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A homogenization-based model for estimating effective thermal conductivity of unsaturated compacted bentonites

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ABSTRACT

A homogenization-based effective thermal conductivity model was proposed for unsaturated compacted bentonites. The microstructure of soils was approximated with pores of spheroidal shape, diverse sizes and random orientation, and solid matrix of homogeneous properties (or soil particles of the same assumptions with pores for the self-consistent approach). With the consideration of preferential invasion of the wetting fluid (water) into pores of smaller sizes and by virtue of the analytical solution to Eshelby's inclusion problem in heat conduction, the model was developed using homogenization techniques such as the dilute, Mori–Tanaka (MT), interaction direct derivative (IDD) and self-consistent (SC) schemes for different consideration of the interactions between pores and the solid phase. The proposed estimates are dependent on the thermal conductivities of the solid, liquid and gas phases, porosity, the degree of saturation, and the aspect ratios of pores and/or soil particles. The proposed model was validated against five sets of laboratory measurement data on the MX-80, FEBEX, Kunigel-V1 and GMZ01 bentonites. Compared to Chen's series–parallel structural model recently developed for unsaturated compacted bentonites (Chen et al., 2014), the proposed model not only overall exhibits better performance, but as a great advantage, has much clearer physical mechanisms and significantly reduces the number of parameters by three or four, depending on the homogenization schemes adopted. It is demonstrated that the predictions by the MT, IDD and SC schemes strictly fall within the Weiner bounds and the Hashin–Shtrikman bounds over the full range of porosity and saturation, with the SC estimates overall having slightly better performance than the MT and IDD estimates.

1. Introduction

Bentonite has been considered as an engineered buffer/backfill material for deep geological disposal of high-level radioactive wastes (HLW) because of its low permeability, good swelling capacity and chemical buffering capability, etc. The thermal conductivity of compacted bentonite is a vital property that remarkably influences the transfer of decay heat and the coupled thermo-hydro-mechanical and chemical (THMC) processes in the barrier system [1–3]. Determination of the effective thermal properties of compacted bentonites, therefore, becomes essential for optimization design and safety assessment of the geological repositories [1–4]. In recent three decades, a number of experimental tests were performed to examine the heat transfer behaviors of compacted bentonite materials [5–14], showing that the effective thermal conductivity of bentonites is strongly dependent on their mineralogical composition, dry density, porosity and water content, etc.

The experimental measurements [15,16], however, are always limited and only available in certain well-controlled conditions. For the purpose of extrapolation, a great number of empirical models [5,6,17–20], statistical models [21–24] and structural models [1,3,25–27] were proposed for estimating effective thermal conductivities of two-phase or three-phase porous media with varying saturation, porosity and/or dry density, in which some of the models were particularly developed for bentonite materials [1,3,5–7,19]. It remains a difficult task, however, to relate the heat conductivity properties to the microstructure of compacted bentonites in the above phenomenological models, due to the complexity of the microstructural features of bentonite materials. Microstructure examinations [10,11,28–31] have demonstrated a hierarchical structure of pore spaces, with intra-particle pores, inter-particle pores and inter-aggregate pores within the microstructure of compacted bentonites. The pore size distribution (PSD) curves of compacted bentonites are typically bimodal

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[10,11], with the dominant smaller pore size mode insensitive to compaction or mechanical loading.

Micromechanical approaches provide an alternative that possibly better relates the microstructural features to the effective thermal properties for materials with inhomogeneities. Earlier models [32–35] applied the idea of random phase distribution using the flux concept. Later development of the models [36–42] relied on the analytical solution to the Eshelby's type inclusion problem [43] and formulated the effective thermal conductivity of saturated or partially saturated soil, rock and concrete materials with randomly or arbitrarily oriented pores, voids and cracks of diverse ellipsoidal shapes, using various homogenization techniques such as the dilute scheme, the self-consistent (SC) scheme [44,45], the Mori–Tanaka (MT) scheme [46], the differential scheme [47], the Hashin–Shtrikman type (HS) scheme [48] and the interaction direct derivative (IDD) scheme [49]. However, the micromechanical approaches are less reported to apply to compacted bentonites.

