Large eddy simulation of hydrodynamic instability in gaseous detonations

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Abstract
Despite decades of research on the detonation phenomenon our general understanding of unstable detonation propagation is still highly incomplete. For instance, the state of the turbulent reaction zone and the consumption mechanism of unreacted gas pockets have remained mostly unexplored. It has been shown that in strongly unstable detonations diffusive turbulent mixing plays a key role in propagation. However, in weakly unstable detonations the main shock front is responsible for the initiation of the reaction and turbulent phenomena are of minor importance. In general, the simulation of detonations with resolved reaction zones is becoming progressively easier by the availability of adaptive mesh refinement and high performance computing. However, so far the effect of sub-grid scales in reaction zones of unstable detonations has not been taken into account. In the case of highly unstable detonations, a clear need for sub-grid scale modeling of has been already identified. This work therefore aims at evaluating the role of sub-grid scales in the reaction structure of an unstable detonation configuration.

A large eddy simulation (LES) is utilized in the present work to investigate the structure of detonation and the evolution of hydrodynamic instabilities (i.e., Richtmyer-Meshkov and Kelvin Helmholtz instabilities) in unstable detonations, which are characterized by turbulent reaction zone structure. The governing equations for compressible, reacting flows are Favre filtered and turbulence closure is achieved using the dynamic Smagorinsky subgrid model. The Arrhenius law model based on filtered quantities is employed for the subgrid scale reaction rate. The dependency of the detonation structure on the grid resolution is investigated and the structures obtained by LES are compared with the predictions from solving the Euler and Navier-Stokes (N.S.) equations directly.

The results indicate that to predict irregular detonation structures to be at least in qualitative agreement with experimental observations, the dissipation in small-scale structures should be taken into account. Thus, large eddy simulation with high grid resolution more than 600 cells per half reaction length is required. In low grid resolution scenario, in which numerical diffusion dominates, the structures obtained by solving the Euler or N.S. equations and LES are qualitatively similar. When high grid resolution is employed, the detonation structures obtained by solving the Euler or N.S. equations directly are roughly similar; yet equally in disagreement with the experimental results. We find that for high grid resolution only the LES predicts detonation sub-structures correctly, which we attribute to the increased dissipation provided by the sub-grid scale model. Because the diffusion introduced by subgrid scale (SGS) motions, increases the effect of dissipations, suppresses the vortices that undergo Richtmyer-Meshkov and Kelvin-Helmholtz instabilities. Such an effect also leads to a more rapid consumption of the gases engulfed in the rolling flow of large vortices, as well as, disappearance of long tailed funnel of unreacted gases behind the main shock.