Modelling electrokinetic two-phase flows applicable to porous media

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The simulation of electrolytic multiphase flow is a highly complex task that requires to simulate a large number of explicit particles or to solve a highly coupled set of non-linear partial differential equations, namely the Navier-Stokes and the Nernst-Planck equations in a continuous picture. At the cost of the molecular details, the continuum scale description enables the investigation of larger-scale systems that are relevant for oil-recovery and biological systems, which are inaccessible with particle-based approaches. An application is the electrophoresis of liquid droplets, which displays various complex phenomena incluing phase separation and transport in biological systems. Different solving techniques are used to solve the equations for the continuum scale, e.g. continuum (mesh) based solvers such as finite element methods and finite-volume approaches. Our choice of solver is based on the lattice-Boltzmann (LB) method, which is a well-established tool to solve the Navier-Stokes equations on a mesh for mesoscale simulations in porous media. We implemented a color-gradient extension for LB [1] to simulate immiscible multiphase flow as well as a custom Nernst-Planck solver to describe dissolved charged chemical species [2]. By developing a coupling between these two methods, we allow for the inclusion of preferential solubilities of the chemical species. For the implementation, the pystencils/lbmpy [3] framework is used, providing a highly optimized code-generation tool for CPU and GPU that allows for rapid prototyping of stencil-code in Python. In order to assess our model, we conduct a simulation study of freely suspended liquid droplets under application of an external electric field.

References

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