This study presents a homogenization-based model for estimation of the effective thermal conductivity of unsaturated compacted bentonites. The pores and solid particles of compacted bentonites are assumed to be of spheroidal shape and random orientation, and this assumption is partly supported by microscopic observations [31]. At a given saturation, smaller pores are assumed to be preferentially occupied by the wetting fluid (water), with the rest being occupied by the non-wetting fluid (air). The model is developed with the help of the PSD function, but its final expression depends only on the thermal conductivities of the solid, liquid and gas phases, porosity, the degree of saturation and the aspect ratios of pores and/or solid particles. The dilute, MT, IDD and SC homogenization schemes are adopted for different considerations of the interactions between the solid, liquid and gas phases and the effect of their spatial distributions on the effective thermal conductivity. Compared to the series–parallel structural models recently developed by Tong et al. [1] and Chen et al. [3] for unsaturated bentonites, the proposed model not only has clearer physical mechanisms, but significantly reduces the number of parameters by three or four, depending on the homogenization schemes. Validation studies against five sets of laboratory data on the MX-80, FEBEX, Kunigel-V1 and GMZ01 compacted bentonite materials [7–9,12,13] show good agreements between the model predictions and the laboratory measurements if proper homogenization methods are adopted. It is demonstrated that the SC estimates are slightly better than the MT and IDD estimates, and the performance of the proposed model is overall better than the series–parallel structural models. The effective thermal conductivity model, although developed for compacted bentonites, can be readily applied to other types of soils or three-phase media.

2. Model development

2.1. Conceptual model

Compacted bentonite materials are characterized as a three-phase mixture, which contains pores and voids surrounded by solid particles and filled with fluids (liquid water and/or gas mixture). Observations with X-ray micro CT [31] showed that the solid particles or aggregates of bentonites are typically of ellipsoidal shape. The shape of pores could be much more diverse, but for simplicity, this study assumes the pores also to be of spheroidal shape. The size of pores is characterized with radius a and aspect ratio ω, as shown in Fig. 1. The orientation of pores is represented by a unit vector $\boldsymbol{n}$ along the symmetry axis. At the microscopic scale, the thermal conductivity of pores is assumed to be isotropic (denoted by λ_p), and it takes the thermal conductivity value of water ($\lambda_p = \lambda_w$) or that of gas ($\lambda_p = \lambda_g$), depending on whether the pores are occupied by water or gas. The thermal conductivity of the solid phase is also assumed to be isotropic, and denoted by λ_s.

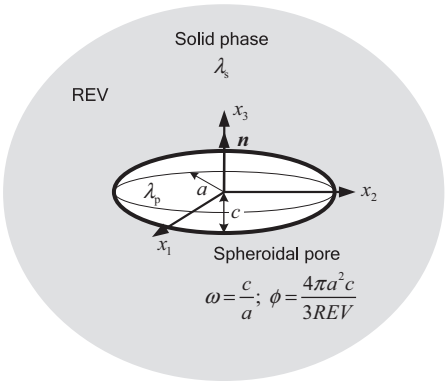

Fig. 1. A single spheroidal pore in REV.

A soil material typically contains numerous pores of different size, shape, orientation and arrangement. The size of pores can be characterized with a pore size distribution (PSD) function $f(r)$, where r is the characteristic radius of pores. For compacted bentonites, the PSD curves are typically bimodal [10,11], with the smaller dominant pore size mode corresponding to the pores inside aggregates and the larger dominant pore size mode corresponding to the inter-particle or inter-aggregate pores. The volume fraction of pores of size in the range $[r, r + dr]$ is denoted by $d\phi = f(r)dr$, as shown in Fig. 2. Proper classification of the pore shapes into finite groups and accurate determination of the pore shapes may be technically difficult, and as a first approximation, a simple assumption is made here that all pores of different sizes have a uniform aspect ratio ω. Furthermore, the pores are expected to have random orientations for compacted soils that are manufactured by sieving with fine mesh and compaction under well-controlled conditions, and hence the volume fraction of pores of orientation $\boldsymbol{n}$ and with size in $[r, r + dr]$ is statistically represented by $d\phi(\boldsymbol{n}) = f(r)dr/4\pi$.

With the above considerations, the overall thermal conductivity of compacted bentonites is isotropic. Estimates of the effective thermal conductivity could be developed by virtue of the analytical solution of thermal conductivity of an infinite homogeneous solid phase embedded with a single ellipsoidal inclusion and using various homogenization approaches such as the dilute, MT, IDD and SC schemes.

2.2. Solution of one inclusion

Consider a representative elementary volume (REV) in which a single spheroidal pore is embedded in an infinite homogeneous solid phase, as shown in Fig. 1. The effective thermal conductivity of such a pore-matrix system is the solution to the Eshelby's inclusion problem (e.g. 37, 39), which provides a basis for

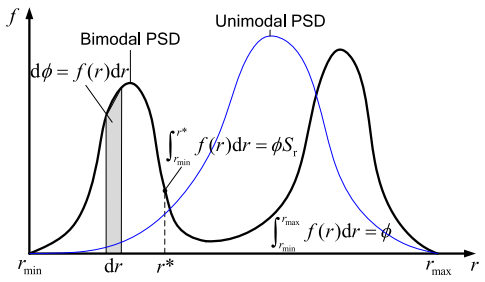

Fig. 2. Pore size distribution of soils.