory measurement data on the Kunigel-V1, MX-80, Kyungju, and GMZM bentonite–sand mixtures. It is demonstrated that although with simplified considerations of the microstructural features and mechanisms, the model predicts the effective thermal conductivity of the bentonite–sand mixtures with a fairly good agreement.

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1. Introduction

Bentonite–sand mixtures have been widely considered as a potential engineered buffer that could be placed between high-level radioactive wastes and host rocks in the process of deep geological waste disposal. Compared to pure bentonite materials, bentonite–sand mixtures have better thermal conductivity, relatively higher strength and lower compressibility, and very low hydraulic conductivity. The effective thermal conductivity of bentonite–sand-based buffer materials is one of the physical properties that remarkably influence the transfer of decay heat and the resultant coupled thermo-hydro-mechanical-chemical (THMC) processes in the barrier system [1–3].

Experimental tests [4–10] were performed to examine the thermal conductivity of the compacted bentonite–sand mixtures, showing that the heat-conductive property is strongly dependent on the soil structure and phase composition, such as mineral constituents, dry density, porosity, and water content. Few efforts were made to develop theoretical or empirical models for generalizing the experimental results to any possible states. For instance, Ould-Lahoucine et al. [6] adopted the idea of random phase distribution to estimate the effective thermal

conductivity of the bentonite–sand mixtures using different models such as Fricke's model [11], Maxwell's model [12], Bruggeman's model [13], and Johnson's model [14]. However, the microstructural features of the bentonite–sand mixtures were not properly considered in the existing models. It has been shown [15] that the bentonite–sand mixtures typically display a bimodal shape of pore size distribution (PSD) curve, as plotted in Fig. 1, with the dominant smaller pore size mode corresponding to the intra-particle pores and the larger one to the inter-particle and/or inter-aggregate pores [15–17].

Homogenization methods provide an alternative that possibly better relates the microstructural features to the effective thermal properties for materials with inhomogeneities. This approach has been frequently applied to saturated or partially saturated soil, rock, and concrete materials [18–22], but not to bentonite–sand mixtures. In this study, a homogenization-based effective thermal conductivity model was developed for unsaturated compacted bentonite–sand mixtures using homogenization techniques. The model was developed by using the analytical solution to the inhomogeneous inclusion problem in heat conduction [23] and by assuming the pores and sand particles to be of spheroidal shape and random orientation based on the microscopic observations [15]. The Mori–Tanaka (MT) scheme [24] and the interaction direct derivative (IDD) scheme [25] are adopted for different considerations of the interactions between the pores, sand particles, and the solid phase. The proposed model is validated against four sets of laboratory data on

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the Kunigel-V1 [6], MX-80 [7], Kyungju [9], and GMZM [10] compacted bentonite–sand mixtures, showing good agreement between the model predictions and the laboratory measurements and an overall much better performance than Johnson's model [14].

2. Model development

2.1. Conceptual model

As conventional compacted bentonite materials [2,3], the bentonite–sand mixture is regarded as a three-phase medium, with the pores occupied by water and air at partially saturated states and the solid phase being composed of bentonite and sand particles, as shown in Fig. 2. Denoting the porosity and the degree of saturation of the mixture by ϕ and S_r , respectively, one obtains the following relationships:

$$\phi_w = \phi S_r, \quad \phi_g = \phi(1 - S_r), \quad \phi_m = 1 - \phi - \phi_s \quad (1)$$

where ϕ_m and ϕ_s are the volume fractions of bentonite matrix and sand particles, respectively, ϕ_w and ϕ_g the volume fractions of pores occupied by water and gas, respectively.

In this study, both the pores and the sand particles of different size, shape, orientation and arrangement in the compacted bentonite–sand mixture are regarded as inclusions in the bentonite matrix, as shown in Fig. 2. Although the bentonite particles and the additive sand particles have been observed to be typically of ellipsoidal shape [15], the geometry of pores could be much more diverse. As a first approximation, this study assumes the inclusions to be of spheroidal shape for simplifying the model development, with ω_p and ω_s for overall representing the aspect ratios of the pores and the sand particles, respectively. The pores and the sand particles are assumed to be randomly oriented. According to the Young–Laplace equation, the pores with a smaller radius will be preferentially occupied by water and the rest by air. At the microscopic scale, the thermal conductivity of pores (λ_p) is assumed to be isotropic, and at a given degree of saturation S_r , it takes the thermal conductivity of water (λ_w) for the smaller pores of a volume fraction of $\phi_w = \phi S_r$ and the thermal conductivity of gas (λ_g) for the rest of the pores $\phi_g = (1 - \phi)S_r$. The thermal conductivities of the sand material and the bentonite matrix are also assumed to be isotropic, and are denoted by λ_s and λ_m , respectively.

