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The Simulation of Detonations Using a Monte Carlo Method

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ABSTRACT

We report the successful simulation of detonation waves using the direct simulation Monte Carlo (DSMC) method. The simulations provide 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. The systems treated are simplified and clarified by restriction to the reaction $A + M \rightarrow B + M$ with variable energy release and rate characteristics and with ideal and calorically perfect gas reactants and products. Results are compared with the predictions based on the Chapman-Jouguet condition.

INTRODUCTION

The Direct Simulation Monte Carlo (DSMC) method [1,2] has been found remarkably successful for predicting and understanding a number of difficult problems in rarefied gas dynamics. Extension to chemical reaction systems has provided a very powerful tool for reaction systems with non-thermal distributions, with coupled gas-dynamic and reaction effects, with concentration gradients, with emission and absorption of radiation, and with many other effects difficult or impossible to treat in any other way. Examples of systems which may be treated include flames and explosions, shock waves and detonations, reactions and energy transfer in chemical laser cavities, upper atmosphere reactions and radiation effects, fluorescent lamp discharges, and many, many others. In this paper we describe the application of the DSMC method to the problem of detonations, a classic and an extreme example of the coupling of gas dynamics and chemical reactions.

Although a Monte Carlo simulation of a gas was described by Lord Kelvin in 1901 [3], it was not until the 1960's that the use of such simulations became practical for solving problems in the field of rarefied gas dynamics. The combination of an efficient sampling developed by Bird in 1963 [1] with high speed computers made possible the nearly exact simulation of a large number of systems which had previously been impossible to analyze. The current generation of computers makes it possible to consider much more ambitious applications: those in which chemical reactions are important. Since chemical reactions are in most cases relatively rare events, the numbers of collisions which must be calculated for reaction systems are likely to be large compared to those for the dynamics of inert gases. The applications are, for the present, restricted to fairly reactive systems at reasonably low gas densities, but it is precisely these systems which depart farthest from equilibrium distributions and which are most difficult to treat. In the case of detonations we have very reactive systems and in place of low gas densities we have very small length dimensions.

Some years ago we used Bird's direct simulation method for treating complex problems in the redistribution and relaxation of energy among the electronic states of a dilute gas [4,5]. One of these involving the coupling of rarefied gas dynamics and chemistry is the simulation of a 2-D free-jet flow with electronic relaxation, which has applications in laser isotope separation. The molecules were treated as hard spheres of five different energy states with the collision dynamics obtained from a statistical model satisfying all the requirements of energy and momentum conservation, microscopic reversibility and equilibrium. The results were found useful in understanding the expansion of high temperature uranium gas from a slit source [5]. Other systems examined thus far include homogeneous isotropic systems for an exothermic bimolecular reaction [6], a Lindemann-Christiansen reaction system [7], an energy-

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dependent unimolecular reaction [8], and a dissociation-recombination system [9]. In these studies we found the number of sample molecules required for adequate simulations to be far lower than we could have imagined.

The DSMC simulation of reactive systems has been reviewed in detail by Bird [2]. Energy transfer among metastable species has been treated with DSMC by Nishimura and Shibata [10]. Modelling of vibrational exchange and chemical kinetics has been carried out by Bruno, Capitelli, and Longo [11] and by Longo and Boyd [12]. Koura [13] has applied DSMC in its application to vibrational relaxation of nitrogen. Bird [14] has proposed new chemical reaction models for DSMC.

DETONATIONS

A detonation wave travels at supersonic speed in a reactive gas mixture and is driven by the energy released by exothermic reaction within the wave. The modern theory of detonations began with the work of Chapman [15] and Jouguet [16] about 1900, and their work has been extended by a number of workers, in particular by von Neumann [17], Döring [18], and Zeldovich [19]. Reviews include those by Lewis and von Elbe [20], Hirschfelder, Curtiss, and Bird [21], and Glassman [22].

As for ordinary shock waves it is convenient to use a coordinate system which moves with the wave, such that the detonation wave is stationary. The unburned gases (upstream, subscript 1) enter the detonation wave, are compressed and react, and then exit the wave as burned gases (downstream, subscript 2). For a one-dimensional system the conservation equations become

$$\begin{aligned}\rho_1 u_1 &= \rho_2 u_2 \\ \rho_1 u_1^2 + p_1 &= \rho_2 u_2^2 + p_2 \\ \frac{1}{2} u_1^2 + H_1 &= \frac{1}{2} u_2^2 + H_2\end{aligned}$$

where ρ , u , and p , are the density, velocity, and pressure, respectively, and H is the enthalpy per unit mass. These three equations, together with an equation of state for the gas, provide four equations which relate the five unknowns u_1 , u_2 , p_2 , ρ_2 , and H_2 .

In the model proposed independently by von Neumann, Döring, and Zeldovich the shock wave precedes the reaction. They proved for this model that the velocity u_2 of the burned gases relative to the detonation wave is the local velocity of sound. In this case the velocity D of the detonation wave relative to the upstream velocity u_1 is given by

$$D = \frac{n_2}{n_1} \sqrt{\gamma k T_2 / m}$$

where γ is the specific heat ratio and m is the mean molecular mass for the burned gases. This relation has *not* been proved for cases in which the shock zone overlaps the reaction zone.

