Modeling and Simulation of Materials Mixing with Practical Scale-Resolving Simulation Model

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The modeling and simulation of material mixing flows are challenging due to the complex physics of such problems. They include laminar, transitional, and turbulent flow, instabilities, coherent structures, constant and variable-density flow, low and high Mach number regions, shocks, and turbulent kinetic energy production by shear and buoyancy mechanisms. All these physical phenomena are difficult to represent with traditional turbulence models. Hence, the variable-density flow community has been studying these problems with implicit large eddy simulation (ILES) and, most recently, with the bridging partially-averaged Navier-Stokes (PANS) equations[1]. The latter scale-resolving simulation (SRS) formulation aims only to resolve the flow scales not amenable to modeling, representing the remaining turbulent eddies through an appropriate turbulence closure. As such, the PANS method unleashes the concept of accuracy-on-demand, which is responsible for the model's efficiency. In this work, we study the performance of ILES, PANS, and Reynolds-averaging Navier-Stokes (RANS) equations[2] in predicting two variable-density flows, focusing on the simulated flow physics to understand and interpret the results' accuracy. The selected flows are the Rayleigh-Taylor (RT) gravity-driven mixing flow at Atwood number 0.5 and the Richtmyer–Meshkov shock-driven mixing flow recently measured in the Los Alamos National Laboratory vertical shock tube. The results are compared against numerical and experimental results. The RT simulations confirm that ILES and PANS can produce high-fidelity predictions. In contrast, RANS leads to poor agreement with the reference data. The physical interpretation of the results demonstrates that the fidelity of the simulations stems from the ability to accurately predict the instabilities and coherent structures driving the onset of turbulence and the flow. Whereas ILES and PANS can predict these phenomena accurately, RANS overpredicts the Reynolds stresses in laminar coherent structures regions, dissipating them. Compared to ILES, PANS requires a lower fraction of resolved scales to achieve the same modeling accuracy, reducing the computations' cost. Overall, the physical interpretation of the numerical results illustrates the importance of analyzing the impact of the instabilities and coherent structures driving the flow to the accuracy of the simulations and the development of new turbulence models. We expect a similar outcome for the RM simulations.

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