THE MULTICOMPONENT VERSION OF HMSA CLOSURE FOR CO_2, N_2, AND O_2 SHOCK HUGONIOTS SIMULATION

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Abstract: Both repulsion and attraction molecular interactions influence shock compression process in $C_xN_yO_z$ mixtures. As a result, exact equation of state (EOS) with wide applicability range is required to simulate shock Hugoniots of such systems. A self-consistent Ornstein–Zernike application (SCOZA) based on distribution function integral equation theory (DFIET) is able to solve this problem. As known, hybrid hypernetted chain-softcore mean spherical approximation (HMSA) closure for SCOZA provides accurate results for fluids at high pressures. Unfortunately, this closure was developed for a single component. The van der Waals one-fluid model is convenient to use with HMSA to simulate mixture of dissociated shock products. This model is not able to simulate CO_2 shock Hugoniots at pressures higher than 50 GPa. In this paper, the new multicomponent closure based on HMSA and partial version of virial theorem has been suggested. It is verified by molecular Monte-Carlo simulation at pressures up to 160 GPa with accuracy about 1%–2%.

Keywords: HMSA; SCOZA; DFIET; equation of state; carbon dioxide; nitrogen; oxygen; shock wave; Hugoniots; fluid; Monte Carlo

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