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Programmed Burn Technique**

by

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DETONATION OF HIGH EXPLOSIVES IN LAGRANGIAN HYDRODYNAMIC CODES USING THE PROGRAMMED BURN TECHNIQUE

by

Michael E. Berger

ABSTRACT

Two initiation methods are developed for improving the programmed burn technique for detonation of high explosives in smeared-shock Lagrangian hydrodynamic codes. The methods are verified by comparing the improved programmed burn with existing solutions in one-dimensional plane, converging, and diverging geometries. Deficiencies in the standard programmed burn are described. One of the initiation methods has been determined to be better for inclusion in production hydrodynamic codes.

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I. INTRODUCTION

Several of the Lagrangian hydrodynamic codes presently in production use at Los Alamos Scientific Laboratory make use of the "programmed burn technique" for the modeling of the detonation of high explosives (HEs) within the code. Perhaps the most representative of such codes at LASL are the MAGEE code, a two-dimensional Lagrangian smeared-shock code, and COMBO, a one-dimensional code with both sharp and smeared-shock capabilities. The calculations performed in this study, although primarily one-dimensional, were made with MAGEE due to its greater flexibility. Several case comparisons were also made with COMBO in order to verify that the two HE burn methods are indeed identical, insuring that improvements made with the programmed burn in the MAGEE code would also be applicable to COMBO.

Although there are many variations, the basic premise of the programmed burn technique is that the detonation wave travels in all directions at a constant velocity equal to the Chapman-Jouguet (C-J) detonation velocity D_{CJ} . This concept is quite simple in one-dimensional codes; however, it has been necessary to derive several sophisticated

techniques in order to calculate the proper arrival time of the detonation wave in the more complex two-dimensional geometries. These arrival times (called burn times, BT) plus the time required for a cell to burn at D_{CJ} (called the burn interval, BI) are stored for each HE cell. When the detonation wave reaches and proceeds into a cell, the chemical energy ϵ_c is proportionally added to that cell at time T according to the burn fraction $\Delta T/BI$ until the cell has completely burned and the total chemical energy has been added to that cell. The parameter ΔT is the problem time step.

Of course, several other methods exist for modeling the detonations of high explosives in 2-D Lagrangian, smeared-shock hydrodynamic codes. Among these are the C-J volume burn, where the chemical burn energy is added to a compressed cell according to the volume burn fraction with respect to the Chapman-Jouguet volume v_{CJ} . In addition, there is the combination of the programmed burn and C-J volume burn which incorporates both techniques running side by side and lets the relative value of the burn fraction, be it programmed burn or C-J volume burn, determine the method to be used. This is presently used in the HEMP code.¹ A C-J volume burn may be initiated by a programmed

burn, a piston, or a hot spot. All of these methods assume that the chemical reaction occurs instantaneously and that the reaction zone has no thickness.

There are several advantages of the programmed burn technique in both MAGEE and COMBO, which justifies improving and maintaining it in the codes. The first advantage is, of course, the vast amount of experience that has been gained over the years by using this technique in the two codes. It does not quench when the geometry is such that the detonation wave must traverse a corner. Burn prescriptions are easily incorporated and the method is quite flexible. Finally, once the burn has been programmed, it is computationally very fast during equation-of-state execution.

With all computational schemes, the programmed burn also has its disadvantages. The first of these is that it has a slow initiation which ultimately yields insufficient energy being delivered by the HE system and thus lower pressures. An example of this in a simple one-dimensional slab geometry is shown in Fig. 1. Further evidence of this in 1-D converging and diverging geometries can be seen in Figs. 2 and 3. An additional failure of the programmed burn is in highly converging systems where the detonation front proceeds at its constant velocity (programmed) while the shock outruns the detonation (due to convergence), pre-compressing the solid HE and

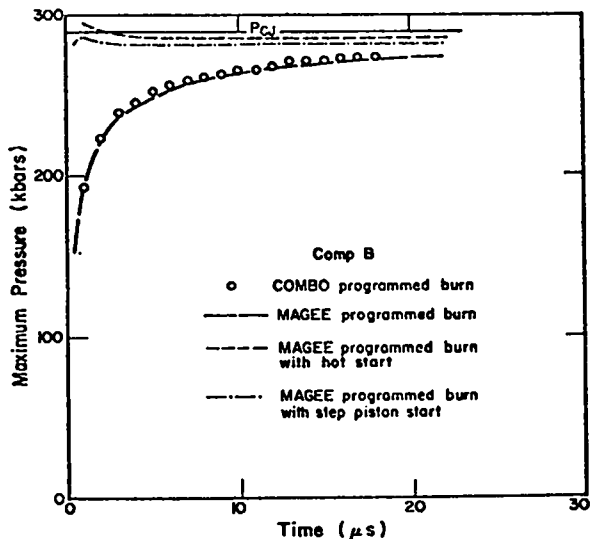


Fig. 1.

