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Computations of fluid mixtures including solid carbon at chemical equilibrium

EMERIC BOURASSEAU, CEA

One of the key points of the understanding of detonation phenomena is the determination of equation of state of the detonation products mixture. Concerning carbon rich explosives, detonation products mixtures are composed of solid carbon nano-clusters immersed in a high density fluid phase. The study of such systems where both chemical and phase equilibriums occur simultaneously represents an important challenge and molecular simulation methods appear to be one of the more promising way to obtain some answers. In this talk, the Reaction Ensemble Monte Carlo (RxMC) method will be presented. This method allows the system to reach the chemical equilibrium of a mixture driven by a set of linearly independent chemical equations. Applied to detonation product mixtures, it allows the calculation of the chemical composition of the mixture and its thermodynamic properties. Moreover, an original model has been proposed to take explicitly into account a solid carbon meso-particle in thermodynamic and chemical equilibrium with the fluid. Finally our simulations show that the intrinsic inhomogeneous nature of the system (i.e. the fact that the solid phase is immersed in the fluid phase) has an important impact on the thermodynamic properties, and as a consequence must be taken into account.