In order to simplify the calculations reported here and to clarify the results by eliminating extraneous effects, we consider the special case of the reaction of $A + M \rightarrow B + M$ in which the masses of A, B, and M are equal. Further, the gases are ideal and calorically perfect and have constant heat capacities as for monatomic species. The energy release on reaction is fixed at the amount Q (per molecule A reacting), the energy per molecule is $3/2 kT$, the enthalpy exclusive of Q is $5/2 kT$, the mass is fixed at m , and the equation of state is $p = nkT$ where n is the number density of molecules. The constant k is the Boltzmann constant.

With these simplifications the conservation equations above become

$$\begin{aligned}n_1 u_1 &= n_2 u_2 \\ n_1 m u_1^2 + n_1 k T_1 &= n_2 m u_2^2 + n_2 k T_2 \\ Q + \frac{1}{2} m u_1^2 + \frac{5}{2} k T_1 &= \frac{1}{2} m u_2^2 + \frac{5}{2} k T_2\end{aligned}$$

These may be recombined with the equation of state to give the relation

$$\frac{p_2}{p_1} = \frac{4 + 2 \frac{Q}{k T_1} - \frac{n_1}{n_2}}{4 \frac{n_1}{n_2} - 1}$$

This gives the Hugoniot relations for the system. They are often plotted on a Rankine-Hugoniot diagram as curves of p_2/p_1 vs. n_1/n_2 (or ρ_1/ρ_2), an initial or shock Hugoniot curve for the unburned ($Q = 0$) gases and a final Hugoniot curve for the burned ($Q = Q$) gases. In passing through the detonation wave the system passes from one Hugoniot curve to the other. The point on the initial curve is fixed by the initial conditions. The point on the final curve depends on the detailed characteristics of the detonation wave.

The cross-section S_r for the reaction $A + M \rightarrow B + M$ is specified as a function of collision energy E_{rel} and a minimum energy E^* required for reaction as well as a steric factor P_r and the hard-sphere cross-section S for all collisions,

$$\begin{aligned} S_r &= P_r S, & E_{rel} &\geq E^* \\ S_r &= 0, & E_{rel} &< E^* \end{aligned}$$

In a system with a Maxwellian distribution of relative velocities this model gives the second-order rate constant k_{rate} [23]

$$k_{rate} = P_r S \sqrt{\frac{8kT}{\pi\mu}} e^{-\frac{E^*}{kT}} \left(1 + \frac{E^*}{kT} \right)$$

where μ is the reduced mass for A - M pair.

DSMC CODE

DSMC simulations were carried out for a variety of conditions using both transient and steady-state codes. The transient code was a 3-D code with the option of either periodic boundaries or solid-wall outer boundaries in each direction. It was run in a time-accurate manner, and the time-accurate results were obtained from the ensemble average of numerous instances of each run. The steady-state code was a 1-D code with an adjustable velocity at the upstream entrance and a vacuum condition at the downstream exit. Results reported here are those for the transient code. Essentially identical results were obtained with the steady-state code.

The programs were written in a modular fashion, using Fortran-90. Fortran-90 (and Fortran-95) have some real advantages over previous versions of Fortran, such as array syntax, free format source code, modules, and allocatable arrays. In addition, this code can be used with OpenMP, MPI, or High Performance Fortran compiler directives to run on parallel computers or clusters of Personal Computers [24, 25].

The molecules were treated as hard spheres. The unburned or reactant gases were specified as pure A. The species M was either A or B. For collisions of A with A only one A was allowed to react. The energy released by reaction was added to the initial relative kinetic energy of the collision partners and distributed as for the collision of hard spheres.

The transient code in the 1-D mode had 5000 cells in the x-direction 1 cell in the y- and z-directions. Periodic conditions were used in all three spatial directions. Other cases were run that used solid walls at each end of the grid in the Y-direction. The detonation was started by either suddenly increasing the temperature in one of the cells (to simulate an ignition source), or by simply specifying that the wall temperature was relatively high (e.g. 1000K). Both methods ignited the gas and produced similar detonations. For most of the current simulations we used 500 time steps, 250,000 particles and 5000 cells. Each simulation was run on a 166 MHz Pentium laptop in roughly 2.5 hours and required 9 megabytes of memory. The computations required roughly 30 billion floating point operations.

RESULTS

Profiles of the detonation wave for a typical simulation are shown in Figure 1. For this run the cell length was specified as one mean free path for unburned gases and the mass m was 50 gm/mole. For the reaction parameters we have the activation energy $E^* = 5.0$ kcal/mole, the steric factor $P_r = 0.2$, and the energy release $Q = 20.0$ kcal/mole.

