Fluctuating hydrodynamics of complex fluid mixtures

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Fluctuating hydrodynamics is a powerful tool for modeling of nonequilibrium phenomena at the mesoscale, where it is no longer possible to use fully atomistic models, but where fluctuations still need to be explicitly modeled. This talk will contain a review of our recent work on computational FHD of complex multispecies liquid mixtures.

In [1] we developed a low Mach number FHD formulation describing transport of mass and momentum in a multispecies mixture of incompressible miscible liquids at specified temperature and pressure. The formulation applies to non-ideal mixtures of arbitrary number of species, without the need to single out a 'solvent' species. We studied the development of giant nonequilibrium concentration fluctuations in a ternary mixture subjected to a steady concentration gradient.

In [2] we formulated and studied computationally the compressible FHD equations for reactive multispecies fluid mixtures. We studied the suppression of non-equilibrium long-ranged correlations of concentration fluctuations by chemical reactions, as well as the enhancement of pattern formation by spontaneous fluctuations. In [3] we developed numerical methods for FHD of reaction-diffusion systems. We demonstrated and quantified the importance of thermodynamic fluctuations to the formation of a two-dimensional Turing-like pattern, and examined the effect of fluctuations on three-dimensional chemical front propagation, to show that fluctuations accelerate pattern formation in spatially homogeneous systems, and lead to a qualitatively-different disordered pattern behind a traveling wave. In ongoing work that will be discussed, we propose a low Mach FHD formulation for reactive mixtures that combines the methods developed in [1] and [3].

In recent work [4], we have formulated and studied computationally the low Mach number fluctuating hydrodynamic equations for (non-reactive) electrolyte solutions. This enables the study of hydrodynamic transport in mixtures of charged species at the mesoscale, down to scales below the Debye length, where thermal fluctuations have a significant impact on the dynamics. In the stochastic setting, our model captures the predicted dynamics of equilibrium and nonequilibrium fluctuations. We also identify and model an instability that appears when diffusive mixing occurs in the presence of an applied electric field.

[l] A. Donev and A.J. Nonaka and, Physics of Fluids **27**, 037103 (2015).

[2] A.K. Bhattacharjee, K. Balakr, J. Chem. Phys. **142**, 224107 (2015).

[3] C. Kim, A. Nonaka, J. B. Bell,, J. Chem. Phys. **146**, 124110 (2017).

[4] J.-P. Peraud, A. Nonaka, A. Ch, Phys. Rev. F **1**, 074103 (2016).