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MODELING OF DETONATION: ROLE OF VACANCIES IN THE INITIATION OF DETONATION IN AN ENERGETIC CRYSTAL

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Abstract
We have employed the method of molecular dynamics in a preliminary study of the initiation of detonation in an energetic molecular crystal containing vacancy defects. The model was a two-dimensional filament of 8 x 240 diatomic molecules which were capable of undergoing exothermic dissociation. The reaction was initiated at one end of the filament by heating. The ensuing dynamics of detonation was followed by calculating the motions of the dissociating molecules as a function of time. The results showed that with this particular model, there was a tendency for the vacancies to diffuse by thermal motion, and that the net effect of the vacancies was the reduction of the caging effect on dissociation. This in turn produced a measurable effect on the initiation of detonation, the reaction rate, the energy and the stress profiles, and the shock propagation velocity. In order to study the effect of a cluster of vacancies on initiation, it will be necessary to modify the interatomic-intermolecular potentials so as to stabilize the vacancy configuration.

A special feature of this investigation was that the computational work was performed entirely on a personal computer driving a 32-bit coprocessor board. It was found that the use of such a system for doing large-scale modeling of scientific problems was both practical and cost-effective.
I. INTRODUCTION

The problems of initiation of detonation are important to our understanding of dense explosives and their use. These problems have been extensively studied from the macroscopic viewpoint [1-7]. It is generally thought that reactions start at local "hot spots" in the material under shock compression. These are believed to be caused by defects such as porosity, grain boundaries, dislocations, etc. But the nature and the energetics of the "hot spots" in response to different forms of excitation are not completely clear. Sharma, et al. [7] found, for example, that the effects of thermal heating and electron beam on the the initiation of reactions in TATB are different from those of UV excitation and impact.

To understand these problems of detonation, we need to develop our insight into the processes of energy transfer and energy sharing in condensed systems on a molecular scale. These energy exchange processes are in fact of very general interest in physics and chemistry. In the past these have been studied mostly in the gas phase [8]. But with the development of lasers, computers and chemical studies in the picosecond regime, investigations of these problems in condensed phases also have become active, because it is now possible to study the details of energy transfer on the time scale of real chemical experiments [9-12]. These developments also have encouraged investigators in various countries to conduct model studies of detonation by means of molecular dynamical simulation [13-17].

The method of molecular dynamics (MD) is now well established. From the viewpoint of detonation studies, however, our knowledge of the intermolecular potentials for complex molecules is still too rudimentary for MD to simulate real chemical reactions, which in any case obey quantum mechanical laws rather than classical laws of motion. On the other hand, in the high temperature environment of detonation, we expect that MD would give an accurate description of the motion of the atoms and molecules, consistent with the assumed set of model potentials. These details may be expected to provide information on the energy flow among the molecules, and thus allow us to investigate in considerable detail those energy transfer processes and initiation mechanisms which depend on the motion and the geometric arrangement of the molecular system.

In this report we discuss some preliminary results of an MD study of the role of vacancy defects on the initiation of detonation in a crystalline model of diatomic molecules capable of undergoing sustained exothermic dissociation reactions, leading to detonation, when the system was subjected to local heating or shock compression.

The model used in this investigation is described in Section II. In Section III we report briefly on our experience with a personal microcomputer system that was used for all the computations and graphics. This is a special feature of this project, and the relatively low cost and high efficiency of the system is noteworthy and may be of interest to other investigators. In Section IV we discuss the results, and in Section V we give our conclusions and discuss our view on the direction of future work.

II. MODEL

The model used here was basically the same diatomic molecular crystal described in Refs. [13,14]:
Here $A_2$ is a diatomic molecule prepared in its metastable, predissociative state, $k_1$ and $k_2$ are the rate constants for the forward and reverse reactions, $A$ is the dissociated free atom, and the energy term is the energy released by the dissociation reaction. This model was chosen mainly for its simplicity, but as we showed in [13,14], the dynamical characteristics of the model were well-behaved, whether the dissociation was exothermic or endothermic.

