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High Fidelity Modeling of Turbulent Mixing and Chemical Kinetics Interactions in a Post-Detonation Flow Field NEERAJ SINHA, ANDREA ZAMBON, JAMES OTT, MICHAEL DEMAGISTRIS, CRAFT Tech — Driven by the continuing rapid advances in high-performance computing, multi-dimensional high-fidelity modeling is an increasingly reliable predictive tool capable of providing valuable physical insight into complex post-detonation reacting flow fields. Utilizing a series of test cases featuring blast waves interacting with combustible dispersed clouds in a small-scale test setup under well-controlled conditions, the predictive capabilities of a state-of-the-art code are demonstrated and validated. Leveraging physics-based, first principle models and solving large system of equations on highly-resolved grids, the combined effects of finite-rate/multi-phase chemical processes (including thermal ignition), turbulent mixing and shock interactions are captured across the spectrum of relevant time-scales and length scales. Since many scales of motion are generated in a post-detonation environment, even if the initial ambient conditions are quiescent, turbulent mixing plays a major role in the fireball after-burning as well as in dispersion, mixing, ignition and burn-out of combustible clouds in its vicinity. Validating these capabilities at the small scale is critical to establish a reliable predictive tool applicable to more complex and large-scale geometries of practical interest.

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