Multi-Sphere Hydrodynamic Models of Suspensions and Porous Media

by

Ronald Jefferson Phillips

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Abstract

A method has been derived for calculating hydrodynamic interactions in unbounded suspensions and porous media comprised of spherical particles. The method relies upon a separation of these interactions into far-field and near-field components. The far-field, or long-range interactions are calculated in terms of an expansion in moments of the force density of each particle surface about its center, and in principle can be carried out to any level of accuracy that is desired. These far-field interactions are properly renormalized and are summed using an accelerated convergence scheme known as the Ewald summation technique. The near-field, or short-range interactions are accounted for in a pairwise additive fashion using the exact, two-sphere interaction results available in the literature.

This new method of calculation, referred to as the "Stokesian dynamics" method, has been used to calculate transport properties of both spatially periodic and disordered suspensions and porous media. The studies on spatially periodic media allowed the accuracy of the method to be examined through comparisons with the relatively complete set of results available for those systems. Properties such as the hydraulic permeability, sedimentation velocity and shear viscosity were calculated for cubic arrays of spheres. It was found that, in almost every case, Stokesian dynamics gave highly accurate results over the full range of volume fractions possible for hard spheres.

Calculations for disordered media were accomplished by Monte Carlo simulation, in which a series of disordered samples were generated and their transport properties calculated and averaged. In addition to the properties mentioned above for periodic media, short-time self-diffusion coefficients and short-time hindered diffusion coefficients were calculated for single, Brownian particles disordered suspensions and porous media, respectively. The results were compared with other theoretical and experimental results reported in the literature, and again excellent agreement was obtained in almost every case. It should be emphasized here that Stokesian dynamics allowed all the transport properties listed above to be calculated from a single theoretical framework, and also permitted what theoretical predictions do exist for disordered systems to be extended to arbitrarily high volume fractions.

Finally, two approaches have been developed for calculating long-time, macroscopic transport coefficients for a spherical solute in a matrix of fibers. The first method is an effective medium approach based on Brinkman's equation, and has the advantage of being applicable to systems for which very little microstructural information is available. In the second, and more rigorous calculation, the Stokesian dynamics method is used to obtain short-term, or local hydrodynamic coefficients for spherical particles in arrays of bead-and-string fibers. These local coefficients are used to evaluate global coefficients, which govern transport over macroscopic length scales, through application of generalized Taylor dispersion theory. Numerical results have been obtained for two different spatially periodic fiber lattices over a wide range of volume fractions, and for ratios of solute radius to fiber radius ranging from 0.5 to 5. Comparisons between the effective medium model and the generalized Taylor dispersion theory results consistently showed good qualitative agreement, and agreed quantitatively at volume fractions low compared to the critical volume fraction (i.e., the volume fraction where macroscopic transport ceases). In addition the effective medium model predictions of hindered transport coefficients were found to be in excellent agreement with experimental data obtained from the literature, without the use of adjustable parameters.

Thesis Supervisor: William M. Deen
Title: Professor of Chemical Engineering