All atoms were considered to be independent particles which interacted with one another through a compound Morse potential $V_1 - V_2$:

\[
V_1 = E\{\exp[-2a_1(R-R_{1})]-2\exp[-a_1(R-R_1)]\}, \quad \text{for } R>R_{\text{dis}}; \tag{1a}
\]
\[
V_2 = b_2E\{\exp[-2a_2(R-0.15R_{1})]-2\exp[-a_2(R-0.15R_1)]\}+QE, \quad \text{for } R<R_{\text{dis}}. \tag{1b}
\]

$V_1$ and $V_2$ are both in energy units of $E$ taken here to be unity. $R=R_{ij}$ is the distance between atoms $i$ and $j$, $R_1=1$ is the unit of distance, $a_1=\ln 2/0.255$, $a_2=\ln 2/0.05$, and $Q=32$. The range of interaction for $V_1$ was limited to $R=1.2$ in order to reduce the number of neighbors whose interaction must be computed. The zero of energy for both $V_1$ and $V_2$ was moved to $-0.8241$. For $R>1.2$, the interparticle potential energy and the interparticle force were both set equal to zero. The atomic mass $M$ was also taken to be unity, and the unit of time was then $R_1\sqrt{M/E}$.

For $R<R_{\text{dis}}$, atoms $i$ and $j$ formed a molecule, and interacted through $V_2$. Once formed, the molecular bond was assumed to be saturated, so that other neighbors $k$ of atom $i$ interacted with $i$ through $V_1$, even if $R_{ik}$ were less than $R_{\text{dis}}$. For $R>R_{\text{dis}}$, the molecule $ij$ was considered to be dissociated, and $i$ and $j$ now interacted through $V_1$.

The depth of the well $b_2$ for the potential $V_2$ determined the strength of the molecular bond and hence the relative degree of stability of molecule $ij$. We found that with $b_2 = 0.4$, a value used earlier in [13,14], the molecules near the vacancies would dissociate rather too easily, even at quite low temperature (average kinetic energy around 0.002), almost as soon as the vacancies were introduced into the model. This made it difficult to investigate the separate role of vacancies in the initiation of detonation. We therefore calculated the cases with $b_2$ set to 1.0 and 4.0. This increased the stability of the molecules, but did not completely remove the difficulty, because the potential well of $V_2$ binding different molecules together was also too shallow by the shifting of the zero energy axis as described above. This made the vacancies diffuse easily by the thermal motion of the molecules. Thus a cluster of vacancies would in time become a distributed system of vacancies. This point,
i.e., the simulation of stable defects, must be further considered in future studies.

The system modeled here was a two-dimensional (2-D) fcc crystalline filament of molecular $A_2$. Previous studies of 2-D and 3-D cases showed that both the 2-D and the 3-D models exhibited properties of energy transport in agreement with experiments, whereas the 1-D model did not [18]. We chose the 2-D model for this study because it was simpler than the 3-D model, and for comparable amounts of computer memory and numerical computation, the 2-D model allowed the use of a larger dimension in the transverse (X-) direction. This was especially important for defects such as vacancy clusters and dislocations with extended strain fields, and a larger dimension in the transverse direction would tend to reduce the effect of the transverse boundary on the defects. Our present model was 16 cells wide, each cell normally containing one diatomic molecule. The boundary condition in the transverse direction was assumed to be periodic.

Further to reduce the amount of computation required, we initially divided the filament into shorter block of 8 cells in length, and imposed periodic boundary condition also in the longitudinal (Z-) direction, except at the free boundary of the first block at $Z = 0$ where the boundary condition was mirror reflection. In this way the initial condition of the semi-infinite half plane could be represented by the equilibrium condition of a single block of 128 molecules (256 atoms). A cell was considered to be a vacancy site if it did not contain any atom. For a vacancy cluster, we initially assigned a cluster of 10 vacancies in each block of 128 cells. When $b_2$ was large (1.0 and 4.0) and the system initially at a low temperature, the thermal motion of the molecules, while not sufficient to cause molecular dissociation, was enough to bring about motion of the vacancies, so that the configuration of the cluster was continually changing, and in time, the vacancy cluster would become a distributed system of vacancies, as discussed above. With the assumed periodic boundary condition for each block, this was then equivalent to a 2-D crystallite containing a distribution of micropores.