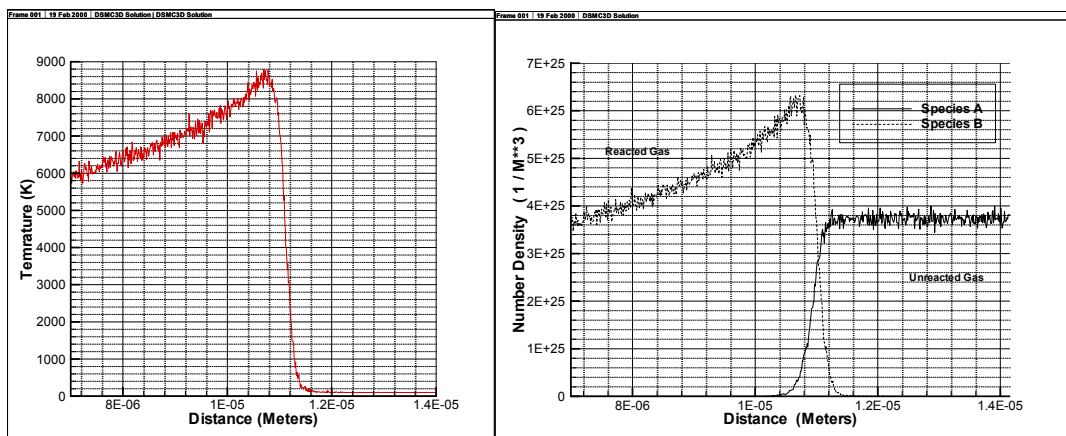


Figure 1. Temperature and species concentration levels for a reaction with 20 Kcal energy release (see text).

The profiles in Figure 1 show a detonation wave travelling from left to right into an undisturbed gas at 100K. The peak temperature reaches approximately 8500K, and after the wave passes the gas expands and the temperature is reduced. The number densities of the two species is also shown in Figure 1. The number density discontinuity is not symmetric, having a fairly long tail in the reacted flow region. In addition, the location of the discontinuity in the number density and the temperature plots are shifted from each other by roughly 5 mean free paths.

The variation of some of the detonation wave characteristics are shown in Figure 2. The conditions are the same as those listed above except that the energy release Q is varied in the range of 5 to 25 kcal/mole. The detonation velocities D and the temperatures T_2 predicted for the Chapman-Jouguet condition are also shown for comparison.

The calculations produce a variety of interesting results. Temperature, density, and reaction-rate peaks may be separated. Temperature and density maxima depend strongly on the reaction rate. The thickness of the reaction zone varies strongly with the conditions.

CONCLUSION

This paper presents some preliminary results for simulations of detonations. The results provide some interesting tests for some of the earlier theoretical models of detonations. In the future we hope to model more complex reactions, as well as 3-D results. We are especially interested in performing detonation simulations inside closed containers.

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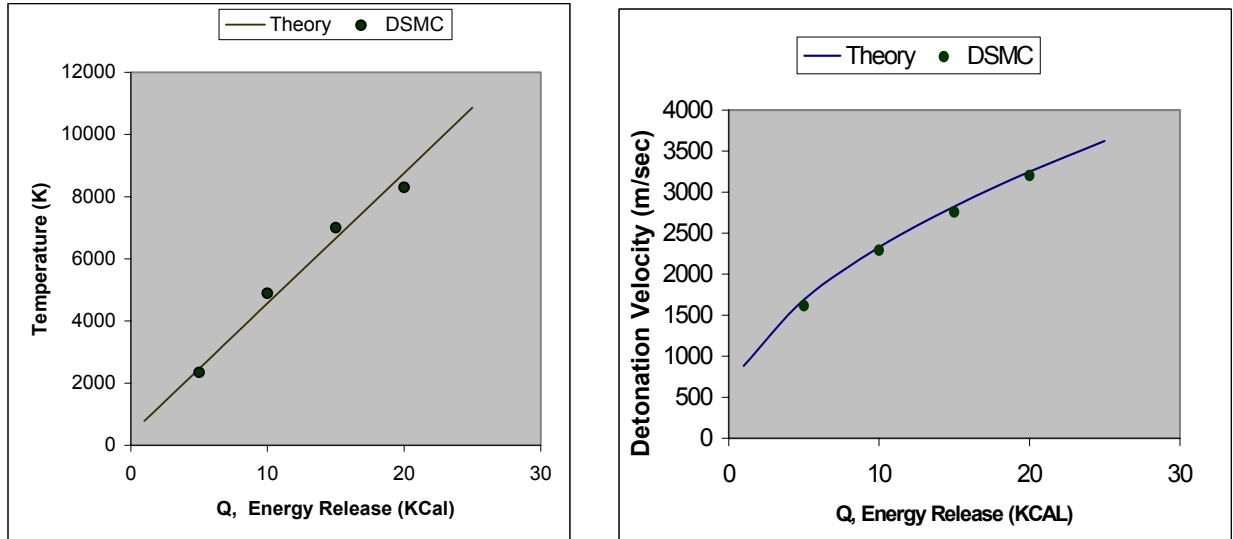


Figure 2. Peak temperature (T) and Detonation velocity (D) vs. energy release Q .

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