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Improvements of the CARTE thermochemical code dedicated to the computation of properties of explosives NICOLAS DESBIENS, VINCENT DUBOIS, CHRISTOPHE MATIGNON, REMY SORIN, CEA, DAM, DIF
— Predicting the thermodynamic properties of detonation products and the detonation parameters of explosives with thermochemical codes requires both the use of very accurate theoretical equations of state of fluid species and a precise calibration of the parameters of the species potentials. In this work, we present the methods used in the CARTE[(1)] thermochemical code. The detonation product mixture is split in two phases (fluid phase plus condensed phase for the carbon). The improved KLRR[(2)] method and a modified Van der Waals – one fluid model[(3)] are used to compute the properties of the mixture. The usual Ree – Van Thiel equation of state for carbon is used. Ionic/polar species are taken into account by the use of methods already published in the literature[(4)]. We also consider a multiphase EOS model of carbon which evolves with the chemical composition of the explosives. The calibration of the parameters is then performed with a Monte Carlo minimisation method against a wide range of both theoretical and experimental data. This reference data base is mainly composed of shock or static compression data. Finally, we present some results obtained on a wide range of explosives. (1) Dubois et al., Chem. Phys. Lett., 494, 2010, p 306 (2) Victorov et al., Proc. of the 13^{th} Int. Deto. Symp., 2006 (3) Desbiens et al., Proc. of 8^{th} New Models and Hydrocodes, 2010 (4) Bastea et al., Proc. of the 13^{th} Int. Deto. Symp., 2006

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