Before the start of computation, the periodic block (with or without vacancies) was first equilibrated and relaxed to a low potential energy configuration. At the start of computation, time $t = 0$, several periodic blocks were brought together to form the beginning of the filament. An initial temperature of about 0.002 in kinetic energy (low compared with the well depth $b_2$) was assigned, and the mirror boundary condition was imposed at the free surface. A brief period of time (600 time steps at 0.0025 per step) was allowed for the filament to adjust to the new temperature and the new boundary condition at the mirror plane. Then the first 8 lattice planes next to the mirror plane were rapidly heated by addition of a known amount of kinetic energy. After that the system was allowed to evolve without any further disturbance.

The rapid heating initiated the dissociation of some molecules and generated a large disturbance in the form of a thermal conduction and shock wave both of which propagated into the filament. As the disturbance traveled along the filament, the longitudinal periodic boundary condition on the various blocks affected by the disturbance of course could not be imposed. However, beyond the head of the disturbance (farthest point from the mirror plane), the crystal was still undisturbed, so that a periodic block could be joined smoothly to the head of the disturbed crystal through the longitudinal periodic boundary condition. As the disturbance advanced, we would move the
periodic block, keeping it just ahead of the disturbance. In this way
the longitudinal periodic boundary served to terminate the
computation at each time step, and thereby reduced the amount of
computation. In a long filament, the saving could approach a factor
of 50%.

The decision as to when the periodic block must be moved was reached
in the following way: In order for the periodic condition to apply,
the motion of the molecules immediately upstream (toward the mirror
plane) of the periodic block must be identical to the motion of their
corresponding images inside the periodic block. Thus if the average
positions of the upstream molecules in one lattice plane differed by
more than a small prescribed amount (0.00005 in this case) from their
corresponding images inside the periodic block, then it would be
necessary to move the periodic block downstream by one plane.

Under the conditions discussed above, we solved for the trajectories
of all the particles of the system as functions of time by using the
numerical method of Refs. [19]. From the positions and velocities of
the particles and the record of the dissociation of the molecules, we
then obtained a description of the dynamics of the detonation
process.

III. COMPUTER SYSTEM

In the past few years, there have been truly rapid advances in all
areas of computer technologies, but especially in microcomputers.
The dramatic increase in the performance of these microcomputers has
been accompanied by an equally dramatic decrease in their costs. In
these circumstances, we considered it useful to investigate the
feasibility of using a small, inexpensive personal computer (PC)
system for doing all the MD calculations required for this study.
Heretofore large-scale scientific computations have been done almost
exclusively with larger, more powerful computers. These computers
are of course needed for their speed, large memory capacity, and
ability to serve many users. However, microcomputer systems are so
much less expensive and more accessible than the larger systems that
in the environment of a small research group, with limited resources,
it might be both advantageous and practical to use the microsystems.
Our experience from this investigation appears to confirm this
expectation.

The equipment we used for this work is listed as follows:

1. Leading Edge Model MH personal computer, 1 mb RAM, 30 mb
   hard disk, 1.2 mb and 360 kb floppy disks, 6-7.16-8 mHz
clock frequency, Intel 80287 math coprocessor. $3300.

2. Definicon DSI 780/2 coprocessor board for 32-bit calcula-
tions, 2 mb memory, 16.7 mHz clock frequency. $2500.

3. Lahey and Quelo Fortran compilers. $1000.

4. Printer and other miscellaneous equipment. $ 500.

Total system cost $7300.

The speed of the Definicon DSI 780 coprocessor board is approximately
equal to that of the VAX 11/780 computer. In the past we have used
the VAX 11/780 (more than one) for this kind of computation. The
cost of computing on the VAX was about $10 per hour. Supercomputers
of the CRAY class are about 50 times faster and about 200 times more costly, and therefore about 4 times more expensive than the VAX per unit of computation. We can make a simple estimate of the cost of computing with our microsystem: If we consider only the amortizing cost, ignore the cost of electricity, supplies, and interests, and assume a three-year life time for the microsystem, then the cost per year is $2433. For our long calculations, if we use 120 hours per week for 30 weeks per year, then the cost would be about $0.68 per hour. This is to be compared with the figure of $10 per hour on the VAX and $40 per hour on the CRAY for the same amount of computation. Thus the cost advantage clearly favors the microcomputer system.

