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Detonation Dynamics in a Non-ideal Gas

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Detonation dynamics in a non-ideal, van der Waals gas exhibiting both classical and anomalous waves are studied. This work extends recent work in inert gases [1] to the reactive regime. Anomalous waves are admissible in a gas if isentropes are non-convex, rendering the sound speed to have the unusual feature of decreasing with increasing temperature [2]. The second law-satisfying anomalous waves considered include rarefaction shock waves, continuous compression fans, and composite waves. Analysis of steady wave dynamics in an inert van der Waals gas reveals that the viscous shock solution is required to discern which among multiple second law-satisfying anomalous waves are achieved in an initial value problem. Shock tube solutions are used for verification of numerical simulations. Highly resolved viscous solutions are obtained with a simple explicit Euler time advancement scheme coupled with a second order central spatial discretization. Inviscid simulations are performed with a third order Runge-Kutta temporal discretization and a fifth order Mapped Weighted Essentially Non-Oscillatory (WENO5M) spatial discretization. The WENO5M method is supplemented with a global Lax-Friedrichs flux-splitting in space, as local flux-splitting methods fail when changes in the sound speed are non- monotonic. We extend the classical program of detonation analysis articulated by Fickett and Davis [3] for ideal gases—algebraic CJ analysis, dynamical systems analysis of steady ZND structure, and unsteady numerical analysis of detonation dynamics—to non-ideal gases with non-convex equations of state. New analysis is done of steady detonation dynamics in a van der Waals gas that exhibits both classical and anomalous behavior. Understanding of anomalous steady wave dynamics in inert flows is used to identify potential complications with Chapman-Jouguet (CJ) and Zel'dovich-von Neumann-Döring (ZND) analysis in and around the anomalous region. Non-convexities of Hugoniot curves in the anomalous region are found to render steady solutions predicted by CJ and ZND analysis inadmissible. Numerical predictions of stable unsteady detonations driven by an anomalous wave are presented, and the detonation dynamics are shown to be consistent with the structure of piston-driven detonations. The van der Waals model is shown to delay the transition to instability of detonations in the classical regime.

References

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