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Multicale modeling of the detonation of aluminized explosives using SPH-MD-QM method[1] QING PENG, Rensselaer Polytechnic Institute, GUANGYU WANG, GUI-RONG LIU, University of Cincinnati, SUVRANU DE, Rensselaer Polytechnic Institute — Aluminized explosives have been applied in military industry since decades ago. Compared with ideal explosives, aluminized explosives feature both fast detonation and slow metal combustion chemistry, generating a complex multi-phase reactive flow. Here, we introduce a sequential multiscale model of SPH-MD-QM to simulate the detonation behavior of aluminized explosives. At the bottom level, first-principles quantum mechanics (QM) calculations are employed to obtain the training sets for fitting the ReaxFF potentials, which are used in turn in the reactive molecular dynamics (MD) simulations in the middle level to obtain the chemical reaction rates and equations of states. At the up lever, a smooth particle hydrodynamics (SPH) method incorporated ignition and growth model and afterburning model has been used for the simulation of the detonation and combustion of the aluminized explosive. Simulation is compared with experiment and good agreement is observed. The proposed multiscale method of SPH-MD-QM could be used to optimize the performance of aluminized explosives.

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