The most serious disadvantage of the microsystem, in our experience, has been that it is essentially a single-user, single-task system. However, at the relatively low capital cost of the equipment, it is possible to add a second system as the need arises, for example, for processing the data generated by the first system. The total cost would still be low. In fact, toward the end of the present project, when the deadline for completion was pressing, we did acquire a second computer (Item 1 above) and a plotter. By that time the cost of the computer had decreased by about 15%. We did not get a second Definicon coprocessor board. The price of this board did not change in the recent months, but its capability has improved from 16.7 mHz to 20 mHz, even 25 mHz. These points illustrate the flexibility of the PC system: It can be adjusted relatively easily according to need, and full advantage can then be taken of the most current improvements in technology. Thus we are able to conclude from our own experience that the use of microcomputers for the MD type of calculations is not only feasible, but also highly effective in cost. Our application certainly is not unique, and it seems safe to say that comparable advantages would exist in other situations as well.

IV. RESULTS

A test case without any vacancy and with $b_2^2 = 0.4$, as in Ref. [14], was first run to test the various Fortran programs after they were installed in the microcomputer system. The results were found to be in good agreement with previous results [14]. But when vacancies were introduced, it was found that they moved about freely by thermal diffusion, as discussed above. To make matters worse, from the viewpoint of modeling detonation, the molecules also tended to dissociate rather easily, even when the temperature was kept at about 0.1 in average kinetic energy, which was low compared with the well depth of 0.4. And as soon as one or two molecules dissociated and released energy into the system, the other molecules quickly followed. This was a form of initiation of detonation, violent and rapid and uncontrolled, because of the low activation energy for dissociation and the large amount of energy released. The situation was in fact similar to our earlier results [13] when we modeled the exothermic dissociation without reference to detonation. The mechanism involved here clearly was the reduced effect of caging when some molecules were next to vacancies. But the rapid dissociation reaction tended to obscure other competing mechanisms, such as the effect of "hot spots", which we also wished to investigate. In order to develop a more complete understanding of the effect of vacancies, it is therefore necessary to determine how the different mechanisms are affected by the system parameters such as the well depth $b_2$, the energy release, and the structural configuration of the system. In this preliminary investigation, we undertook to study the effects of several of these parameters.
After the first test case, we studied a total of six cases as listed in Table I. Four parameters were adjusted. They were: the number of vacancies, \( b_2 \), the volume of the system, and the amount of heating. Except for case \( F \), the volume of the periodic block was adjusted to keep the initial pressure at equilibrium approximately zero. And except for case \( C \), the amount of heating was approximately the same. The temperature of the heated planes at the end of heating, however, was affected both by the heat added and by the energy released from dissociation, and so was not the same for the various cases.

The results obtained here turned out to be qualitatively similar to earlier results of Refs. [14]. We shall discuss the detonation wave profiles for three representative cases, pointing out the important features, and as illustrations of the capability of MD studies. Detailed and quantitative analyses of the results will be left to future studies. Fig. 1 shows four sets of profiles of the detonation wave for Case \( B \) at time step \( J=5000 \). The mirror plane was at plane zero, and the shock wave traveled to the right. The data were obtained by averaging over three lattice planes and over 80 time steps. The shock front was about 5 lattice plane thick, at around plane 165. The normal stress components \( S_{XX} \) and \( S_{ZZ} \) and their average (Fig. 1A) were essentially the same over the entire profile, showing that stress relaxation occurred in this case with the velocity of the shock travel and that there was hydrostatic pressure behind the shock front. Fig. 1B shows profiles of the number of particles in molecular form, as dissociated free atoms, and the sum of the two. Ahead of the shock front, there was no dissociation, so that the number of free atoms was zero. In this region the total number showed rather large fluctuations on account of the vacancies in the system. Dissociation started after the passage of the shock.

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**Table I Initial Conditions for the Various Cases.**