Maximum cell pressure vs time comparing the different programmed burn methods in a 1-D slab geometry detonation. The theoretical Taylor wave solution is represented by the solid line, p_{CJ} .

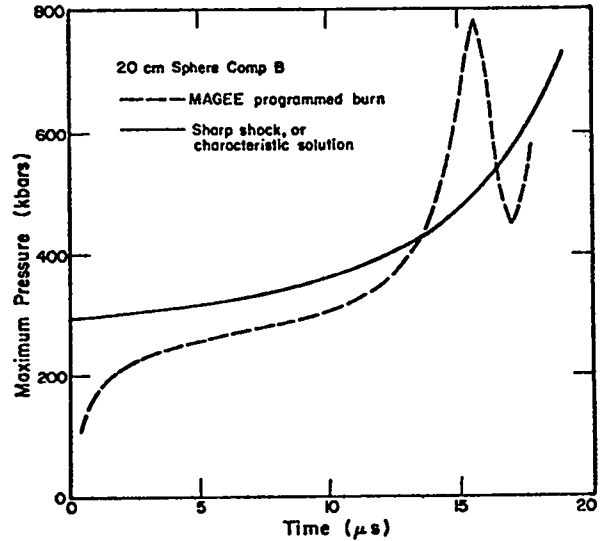


Fig. 2.

Maximum cell pressure at detonation as a function of time comparing the standard MAGEE programmed burn with the sharp-shock and MOC solutions in a 1-D spherically converging system. The solid curve is representative of the true C-J solution (Ref. 4).

resulting in energies and pressures in unburned HE as if the detonation products had been compressed. When the programmed burn does tell these cells to detonate, they do so at unusually high pressures and energies, resulting in chaos. Two other disadvantages of the programmed burn, at least in a 2-D code, are that the calculation of burn times is quite

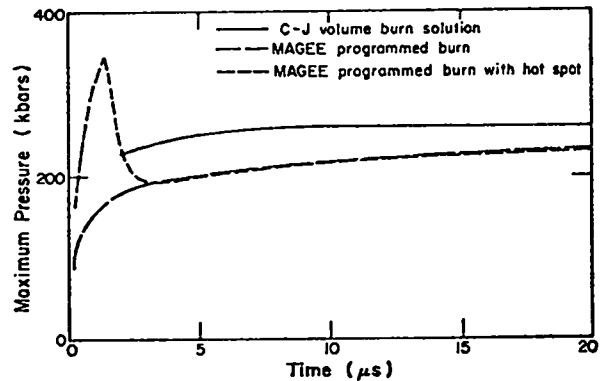


Fig. 3.

Comparison of maximum cell pressure at detonation vs time for different programmed burn methods and the C-J volume burn in a 1-D spherically diverging system. The C-J volume burn, solid curve, is representative of the C-J solution (Ref. 4).

cumbersome and complex burn prescriptions (modification of energies, C-J pressure, etc.) are required to match experimental data.

The purpose of the present study was to develop techniques in which the programmed burn can be used to calculate simple problems properly and, in particular, obtain valid solutions to C-J problems. These methods must be suitable for incorporation into production hydrodynamic codes, i.e., MAGEE and COMBO, in a form that requires little if any action on the part of the user. Once this has been accomplished, attention can be given to the more difficult task of including real detonation effects, e.g. buildup,² in order to match experiments without the user input of burn energy modifications.

II. PRESENT PROGRAMMED BURN SOLUTIONS TO THREE SIMPLE 1-D PROBLEMS

The inadequacies of the present programmed burn can best be demonstrated by using it to solve three simple one-dimensional problems. These are a 1-D slab of HE, a 1-D converging sphere and a 1-D diverging sphere. For comparison, the Taylor-wave self-similar solution exists for the slab geometry, and C-J volume burn, sharp shock, and method of characteristics (MOC) solutions are available for the spherical geometries.

In all cases, Composition B (hereafter called Comp-B) was used as the HE with the following parameters:

Initial density, $\rho_0 = 1.714 \text{ gm/cm}^3$
C-J volume, $v_{CJ} = 0.423 \text{ cm}^3/\text{gm}$
C-J pressure, $p_{CJ} = 290.4 \text{ kbar}$
C-J detonation velocity, $D_{CJ} = 0.7991 \text{ cm}/\mu\text{s}$
Specific heat ratio, $\gamma = 2.77$
Detonation energy per cm^3 , $\rho_0 \epsilon_0 = 0.2381 \text{ Mbar-cm}^3/\text{cm}_0^3$

The LASL HE equation of state, which is a variation of the γ -law EOS,³ was used.

