

Abstract Submitted
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Vibrational nonequilibrium in chain branching reactions of hydrogen combustion using quasi-classical trajectory analysis¹ STEPHEN VOELKEL, University of Texas at Austin, VENKAT RAMAN, University of Michigan, PHILIP VARGHESE, University of Texas at Austin — In high-speed reactive flows in scramjets, thermal nonequilibrium is introduced in the flow via shock waves. Though rotational and translational energy modes relax back to equilibrium quickly, vibrational relaxation is comparable to the bulk mixing and reaction timescales. The discrepancy between vibration and rotation/translation energy distributions can dramatically alter on the initiation of the fuel oxidation process. For continuum-scale applications, thermal nonequilibrium effects are derived from the rovibrational state-specific reaction and scattering rates associated with the chemical mechanism. In this work, the state-specific reaction rates are calculated for the chain branching reactions in the hydrogen combustion mechanism using a quasi-classical trajectory (QCT) framework. The state-specific rates are incorporated into a multiple temperature continuum-scale model whereby each species is characterized by a Boltzmann distribution parametrized by its own vibrational temperature. The flame ignition rates are implemented in a CFD code to simulate a reactive coflow.

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