<table>
<thead>
<tr>
<th>Case</th>
<th>No. of Vacancies (^1)</th>
<th>( b_2 ) (^2)</th>
<th>Initial Conditions (^3)</th>
<th>Heat Added (^4)</th>
<th>Total Time Steps (^5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0 (256)</td>
<td>4.0</td>
<td>Vol. 121.8</td>
<td>Temp. 0.0021</td>
<td>Pres. -0.0898</td>
</tr>
<tr>
<td>B</td>
<td>10 (236)</td>
<td>4.0</td>
<td>Vol. 116.6</td>
<td>Temp. 0.0013</td>
<td>Pres. -0.0039</td>
</tr>
<tr>
<td>C</td>
<td>10 (236)</td>
<td>1.0</td>
<td>Vol. 116.6</td>
<td>Temp. 0.0346</td>
<td>Pres. 0.3530</td>
</tr>
<tr>
<td>D</td>
<td>10 (236)</td>
<td>1.0</td>
<td>Vol. 116.6</td>
<td>Temp. 0.0023</td>
<td>Pres. 0.1559</td>
</tr>
<tr>
<td>E</td>
<td>0 (256)</td>
<td>1.0</td>
<td>Vol. 121.9</td>
<td>Temp. 0.0014</td>
<td>Pres. -0.1847</td>
</tr>
<tr>
<td>F</td>
<td>0 (256)</td>
<td>1.0</td>
<td>Vol. 144.0</td>
<td>Temp. 0.0017</td>
<td>Pres. -3.2508</td>
</tr>
</tbody>
</table>

**Notes:**

1. First number refers to number of vacancies and second number to number of atoms in each periodic block.
2. Well depth of potential \( V_2 \), equation (1b).
3. Volume of periodic block in \( R_b \), temperature refers to average kinetic energy of each atom in unit of \( E \), pressure in units of \( E/\text{unit volume} \).
4. Energy added per atom in the 8 planes next to the mirror plane.
5. Each unit of \( J \) corresponded to 0.0025 unit of time.
front, at plane 155, and did not occur smoothly over space on this scale of averaging. The main reactions occurred between planes 150 and 90. This region may be considered as the reaction front. The reaction was complete at plane 65.

The kinetic temperature profiles (Fig. 1C) showed that the kinetic energy $E_{KZ}$ associated with the Z-component of velocity differed considerably from $E_{KX}$ within the reaction front. This was similar to our earlier results obtained for reactive systems [14] and for the shock compression of non-reactive systems [19]. In Fig. 1D we have plotted the kinetic energy of those atoms still in the molecular form, per degree of freedom of the molecules. After complete dissociation, the kinetic energy of the "molecules," say, between plane 60 and the mirror plane, was not meaningful. The curves in that region were therefore omitted. We see here that within the reaction front the kinetic energy was mostly in the translational degrees of freedom, and very little in the rotational and vibrational degrees of freedom. From the lack of equipartition of the kinetic energy in the various degrees of freedom, we conclude that energy relaxation processes were occurring during dissociation. But between plane 90 and the mirror plane, $E_{KX}$ and $E_{KZ}$ (Fig.1C) were substantially the same and there was no further energy relaxation, except near the mirror plane where the system was initially heated.

Figs. 2A to 2D show the corresponding situation at $J=4000$ for Case D in which only $b_2$, the well depth of potential $V_2$, was changed from 4 to 1. The shallower $b_2$ made it easier for reactions to occur. Fig. 2B shows that dissociation started almost at the foot of the shock front, at plane 150, and was complete at plane 100. The rate of dissociation was therefore faster than in Fig. 1. This higher rate of energy release was responsible for the higher pressure and kinetic temperature profiles (Figs. 2A and 2C) than in Case B. The shock wave velocity was also higher, if we were to compare the two cases at the same value of $J$. These results indicate that the model was capable of providing a self-consistent account of the thermal-mechanical coupling within the system, as well as the effect of the energy content on the rate of reaction, even when there was large departure from thermal equilibrium.

Fig. 3 is a series of profiles of the particle number at different times for Case F in which the volume was expanded to decrease the density of the system. We have already mentioned that vacancies tended to become distributed by diffusion in our model. If the effect of caging, i.e., the average number of neighbors surrounding a molecule ready to dissociate, is important, then we should observe similar effects on the initiation of detonation in a system with distributed vacancies as in a system without vacancy but at lower density. The results displayed in Fig. 3 confirm this expectation. In particular, they show that dissociation reactions started almost as soon as the arrival of the shock wave. But when there were no vacancies, and when the volume was not expanded, Cases A and E (not shown here), the start of dissociation was later.