In all cases, the characteristic length or radius of the HE was chosen as 20 cm, and 100 cells were used, for a cell length of 0.2 cm. Although MAGEE is a 2-D code, only one cell width was used to minimize computation time. It was quickly discovered that the detonation of HE in MAGEE is quite sensitive to the cell aspect ratio, i.e., width-to-length ratio. For aspect ratios not close to one, small instabilities appeared in the form of oscillation of pressures, energies, etc. This effect was traced to the dependence of the artificial viscosity q on the square

root of the cell area; thus, different aspect ratios would give different values of q . In all problems, therefore, the width dimension was chosen such that the aspect ratios in the HE were very nearly equal to unity. The detonation was initiated at a free surface in the slab and converging geometries. In the diverging geometry, the detonation was initiated at the fixed center and proceeded to a free surface.

For the slab geometry, the results of the standard MAGEE programmed burn are shown in Fig. 1 as the large, dashed curve. Superimposed on this curve are the COMBO results for the same geometry, indicating good agreement of the smeared-shock, programmed burns in the two codes. However, it is also seen that both the MAGEE and COMBO results differ drastically from the Taylor-wave solution for this geometry, represented by the straight line p_{CJ} . This clearly demonstrates the inadequacy of the present MAGEE-COMBO programmed burns as applied to simple theoretical problems.

The standard MAGEE programmed burn results for the spherically converging case are shown in Fig. 2. Again it is seen that the pressure starts off low, when compared to the sharp shock and MOC solutions, and increases. However, in this case the increase becomes quite rapid at about 12 to 13 μs , giving rise to an instability. What happens is that the standard programmed burn does not allow the detonation velocity to increase, due to convergence. Thus, the shock outruns the programmed detonation, compressing the condensed HE cells prior to their programmed detonation. Since the equation of state is for the HE products, this compression results in high pressures and energies in these cells even before they detonate. When the chemical energy is added to these cells according to the programmed burn, the unusually large pressures exhibited in Fig. 2 result. Therefore, in addition to its "slow" start, the present programmed burn method has the added disadvantage of maintaining a constant detonation velocity in converging geometries, whereas the detonation velocity actually increases with convergence. This effect, however, appears to influence the model only when the radius ratio R/R_0 is less than 0.7 where R_0 is the initial radius of the system.

Results for the standard MAGEE programmed burn in a spherically diverging geometry are compared with a C-J volume burn solution in Fig. 3. The C-J volume burn is accepted as representative of the actual solution to this problem.² Again, the standard programmed burn exhibits the low initial pressure, as do the previous two cases. In the diverging geometry, as with the slab geometry, the pressure never reaches the theoretical value as time progresses. An apparent reason for this is that the

smearing of the shock "rounds" the pressure profile such that the peak pressure is not reached. This is discussed in more detail later.

The above three simple cases demonstrate the deficiencies of the standard programmed burn as it now exists in MAGEE and COMBO. In order to match experimental data in two-dimensional geometries, the burn energies of the cells must be modified through the use of "burn functions" or "burn prescriptions." As previously noted, the purpose of the present study was to develop techniques with which the programmed burn can be used to calculate simple problems such as the three described above.

III. METHODS FOR IMPROVING THE PROGRAMMED BURN

During the study, two techniques were used to improve the programmed burn. Both are based upon the idea that once the programmed burn is properly initiated, it will maintain itself throughout the remainder of the calculation.

The first method is to initiate the HE with a piston moving at C-J particle velocity ($u_p=0.21$ cm/ μ s for Comp-B). The piston is maintained until the third cell has detonated, at which time the piston is released to the normal boundary condition. This has the advantage of starting the detonation at C-J conditions, and thus the calculation proceeds starting from an ideal state. Although the method works well for simple problems and the so-called "piston problems," it does have the disadvantage of not being easily incorporated in production codes for general problems with arbitrary boundary conditions.

