

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Direct Simulation of Detonations: Applications to the H₂-Cl₂ System¹ PATRICK D. O'CONNOR, Pennsylvania State University, LYLE N. LONG, Pennsylvania State University, JAMES B. ANDERSON, Pennsylvania State University — Earlier simulations in our laboratory showed that ultrafast detonations having steady-state velocities greater than predicted by the Chapman-Jouguet (CJ) and the Zeldovich-von Neumann-Döring (ZND) theories could be produced by very fast model reactions. In this paper we will report matching studies incorporating a realistic treatment of the reaction $\text{H}_2 + \text{Cl}_2 \rightarrow 2 \text{HCl}$ reacting by the Nernst chain reaction mechanism with ignition, propagation and termination steps along with the inclusion of rotational and vibrational degrees of freedom for diatomic species and the realistic treatment of energy exchanges among all species. The H₂-Cl₂ system is the prototypical system for studying detonations both experimentally and theoretically, and is an ideal candidate for investigation. Our simulations are made using Bird's direct simulation Monte Carlo method which produces the full details of the coupled gas-dynamic and reaction effects as well as temperature, velocity, density, pressure, and species profiles for the detonation waves. By comparing predictions with available experimental measurements for the system, we will be able to predict the likelihood that ultrafast detonations can be observed for the H₂-Cl₂ reaction.

¹NSF IGERT Grant No. NSF-DGE-9987589

James B. Anderson
Pennsylvania State University

Date submitted: 30 Nov 2005

Electronic form version 1.4