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A Novel Temperature Non-Equilibrium Reactive Model for Detonation Hydrodynamics

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Detonation waves in gases exhibit a distinctive cellular structure that controls the overall rate of energy release. The cellular structure consists of repeated triple-shock reflections that are driven by the coupling of reactivity to the Mach and transverse shocks [1]. Owing to the wide variations in temperature, the reaction rates can be very large behind the stronger parts of the front. These local hotspot regions, with enhanced reactivity, are believed to control the initiation and propagation limits of detonations. Recently, numerical evidence using molecular dynamics showed that reactivity may be influenced by the presence of local non-equilibrium within the shock wave [2, 3]. Furthermore, reactions were observed to evolve faster than predicted by classical reaction rates based on the assumption of local equilibrium. These enhancements are attributed to the Zel'dovich mechanisms of super-collisions inside the shock structure [4]. Within the shock, the translational temperature in the direction of the shock propagation is higher than the equilibrium post-shock temperature. This can lead to local super-collisions, enhancing the reactivity. The question that arise is: can this effect be modelled quantitatively using kinetic theory in a framework conducive to a hydrodynamic model for the detonation fluid mechanics. The present study reports our progress in answering this important question. In this work, we use a mesoscale model based on moments of the Boltzmann equation. This allows us to accurately model the relaxation process of translational temperature associated with shocks [5, 6]. Furthermore, a new reactive kinetic model accounting for multiple translational temperatures is also formulated.

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