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Computation of streaming potential in porous media: Modified permeability tensor

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ABSTRACT

We quantify the pressure-driven electrokinetic transport of electrolytes in porous media through a matched asymptotic expansion based method to obtain a homogenized description of the upscaled transport. The pressure driven flow of aqueous electrolytes over charged surfaces leads to the generation of an induced electric potential, commonly termed as the streaming potential. We derive an expression for the modified permeability tensor, $\overleftrightarrow{K}_{eff}$, which is analogous to the Darcy permeability tensor with due accounting for the induced streaming potential. The porous media herein are modeled as spatially periodic. The modified permeability tensor is obtained for both topographically simple and complex domains by enforcing a zero net global current. Towards resolving the complicated details of the porous medium in a computationally efficient framework, the domain identification and reconstruction of the geometries are performed using adaptive quadtree (in 2D) and octree (in 3D) algorithms, which allows one to resolve the solid–liquid interface as per the desired level of resolution. We discuss the influence of the induced streaming potential on the modification of the Darcy law in connection to transport processes through porous plugs, clays and soils by considering a case-study on Berea sandstone.

1. Introduction

Electrokinetics refers to a combined consequence of hydrodynamics and electrostatics due to the interplay of a charged medium and an electric field. It plays a pivotal role in a wide gamut of applications ranging from ion batteries [1], waste-water treatment [2–4], soil dewaterification, water deionization etc. [4] to biophysical process such as transport in ion-selective nanochannels [5–7], drug delivery, bacterial growth etc. [8]. The key to understanding the transport phenomena in such devices involves an appropriate resolution and subsequent interlinking of the coupled physics which generally spans over multiple length-scales [9]. For example, flows across porous plugs take place at the coarse-scale where the pressure gradient of ∼1 bar is applied over a length scale of ∼10 mm while the pores are ∼1 µm, and the interfacial phenomena such as electrical double layer occurs at a finer length scale of ∼10 nm across the fine grains. The presence of such varied scales renders a full scale computational modeling of the porous media as a very unattractive and unviable option [10]. To

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alleviate this issue, there are strategies such as volume averaging [11], homogenization etc. [12] which effectively *upscale* the results obtained at a finer scale (often referred to as the microscopic scale) onto the coarse-scale (referred to as macroscale) to essentially bridge the two scales [13,14].

Flows of electrolytes through a porous medium with electrokinetic effects have been a topic of investigation for a large number of studies. From a biophysical perspective, streaming potential plays an important role in the mechanotransduction mechanism which is necessary for the regulation and maintenance of hydrated soft tissues [15]. Naturally occurring clays, bentonite samples and other typical sand samples are amenable to coupled hydrodynamic transport on the application of an external electric field. Such electrokinetic transport plays an important role in geophysical applications such as soil stabilization, decontamination etc. [16]. For rock samples such as sandstone, carbonate or limestone, the streaming potential measurements are important as they link the geological events such as earthquakes to low frequency electrical and magnetic precursors [17]. It was shown that the increase in the pore pressures during seismic movements led to the movement of groundwater which, in turn, may result in measurable electrical signals [18–20]. Moreover, by suitable alteration of the solvent composition, one can have a dramatic alteration in the electrokinetic transport [21].

From a modeling perspective, researchers have considered the flow through random media, fractured media and disordered structures while characterizing the macroscopic manifestations of the microscopic details [22]. These approaches consider the equilibrium conditions, along with suitable perturbations on the base conditions. By discretizing the domain in solid blocks and reconstructing the porous media such as Fontainbleau sandstone, they have obtained the, so-called, coupling parameters [11,13,23]. The homogenization based upscaling technique, whose foundation is in the matched asymptotic expansions, has successfully been applied to several applications such as heat transfer, solutal dispersion, fluid flow etc. in porous media. Owing to its mathematical rigor and physical consistency, several attempts have been made to use these techniques to describe the macro-microscale coupling in the context of transport of electrolytes through porous media [24–26].

One line of approach of determination of the induced streaming potential due to pressure-driven flow of an ionic solution in a complex domain has been based on the fact that the advective transport of the ionic species evaluated by considering the pressure driven component is balanced exactly by reverse electromigration of the ionic species due to the induced electric field [9]. The major aspect which is, however, overlooked in this approach is the fact that the flow is assumed to be independent of the ionic distribution and the induced electric field. This model, therefore, grossly over-predicts the induced streaming potential [27]. The other approach is based on the thermodynamic force-flux relationships described through the Onsager matrix. These relations describe the net flow and total current in a system as a function of the pressure gradient and electric field prevalent in the system described by the coupling matrix. It needs to be mentioned in this context that the cross coefficients in the Onsager matrix are, theoretically, symmetric. However, Auriault and Lewandowska had shown through upscaling that their preliminary results indicate an asymmetry in the Onsager matrix. This implicates that a reformulation of the upscaling procedure is needed in order to describe the flow through the narrow confinements in the porous media [28]. We attempt to address this problem by considering a formulation which is consistent with the fundamental premises of the Onsager matrix by employing a global constraint on the total current to estimate the streaming potential.

Here, we analyze the pressure-driven electrokinetic transport of electrolytes in porous media through a matched asymptotic expansion based method, in an effort to arrive at a homogenized description of the upscaled transport. The article is organized as follows: In Section 2, we first describe the equations which are valid at all the scales. Next, we express the concerned variables as expansions in terms of a small parameter which relates the microscopic and macroscopic characteristic length scales. In Section 3, we portray the salient steps for the determination of an electropermeability tensor that essentially acts as analogous to Darcy permeability tensor for electrokinetic effects. In Section 4, we discuss about the numerical implementation of the proposed methodology highlighting the important stages of the algorithm. In Section 5, we validate our model by comparing our results with the analytical solution for a simplified case of a parallel-plate channel. We then obtain the modified permeability tensor for a few sample cases in both 2-D and 3-D. Finally, as an illustrative example, we employ the technique outlined here to obtain the modified permeability tensor for a reconstructed Berea sandstone sample.

2. Mathematical formulation

We assume that the macroscopic or the coarse-scale porous medium, through which the flow of a Newtonian fluid occurs, is composed of rigid finer-scale or microscopic repeating (periodic) units (Representative volume element, also abbreviated as RVE or equivalently representative elemental volume, abbreviated as REV) whose length-scale, l, is orders smaller than the length scale of the macroscopic medium, L (see Fig. 1). It is assumed that $\varepsilon = \frac{l}{L} \ll 1$ thereby ensuring a *separation of scales*, a criterion crucial to the method of homogenization [12,14]. The coordinate X, when non-dimensionalized using the macroscopic length-scale is given by $\mathbf{x} = X/L$, whereas the same when non-dimensionalized using the microscopic length scale is given by $\mathbf{y} = X/l$.

2.1. Potential distribution in the EDL

Typically, most substrates acquire a net surface charge when they are in contact with an aqueous solution, as attributed to several possible mechanisms [4,29]. In naturally occurring clays, for example, the presence of a surface charge is due