2.2. A homogenization-based effective thermal conductivity model

This study considers the commonly applied homogenization schemes for estimation of the effective thermal properties, including the MT and IDD schemes. With the above conceptual model and by virtue of the analytical solution to the inhomogeneous inclusion problem in heat conduction [21–23,26–28], the effective thermal conductivity of the considered soil mixture is overall isotropic, and can be estimated using different homogenization schemes for consideration of the arrangements of pores and sand particles:

$$\lambda_{\text{eff}}^{\alpha} \delta = \lambda_m \delta + \frac{1}{4\pi} \phi \ell^2 [(\lambda_w - \lambda_m) \phi S_r \mathbf{A}_{\alpha}^w(\mathbf{n}) + (\lambda_g - \lambda_m) \phi(1 - S_r) \mathbf{A}_{\alpha}^g(\mathbf{n}) + (\lambda_s - \lambda_m) \phi_s \mathbf{A}_{\alpha}^s(\mathbf{n})] dS \quad (2)$$

where $\lambda_{\text{eff}}^{\alpha}$ ($\alpha = \text{MT}$ or IDD) is the effective thermal conductivity estimated by the MT or IDD scheme, δ the second-order identity tensor, \mathbf{n} the unit normal of the inclusions, $\ell^2 = \{\mathbf{n}|\mathbf{n}\} = 1$ is the surface of a unit sphere, and $\mathbf{A}_{\alpha}^{\beta}$ ($\beta = w, g, \text{ or } s$) the second-order concentration tensor associated with the pores occupied by water, the pores occupied by air and sand particles, respectively:

$$\mathbf{A}_{\alpha}^{\beta} = \frac{\lambda_m}{(1 - \zeta_{\beta})\lambda_m + \zeta_{\beta}\lambda_{\beta}} (\delta - \mathbf{n} \otimes \mathbf{n}) + \frac{\lambda_m}{2\zeta_{\beta}\lambda_m + (1 - 2\zeta_{\beta})\lambda_{\beta}} \mathbf{n} \otimes \mathbf{n} \quad (3)$$

where ζ_{β} is a geometric parameter related to the aspect ratio ω_{β} of the inclusions [23]. The geometric parameters of pores occupied by water and gas are equal ($\zeta_w = \zeta_g = \zeta_p$) for a uniform aspect ratio of pores ω_p , as assumed in Section 2.1.

Using the identity $\frac{1}{4\pi} \phi \ell^2 \mathbf{n} \otimes \mathbf{n} dS = \frac{1}{3} \delta$, Eq. (2) is simplified as

$$\lambda_{\text{eff}}^{\alpha} = \lambda_m + (\lambda_w - \lambda_m) \phi S_r A_{\text{dil}}^w + (\lambda_g - \lambda_m) \phi(1 - S_r) A_{\text{dil}}^g + (\lambda_s - \lambda_m) \phi_s A_{\text{dil}}^s \quad (4)$$

with

$$A_{\text{dil}}^{\beta} = \frac{2}{3} \frac{\lambda_m}{(1 - \zeta_{\beta})\lambda_m + \zeta_{\beta}\lambda_{\beta}} + \frac{1}{3} \frac{\lambda_m}{2\zeta_{\beta}\lambda_m + (1 - 2\zeta_{\beta})\lambda_{\beta}} \quad (5a)$$

$$A_{\text{MT}}^{\beta} = A_{\text{dil}}^{\beta} [1 - \phi S_r (1 - A_{\text{dil}}^w) - \phi(1 - S_r)(1 - A_{\text{dil}}^g) - \phi_s (1 - A_{\text{dil}}^s)]^{-1} \quad (5b)$$

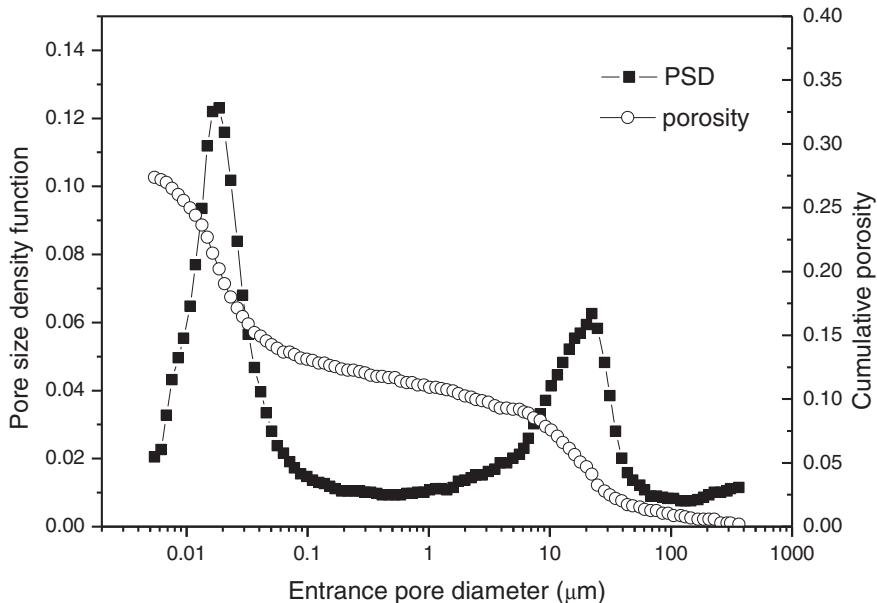


Fig. 1. Pore size distribution and cumulative porosity curve of the MX-80 bentonite–sand mixture (taken after Saba et al. [15]).

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