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Generalized Cahn-Hilliard Navier-Stokes equations for numerical simulations of multicomponent immiscible flows ZHAORUI LI, DANIEL LIVESCU, Los Alamos National Laboratory — By using the second-law of thermodynamics and the Onsager reciprocal method for irreversible processes, we have developed a set of physically consistent multicomponent compressible generalized Cahn-Hilliard Navier-Stokes (CGCHNS) equations from basic thermodynamics. The new equations can describe not only flows with pure miscible and pure immiscible materials but also complex flows in which mass diffusion and surface tension or Korteweg stresses effects may coexist. Furthermore, for the first time, the incompressible generalized Cahn-Hilliard Navier-Stokes (IGCHNS) equations are rigorously derived from the incompressible limit of the CGCHNS equations (as the infinite sound speed limit) and applied to the immiscible Rayleigh-Taylor instability problem. Extensive good agreements between numerical results and the linear stability theory (LST) predictions for the Rayleigh-Taylor instability are achieved for a wide range of wavenumber, surface tension, and viscosity values. The late-time results indicate that the IGCHNS equations can naturally capture complex interface topological changes including merging and breaking-up and are free of singularity problems.

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