In Fig. 3 the peak of the particle number profile appeared to have reached a steady value after $J=2000$. This occurred also in the stress and kinetic temperature profiles. In fact, we found that in Cases C to E, all with $b_2=1$, and in Case B with $b_2=4$, the profiles were either steady or slightly increasing in peak amplitudes toward the end of the calculations. In these cases, the reaction front was able to keep up with the shock front. This indicates that the detonation process was energetic enough to be self-sustaining in these cases. In contrast, Case A showed a small decrease with increasing time in
the peak amplitudes of the stress, kinetic temperature, and density profiles. The data on the start of dissociation also suggest that the reaction front might be falling behind the shock front with increasing time. Further investigation would be required to determine if the decrease in peak stress and kinetic temperature would continue to later times, and whether the observed decrease was due to the smaller energy release (deeper $b_2$) coupled with a slower reaction rate for this case.

V. CONCLUSION AND FUTURE DIRECTIONS

In this preliminary investigation of the effects of vacancies on the initiation of detonation, we have found that because of the weak intermolecular binding energy, a vacancy cluster initially introduced into the model tended to diffuse by thermal motion and become a distributed system of vacancies. This tended to reduce the caging effect of the neighbors surrounding a molecule, thus making the initiation of dissociation easier than in a system without any vacancies. A total of seven cases were studied, at different vacancy contents, densities, different values of $b_2$, and initial heating. We have discussed the results only in qualitative terms. Quantitative analyses of the results must await improvement of the model, to stabilize the configuration of vacancies, in the next phase of this work.

We have also demonstrated that the use of a microcomputer system for large-scale MD calculations was not only feasible, but cost-effective: The cost of using an AT type of personal computer driving a Definicon DSI 780/2 coprocessor board was about 7% of the cost of using a VAX 11/780 computer for doing the same calculations and at comparable speeds.

The results discussed here demonstrate rather clearly the capability of the MD method in providing detailed information on the dynamics of the detonation process. The information includes, in addition to the standard equilibrium properties of the reactive system, such items as the atomic arrangement of the system, the mechanisms of initiation, the energy exchange and energy relaxation processes, the overall rate of reaction, the structure of the shock wave and the detonation wave, their propagation velocities, etc., all under highly non-equilibrium conditions during the detonation process in dense, energetic systems. Moreover, the details produced are consistent with the assumed potentials, and the parameters of the model are easy to control so that their effects on the detonation process may be investigated with a minimum of ambiguity. It is therefore our belief that MD type of studies is potentially able to help us understand more clearly the dynamics of detonation, especially in the microscopic regime, where it is difficult to obtain experimental information, and equally difficult to construct theoretical models.

For this investigation, the next step clearly should be to improve the potential with a view to making vacancy clusters more stable, so that the energy distribution around the clusters may be studied. This will involve lengthier calculations, because additional molecular neighbors would have to be taken into account. The problems of structural defects are important in connection with many thermal, mechanical and other properties of solids. For example, dislocations and grain boundaries and their movement under load affect certain mechanical properties of solids. Under shock loading they are believed to be the source of "hot spots" which affect the initiation of detonation. For our purpose it will therefore be important to
obtain a better model of defects, starting with vacancy clusters.

In addition to the problems of defects, the foregoing discussions concerning the ability of the MD method to produce a consistent set of equilibrium and other dynamical properties of a dissociating system suggest another interesting and perhaps more important problem at this stage of testing of the MD method for modeling detonation. Our idea is to find out to what extent MD results agree with continuum results under comparable conditions. As has been pointed out, a great deal of work has been done with the continuum model, and great deal is known. If we use the MD method to produce a set of data for a reasonable model, including the equations of state of the reactants and of the products, the rates of reaction, and other information, etc., as are required to do a complete calculation of detonation with the continuum model, and repeat the calculation with the MD model under the same operating conditions, the results should be rigorously comparable, and in fact should be identical, if both methods are equivalent. This gives us a method for evaluating the effect of some of the assumptions of the continuum model, especially with respect to the existence of equilibrium. If the results should agree under a wide range of conditions, they would suggest that non-equilibrium effects may be unimportant. If the results should fail to agree in certain respects, then we should be able to examine the reason(s) for the disagreement, and perhaps learn how to modify one or both methods for the purpose of achieving agreement. In either case, the results should provide an objective test of the limitation and the range of validity of both methods. For these reasons, we plan to carry out such a critical comparison at the earliest opportunity.

ACKNOWLEDGEMENT

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REFERENCES


Fig. 1. Detonation wave profiles for Case B at time step J=5000.

Procedure for data averaging as described in text.

Fig. 2. Detonation wave profiles for Case D at time step J=4000.

Fig. 3. Particle number profiles at various times in Case F.