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Equation of state of detonation products based on statistical mechanical theory YANHONG ZHAO, HAIFENG LIU, GONGMU ZHANG, HAIFENG SONG, IAPCM (Institute of Applied Physics and Computational Mathematics), IAPCM TEAM — The equation of state (EOS) of gaseous detonation products is calculated using Ross's modification of hard-sphere variation theory and the improved one-fluid van der Waals mixture model. The condensed phase of carbon is a mixture of graphite, diamond, graphite-like liquid and diamond-like liquid. For a mixed system of detonation products, the free energy minimization principle is used to calculate the equilibrium compositions of detonation products by solving chemical equilibrium equations. Meanwhile, a chemical equilibrium code is developed base on the theory proposed in this article, and then it is used in the three typical calculations as follow:(i) Calculation for detonation parameters of explosive, the calculated values of detonation velocity, the detonation pressure and the detonation temperature are in good agreement with experimental ones. (ii) Calculation for isentropic unloading line of RDX explosive, whose starting points is the CJ point. Comparison with the results of JWL EOS it is found that the calculated value of gamma is monotonically decreasing using the presented theory in this paper, while double peaks phenomenon appears using JWL EOS.

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