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Molecular simulations of Crussard curves of detonation product mixtures at chemical equilibrium: Microscopic calculation of the Chapman-Jouguet state EMERIC BOURASSEAU, VINCENT DUBOIS, NICO-LAS DESBIENS, JEAN-BERNARD MAILLET, CEA-DAM — The simultaneous use of the Reaction Ensemble Monte Carlo (ReMC) method and the Adaptative Erpenbeck EOS (AE-EOS) method allows us to calculate directly the thermodynamical and chemical equilibrium of a mixture on the hugoniot curve. The ReMC method allow to reach chemical equilibrium of detonation products and the AE-EOS method constraints the system to satisfy the Hugoniot relation. Once the Crussard curve of detonation products has been established, CJ state properties may be calculated. An additional NPT simulation is performed at CJ conditions in order to compute derivative thermodynamic quantities like Cp, Cv, Gruneisen gama, sound velocity, and compressibility factor. Several explosives has been studied, of which PETN, nitromethane, tetranitromethane, and hexanitroethane. In these first simulations, solid carbon is eventually treated using an EOS.

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