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Temperature-based model for condensed-phase explosive detonation NICOLAS DESBIENS, CHRISTOPHE MATIGNON, REMY SORIN, VINCENT DUBOIS, CEA, DAM, DIF, F-91297 ARPAJON — Simple reactive flow models for condensed explosives have four requirements: two equations of state (EOS), one for the unreacted condensed-phase explosive, and one for its detonation products, a reaction rate law that converts the explosive in products and a mixture rule to compute the biphasic partially reacted states. Generally, the chemical reaction rates are governed by local temperature. Nonetheless, temperature fields are scarcely known, especially in detonating condensed-phase explosives. Hence this quantity is not provided by the usual unreacted explosive EOS with the required accuracy. As a consequence, for shock initiation and detonation phenomena, rate laws are based on easily measurable properties such as pressure, compression or particle velocity. In this work, we build an EOS for a TATB-based explosive that provides a better estimate of the shocked explosive temperature. This EOS is derived from ab initio simulation results of monocristalline TATB. Then the well-known pressure-based WSD reaction rate law is rewritten to be temperature-dependent. This model is expected to give interesting results as regards shock desensitization and initial conditions variations while remaining very accurate for detonation propagation. Preliminary results will be shown.

Nicolas Desbiens
CEA, DAM, DIF, F-91297 ARPAJON

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