The second method used increased the density and/or detonation energy of the first one to three cells in HE thus initially overdriving the detonation. This method, referred to as a "hot spot" or "hot start," has the advantage of being easily incorporated into production codes. Its major flaw is that the total mass and/or energy of the problem is slightly increased, causing some concern to those who must maintain accuracy of these quantities. However, it was found that by increasing the chemical energy of the first cell by a factor of four to five, a suitable hot start could be obtained without changing the mass and with almost negligible energy increase. In order to obtain a proper hot start, it was determined that a pressure approximately 100 kbar greater than the C-J pressure was required. A second slight disadvantage of the hot start is that it is not entirely compatible with the HE-piston problem. In this case, it is

well-advised to use the piston start mentioned above for proper initiation.

IV. IMPLEMENTATION OF THE INITIATION METHODS ON THE THREE 1-D PROBLEMS

The initiation methods described in Section III were applied to the three simple 1-D problems in Section II. In all cases, the same zoning, boundary conditions, etc., were maintained.

For the slab geometry, the maximum pressures as a function of problem time using both the piston and hot starts are shown in Fig. 1. Both initiation methods bring the pressure within 10 kbars of the theoretical C-J pressure. Further evidence for the improvement wrought by the initiation technique is contained in the pressure-distance profiles of Fig. 4. These profiles are important since they determine how metal plates are moved by the HE. It is seen that the MAGEE programmed burn with a hot start coincides with the theoretical Taylor wave solution for this geometry. This solution is also identical to that obtained with the one-dimensional SIN code⁴ using a C-J volume burn. The loss in the peak pressure during the early part of the standard MAGEE burn is again shown by the dashed profiles.

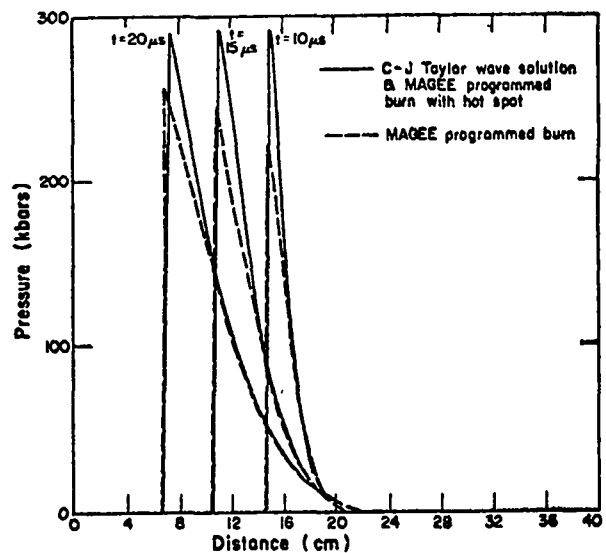


Fig. 4. Pressure-distance profiles in a 1-D slab detonation comparing the C-J Taylor wave solution with the improved and standard MAGEE programmed burn. There is essentially no difference between the Taylor solution and the hot-start MAGEE programmed burn.

Results for the 1-D converging geometry detonation are shown in Fig. 5. Here, the MAGEE programmed burn with a piston start (which is nearly identical to that with a hot start) is compared with the COMBO sharp - shock and the RICKSHAW⁵ MOC solutions. The latter also agree quite well with SIN C-J volume burn calculations. Included in the improved MAGEE programmed burn is a variable detonation velocity (rather than the constant detonation velocity used by the standard programmed burn) which was developed by Mader and Craig.² They found that in spherically converging HE systems, the pressure could be scaled as a function of the inverse normalized radius (R_0/R). This was extended to the detonation velocity to form the relation

$$\frac{D}{D_{CJ}} = 0.22049 \left(\frac{0.2}{\frac{R}{R_0}} \right)^{1.65} + 0.9845$$

for

$$0.25 \leq \frac{R}{R_0} \leq 1.0 \quad ,$$

which applies only to spherical geometry.

The use of this variable-converging detonation velocity keeps the problem from going unstable at late times (large convergence), as happens in Fig. 2. It is not sufficient, however, to prevent a "popping" effect in which, at large convergence, the cell immediately in front of the detonation is compressed due to shock smearing prior to its burning, and thus "pops-off" at a larger than usual pressure when it detonates. This "popping" effect is responsible for the divergence of the dashed curve from the smooth curve in Fig. 5, although it has little effect on the pressure profiles as shown in Fig. 6. Using these profiles and neglecting the "popping," one obtains the extrapolated points in Fig. 7. Thus very good agreement with the sharp-shock and MOC solutions can be obtained with the improved MAGEE programmed burn.

In the spherically diverging case, the use of the hot start does not appear to be as beneficial (Fig. 3) as it was in the slab and converging geometries. The piston start is not feasible in this geometry. However, the calculations for the diverging problem are not as poor as indicated by Fig. 3. If the p-x profiles in Fig. 8 are examined, it is seen that only near the peak do the pressures differ. Although not indicated by Fig. 8, the shock near the peak is considerably rounded due to the artificial viscosity and divergence effects. Thus, the energy delivered by the HE to, for example, a metal plate is very nearly the same for all three cases shown in Fig. 8.

