Study of ultrahigh Atwood-number Rayleigh–Taylor mixing dynamics using the nonlinear large-eddy simulation method

Gregory C. Burton
Center for Turbulence Research, Stanford University, California 94305, USA

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The Nonlinear Large-Eddy Simulation (nLES) method [G. C. Burton, "The nonlinear large-eddy simulation method (nLES) applied to $Sc \approx 1$ and $Sc \gg 1$ passive-scalar mixing," Phys. Fluids **20**, 035103 (2008)] is employed in the first numerical study of multimode miscible Rayleigh–Taylor instability (RTI) in the ultrahigh Atwood-number regime above $A \geq 0.90$. The present work focuses on the dynamics of turbulent mixing at the large density ratios that may be encountered in certain astrophysical contexts and engineering applications. Using the initial condition from the landmark ($N=3072^3$) direct numerical study of Cabot and Cook [W. Cabot and A. W. Cook, "Transition stages of Rayleigh-Taylor instability between miscible fluids," Nat. Phys. **2**, 562 (2006)], the nLES method is first validated in simulations of $A=0.5$ RTI mixing and is shown to recover important statistical measures of the mixing process, such as bubble and spike growth rates and mixing efficiency reported in that study, but at the significantly coarser resolutions typical of most large-eddy simulations. The first simulations of RTI at Atwood numbers $A > 0.90$ are then used to explore the effects of varying the density ratio on mixing dynamics at very high Atwood numbers $0.75 \leq A \leq 0.96$. Spike heights and mixing layer growth rates are shown to be strongly affected by the initial density ratio. An empirical power-law scaling relationship is shown to predict nearly exactly the variation in the ratio of spike to bubble heights as a function of Atwood number. Mixing efficiency is shown to be influenced by the initial density difference but the competition between increased molecular mixing and entrainment largely cancel, producing a relatively modest variation in these flow parameters when compared with the intermediate Atwood-number case. Late-time power spectra show the appearance of an inertial range, indicating that the mixing layer has transitioned to a fully turbulent state. The role of bubble and spike structures in the interscale transfer of kinetic energy is explored for the first time for high Atwood-number RTI flows. Bubble heads (stems) are shown to produce forward (reverse) transfer due to compressive (extensional) straining at intermediate Atwood number. At high Atwood number, however, spike stems are shown to produce forward transfer due to compressive straining generated from the larger spike penetration velocity and the differing spike morphology produced at the higher Atwood number. The study indicates that stable and accurate simulations of ultrahigh Atwood-number mixing may be conducted using the nLES method on grids significantly coarser than used previously to examine RTI flows. © *2011 American Institute of Physics*. [doi:10.1063/1.3549931]

I. BACKGROUND

Rayleigh–Taylor instability (RTI) occurs when a heavier fluid of density ρ_H sits atop a lighter fluid of density ρ_L with a gravitational field vector $\mathbf{g}$ aligned normal to the two-fluid interface and opposed to the density gradient.[1,2] The flow is important to a variety of engineering and scientific applications, such as inertial confinement fusion (ICF), astrophysics, oceanography, and meteorology. For ICF applications, turbulent mixing arising from RTI at the interfaces between capsule shells is directly related to decreasing thermonuclear (TN) yield during an implosion.[3] Similarly, RTI mixing during supernovae collapse directly influences the rate and efficiency of TN burn and the creation of heavy elements.[4] In both ICF applications and astrophysical contexts, Reynolds numbers, defined as $Re_h \equiv h\dot{h}/\nu$ where h is a mixing layer width, $\dot{h}$ is its growth rate, and ν is kinematic viscosity, can exceed $Re_h = 10^4$, and Atwood numbers, defined as $A \equiv (\rho_H - \rho_L)/(\rho_H + \rho_L)$, can exceed $A \geq 0.85$ with some astrophysical conditions approaching $A \to 1$, i.e., a gas-vacuum interface. The growth rate of the RTI mixing layer as well as the efficiency of that mixing are thus key issues in experimental and computational studies of RTI.

In most RTI flows, motion occurs first at the smallest dynamically significant scales, where perturbations at the density interface cause a misalignment of the pressure and density gradients, giving rise to baroclinic torque $\Gamma_{bar} = -(\nabla\rho \times \nabla\rho)/\rho^2$ that sets the system in motion. Heavy fluid falls as spikes into the lighter fluid and the lighter fluid rises as bubbles into the heavy fluid due to buoyancy forces. This movement may create secondary Kelvin–Helmholtz instabilities (KHIs) in the shear layers between individual structures and the local quiescent fluid. Both the RTI and KHI transfer kinetic and scalar energy from the small scales to successively larger scales in the system, through an *inverse cascade* process, i.e., in a direction *opposed* to the usual forward cascade of Kolmogorov theory. As the bubbles

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