Direct Electrohydrodynamic Simulation of Particle Mobility

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Abstract

Introduction:

All particles in suspension have a zeta potential, or surface potential. Its measurement is extremely important for predicting the formulation stability across a wide range of industries including food, ink and pharmaceuticals, water purification and medical devices. Zeta potential is not measurable directly but it can be calculated from an experimentally determined electrophoretic mobility.

Unfortunately, the conversion between mobility and zeta-potential is neither straightforward nor undisputed. Here we use COMSOL to explore this problem, and compare with prevailing solutions.

Use of COMSOL Multiphysics:

Modeling the electrophoretic mobility of an individual charged colloidal particle in a symmetrical electrolyte is a prime example of a strongly coupled Multiphysics problem. Apart from the direct electrical Lorentz force on the colloidal particle, the applied electric field also acts on the ions in the surrounding electrolyte, moving them apart (migration). This creates local concentration gradients that drive diffusion to counter migration. Regions arise where ion concentrations become unbalanced, giving rise to an electrical body force that sets the electrolyte in motion, consequently causing a viscous drag force on the colloidal particle. In addition, the unbalanced ion concentrations distort the electric field, which directly affects the electrical Lorentz force on the particle, and also couples back to the migration of ions and the electrolyte flow. The set of continuum EHD equations are modeled in COMSOL in a 2D rotationally symmetric transient model in weak form PDE mode. Advantage of custom-built equations is that convergence tricks could be implemented, like a logarithmically scaled concentration variable and maximum ion concentration particle packing limits.

Results:

First step was validating the outcome of our model with known literature results. We confirmed that the steady-state mobility values obtained are in excellent quantitative agreement with the numerical results of O'brien and White (1978), as depicted in Figure 2. Now the huge benefit of direct modeling in COMSOL is that it allows to analyze in space and time all factors influencing the particle

mobility, i.e. concentration of co- and counter-ions, the electric field, fluid flow, electrical forces and drag forces.

Conclusion:
Electrophoretic mobility of particles is an important but complex electrohydrodynamic problem. COMSOL direct numerical modeling allows us to explore the various factors influencing the mobility in both space and time. This analysis enhances insight into the rich and complex behavior, and revealed some surprising phenomena.

Reference
R.W. O'Brien et al, Electrophoretic mobility of a spherical colloidal particle, J. Chem. Soc. Faraday Trans., 2 (74), 1607-1626 (1978)

V. Knecht et al, Electrophoretic mobility does not always reflect the charge on an oil droplet, Journal of Colloid and Interface Science, 318, 477-486 (2008)