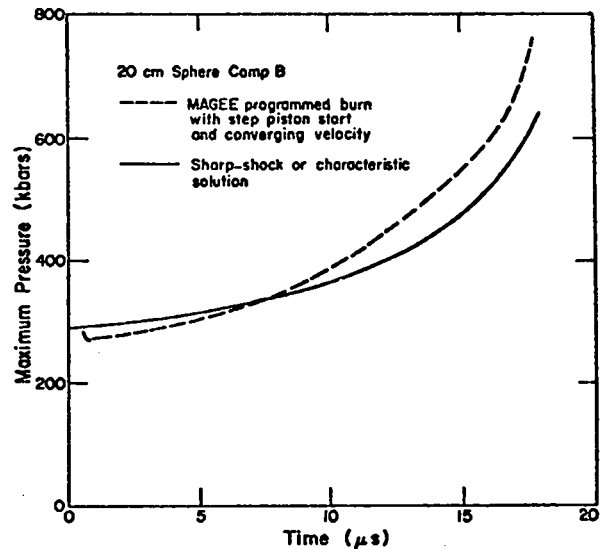


Fig. 5.

Comparison of the maximum cell pressure at detonation as a function of time in a 1-D spherically converging system for the improved MAGEE programmed burn with a variable detonation velocity and the sharp-shock and MOC solutions.

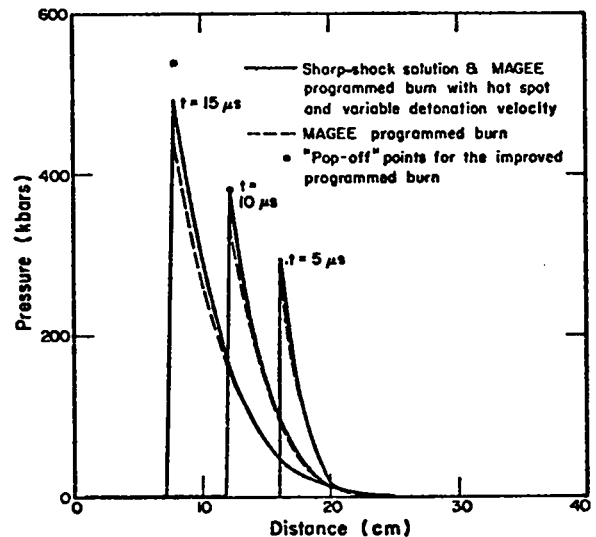


Fig. 6.

Pressure-distance profiles for the sharp-shock and different MAGEE programmed burns in a 1-D spherically converging system. The "pop-off" points for the standard programmed burn at 15 μs is off the graph at 800 kbars.

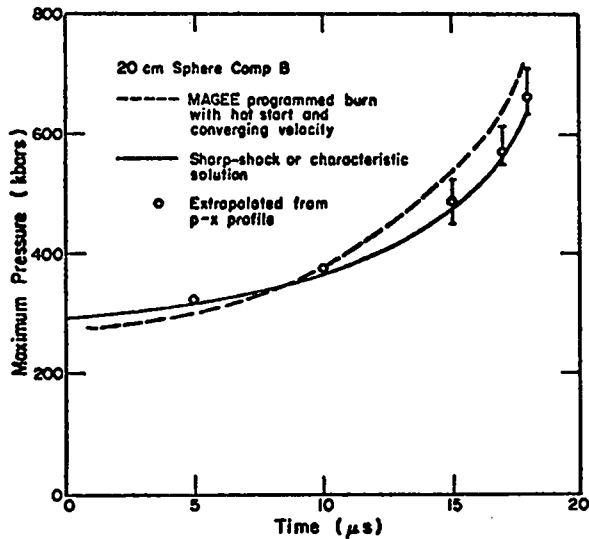


Fig. 7.

Maximum cell pressure at detonation as a function of time in a 1-D spherically converging geometry showing the pressure obtained from the extrapolated $p-x$ profile, Fig. 6, as opposed to the "pop-off" pressure.

