Modeling Reactive Microfluids with Thermal Fluctuations

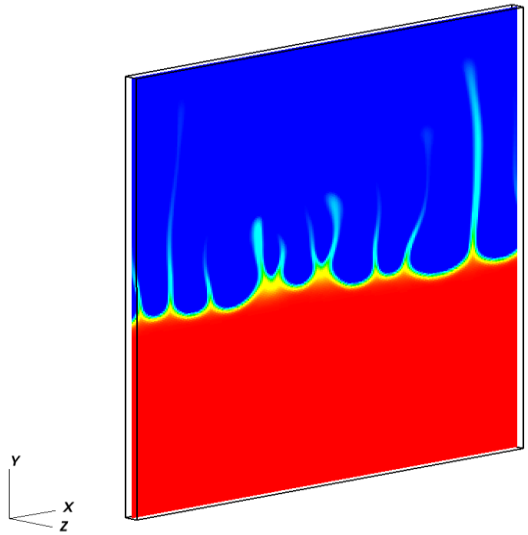
Scientific Achievement

Developed a new simulation method for studying the effect of thermal fluctuations on reactive fluids at the mesoscale and implemented the new approach in an efficient large-scale simulation code.

Significance and Impact

New methodology enables direct detailed observations of the dynamics of a reactive system, which are not usually available from experiments.

One challenging example is an *ideal* experiment of a buoyancy-driven instability (see figure).



Asymmetric fingering observed in a double diffusion instability with a neutralization reaction in a Hele-Shaw cell. This 3D simulation was initiated with natural mass and momentum fluctuations without any artificial perturbation.

Research Details

- An accurate mesoscopic reaction model based on the chemical master equation description is incorporated into the fluctuating hydrodynamics formulation.
- The new method is constructed to efficiently simulate liquid systems, based on an isothermal multi-species Boussinesq approximation and an implicit treatment of viscous momentum dissipation.
- Carefully designed numerical modifications are implemented to handle trace chemical species.
- New simulation methodology can be generalized in a systematic manner to faithfully capture all essential multiphysics in aqueous solutions.

Work performed in collaboration with A. Garcia (SJSU) and A. Donev (NYU)

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