Abstract Submitted
for the SHOCK07 Meeting of
The American Physical Society

Monte Carlo Simulations of the Effect of Cross-potential Variations on the Equation of State of N_2/CO_2 Mixtures and of Detonation Products M. SAM SHAW, Los Alamos National Laboratory — The issues of mixing and cross-potentials were studied with particular emphasis on the implications for detonation products equation of state (EOS) and the prediction of measurable sensitivity to the cross-potential. A large number of Monte Carlo simulations were made with the choice of ensemble depending on the system being studied: NPT for uniform mixing, Gibbs for fluid-fluid phase separation, and Composite for full detonation products with chemical equilibrium and carbon clusters. Simulations with N_2/CO_2 mixtures demonstrate significant sensitivity to the cross-potential in the EOS values for uniform mixtures, in the shape of the isotherms and the location of rapid changes due to fluid-fluid phase separation, and in the location of the fluid-fluid phase separation line in pressure and temperature. Suggestions are made for experimental methods to characterize the cross-potential and mixing properties. Evaluation of the full EOS for HMX based explosives demonstrates an amplified effect of the cross-potential variation through dramatic shifts in thermodynamic equilibrium composition and the resulting EOS.

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Date submitted: 22 Feb 2007 Electronic form version 1.4