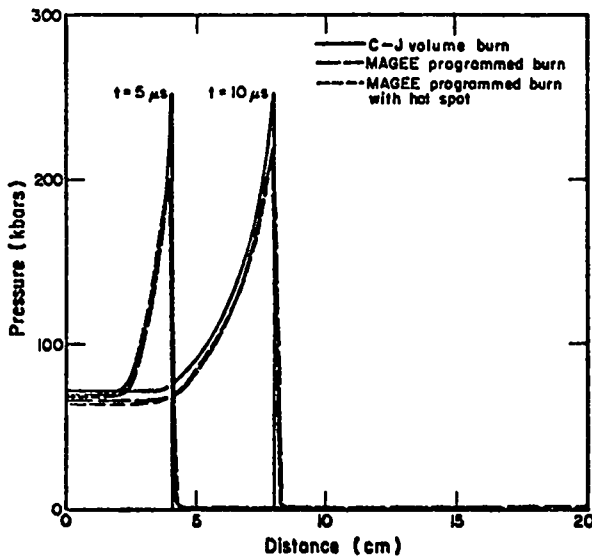


Fig. 8.

Pressure-distance profiles in a 1-D diverging geometry as calculated by a C-J volume burn and two programmed burn methods. The solid curve (C-J volume burn) is considered to be representative of the "best" solution (Ref. 4).

A better indication of the validity of the diverging solution obtained with the hot start can be obtained by comparing the calculated density with that given by the C-J volume burn SIN calculation and experiment, Fig. 9.² Here, it is seen that the programmed burn with a hot start does yield better results than the standard programmed burn.

V. USE OF IMPROVED PROGRAMMED BURN METHODS ON SPECIAL PROBLEMS

In order to test further the improved programmed burn methods developed during this investigation, two additional classes of problems were studied. The first of these were supported detonations in slab geometry. This series of problems was chosen because theoretical solutions can readily be obtained from the Taylor wave solution.⁶ Ideally, the problems should be initiated with the piston starts, stepping the piston velocity to the proper support value after the third cell had burned. However, it was also desired to test the hot start on these problems since this method seems to be more compatible with production codes. Except for the case where the velocity of the supporting piston u_p equals

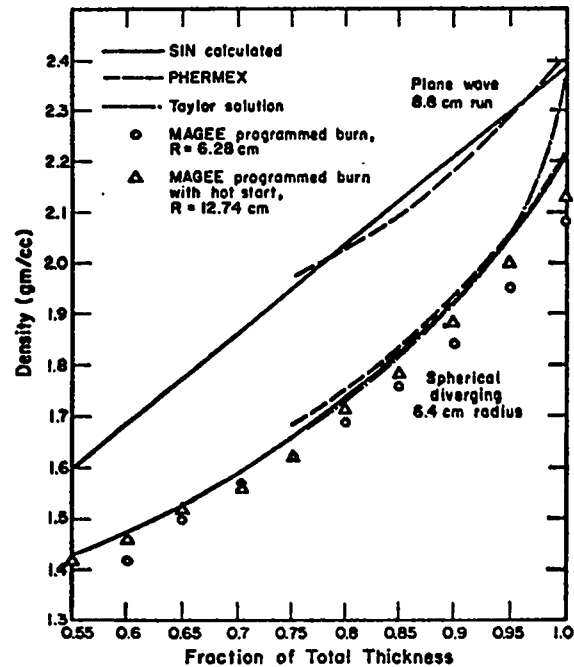


Fig. 9.

Comparison of experimental (PHERMEX) and calculated densities as a function of non-dimensional radius for a 1-D spherically diverging detonation, (Ref. 4).

the C-J particle velocity u_{CJ} , there was very little difference in the solutions for both initiating techniques. When $u_p = u_{CJ}$ and a hot start is used, an overdriven detonation occurs in which the peak pressure p_{max} is not allowed to return to the theoretical value p_{CJ} . Two additional supported problems were run, $u_p = 1/2 u_{CJ}$ and $u_p = 0$ (brick wall). Excluding the boundary condition of the supporting piston, these problems were identical to the slab geometry problems described in Sections II and III.

The peak pressures as a function of time are compared in Fig. 10. It is seen that the standard MAGEE programmed burn is plagued by the same low-pressure/energy problem as that encountered in an unsupported detonation, except for $u_p = u_{CJ}$ where the exact solution is obtained. Pressure profiles comparing the theoretical solutions, improved programmed burn, and standard programmed burn are shown in Figs. 11, 12, and 13. It can generally be concluded that the improved burn techniques yield solutions which are almost identical to the theoretical solutions except, as noted, the use of a hot spot with $u_p = u_{CJ}$.

