

# Hydrodynamics of permeable particles suspensions

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In a sequence of recent papers [1–6], we have studied short-time diffusion and viscosity for suspensions of permeable particles. In this presentation, generic features of the permeable sphere model are discussed. An individual particle is modeled as a solvent-permeable sphere of interaction radius  $a$  and uniform permeability  $k$ , with the fluid flow inside the particle described by the Debye-Bueche-Brinkman equation, and outside by the Stokes equation. The particles are assumed to interact non-hydrodynamically by their excluded volumes. Using a precise multipole method and the corresponding numerical code HYDROMULTIPOLE that account for higher-order hydrodynamic multipole moments, numerical results have been obtained for the hydrodynamic function  $H(q)$ , the short-time translational self-diffusion coefficient  $D_t$ , the sedimentation coefficient  $K$ , the collective diffusion coefficient  $D_c$ , the principal peak value  $H(q_m)$  associated with the short-time cage diffusion coefficient, the short-time rotational self-diffusion coefficient  $D_r$ , and the high-frequency shear viscosity  $\eta_\infty$ , as functions of permeability and volume fraction  $\phi$ . Our results cover the full fluid phase regime, with volume fractions up to  $\phi = 0.45$ .

It has been found that for a given volume fraction, the wavenumber dependence of a reduced hydrodynamic function can be estimated by a single master curve, independent of the particle permeability, given by the hard-sphere model. The reduced form is obtained by an appropriate shift and rescaling of  $H(q)$ , parametrized by the self-diffusion and sedimentation coefficients. To improve precision, another reduced hydrodynamic function,  $h_m(q)$ , is also constructed, now with the self-diffusion coefficient and the peak value,  $H(q_m)$ , of the hydrodynamic function as the parameters. For wavenumbers  $qa > 2$ , this function is permeability independent to an excellent accuracy. The hydrodynamic function of permeable particles is thus well-represented in its  $q$ -dependence by a permeability-independent master curve, and three coefficients  $D_s$ ,  $K$  and  $H(q_m)$  that do depend on the permeability. The master curve and its coefficients are evaluated as functions of concentration and permeability.

The virial expansion of the transport properties in powers of the volume fraction has been performed up to the two-particle level. The two-particle virial coefficients corresponding to two-body hydrodynamic interactions have been evaluated with very high accuracy by the series expansion in inverse powers of the inter-particle distance. Results are obtained and discussed for a wide range of the ratio,  $x$ , of the particle radius to the hydrodynamic screening length inside a permeable sphere.

It is shown that for  $x \gtrsim 10$ , the virial coefficients of the transport properties, and also the total values of the transport coefficients, obtained from simulations, are well-approximated by the hydrodynamic radius (annulus) model. In the annulus model [7], a particle suspended in a viscous fluid is characterized by two radii,  $a_<$  and  $a$ . There exist direct pair interactions. Two particles cannot come too close to each other, with the no-overlap radius equal to the geometrical radius  $a$ . In addition, the particles interact hydrodynamically as the hard non-permeable spheres of the smaller radius  $a_<$ , equal to the hydrodynamic radius of a single uniformly permeable particle.

From the simulation results and the calculated values of the two-particle virial coefficients, we have found that the short-time translational and rotational self-diffusion coefficients of permeable spheres can be scaled to the corresponding coefficients of impermeable particles of the same size. From the scaling relations, accurate analytic approximations for the rotational and translational self-diffusion coefficients in concentrated systems are obtained, useful to the experimental analysis of permeable-particle diffusion. An easy-to-use generalized Saitô formula for  $\eta_\infty$  is presented which provides a good description of its permeability and concentration dependence.

The simulation results for permeable particles are used to show that a generalized Stokes-Einstein-Debye relations between rotational or translational self-diffusion, or sedimentation coefficients, and high-frequency viscosity, are not satisfied. The accuracy of a simplifying cell model calculation of  $\eta_\infty$  is also discussed and its range of applicability assessed.

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