Figure 14 shows the hot spot detonation energy E_c required to produce a Chapman-Jouguet supported detonation with the MAGEE improved programmed burn. This curve is somewhat insensitive in that a ten percent variation in E_c results in only a few kilobars variation in the peak pressure. However, if

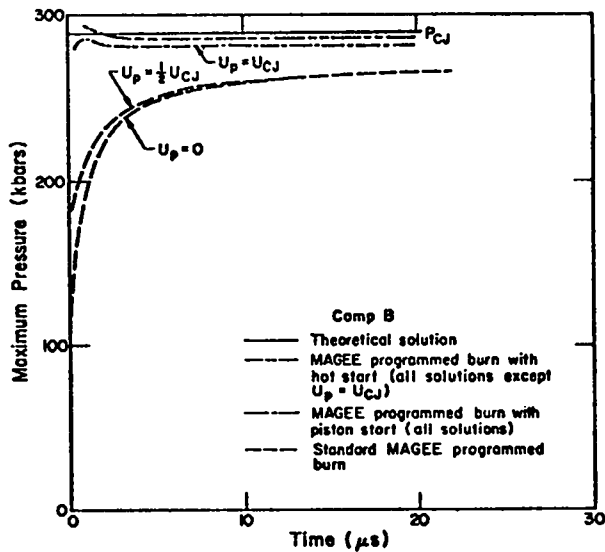


Fig. 10.

Maximum cell pressure as a function of time for a supported detonation in 1-D plane geometry. The different programmed burn methods are compared with the theoretical Taylor similarity solution (solid line).

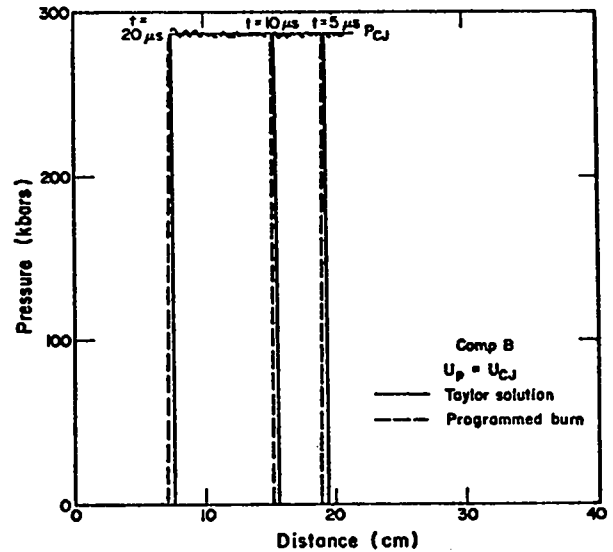


Fig. 11.

Pressure-distance profiles for a supported ($u_p = u_{CJ}$) detonation in 1-D plane geometry. The programmed burn is the standard programmed burn without initiation (see text).

insufficient energy is added to the hot spot, the peak pressure will never reach the C-J value. It must be noted that this type of curve only applies to supported detonations.

The final type of problem run was also in 1-D slab geometry but included a metal plate immediately

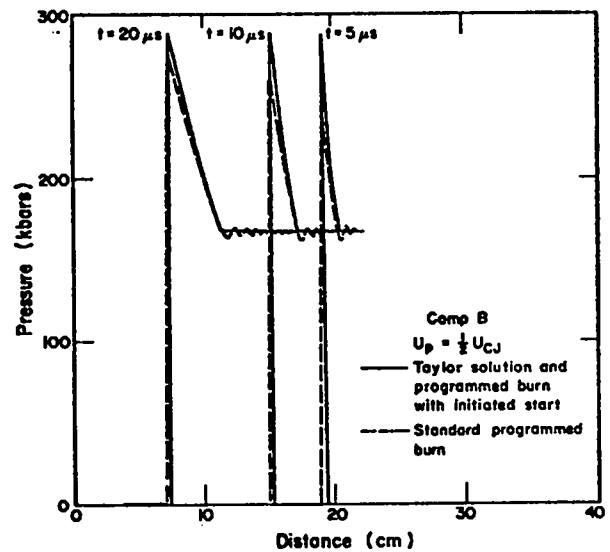


Fig. 12.

Pressure-distance profiles for a supported detonation with $u_p = 1/2 u_{CJ}$ in 1-D plane geometry.

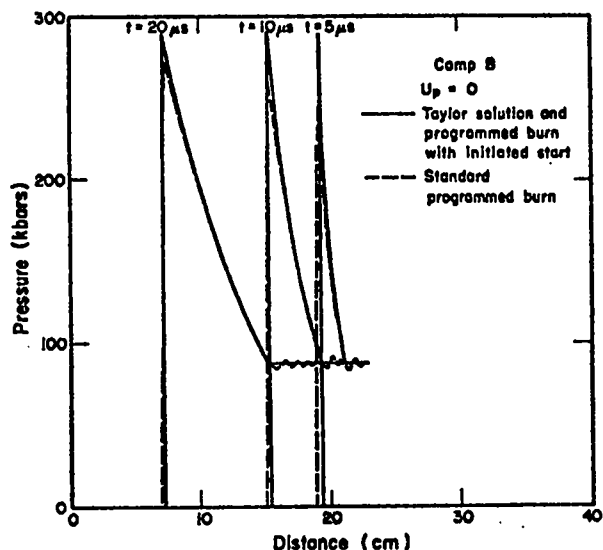


Fig. 13.

Pressure-distance profiles for a supported detonation with $u_p = 0$ in 1-D plane geometry.

adjacent to the hot spot in the HE. Again, zoning, boundary conditions, etc., were the same as used in Sections II and III except that the free surface was now on the outer side of the plate. An additional feature was that 9404 HE was used in addition to Comp-B. The purpose of these problems was to study the effect of the hot spot on the pressure profile, simulating a case around the HE with

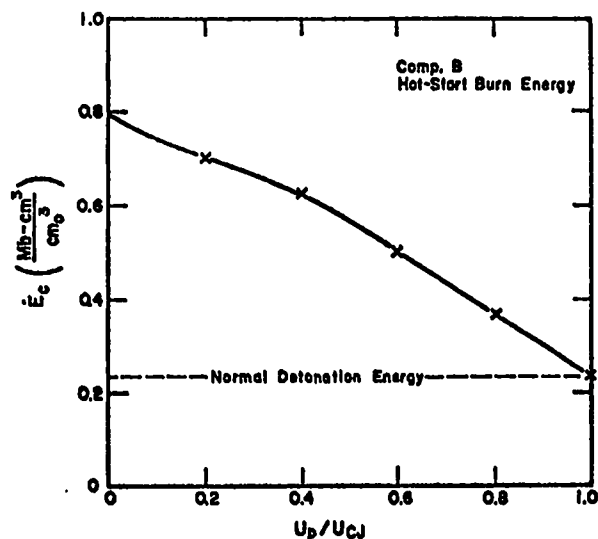


Fig. 14.

Hot-start detonation energy as a function of normalized piston velocity for a supported C-J detonation in Comp-B.

detonation occurring at the case-HE interface. Another reason for studying these problems was to obtain information on the effects of varying the chemical energy, initial density, and number of cells of the hot start.

Results of the study indicate that the metal plate adjacent to the hot spot has little effect on the solution. Pressure profiles are identical to those in Fig. 4 except for a small bump at the trailing edge of the wave caused by interactions of the HE products with the plate. In addition, it was demonstrated that the hot start could be properly modeled by increasing the chemical energy of one cell only by a factor of three or four, making the technique even more suitable to be included in a production hydrodynamic code.

VI. CONCLUSIONS

The standard programmed burn must be properly initiated in order to calculate simple Chapman-Jouguet detonations in 1-D plane, converging, and diverging geometries. Two methods of initiation have been determined—the piston start and the hot start—the latter being more suitable for use in a production hydrodynamics code. By using the hot start, the programmed burn can be used to obtain solutions which agree in both pressure-space profiles and yield peak pressures which agree to within 10 kbars for 1-D plane and converging geometries. The peak pressure in a 1-D diverging geometry can be brought to within 25 kbars of the solutions obtained with sharp-shock and C-J volume burn methods. In order to calculate a converging geometry detonation with a programmed burn, a correction to the detonation velocity must be made to account for convergence. Additional studies indicate that metal plates adjacent to a hot spot do not adversely affect the calculations. It is the author's opinion that the initiation methods are also applicable to other burn techniques. For example, a properly initiated programmed burn can be used to start a C-J volume burn and can even be run in conjunction with a C-J volume burn.

ACKNOWLEDGMENTS

This study is the continuation of the work of G. Brotbeck who initially recognized some of the problems investigated while he was using the COMBO program. The two initiation methods were proposed by C. Mader, and his continued support and interest on almost a day by day basis are greatly

appreciated. The supported detonation studies were suggested by K. Meyer. He also suggested the use of a hot start by increasing chemical energy only. This work was performed in the Theoretical Design Division of the Los Alamos Scientific Laboratory while the author was a member of the High Explosive Working Group. Members of that group who participated in discussions of this study are W. Fickett, G. Wall, W. Mudd, R. Burback, C. Mader, J. Kirkpatrick, and G. Brotbeck.

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