# SOME ISSUES REGARDING THE HYDROCODE IMPLEMENTATION OF THE CREST REACTIVE BURN MODEL

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**Abstract.** CREST is a new reactive burn model that is able to simulate a wide range of shock initiation behaviour in heterogeneous solid explosives including the response to sustained single and multiple shocks, and thin pulse shock inputs. This has been achieved by utilizing entropy-, rather than pressure-, dependent reaction rates. However, the move to entropy-based reaction rates introduces a number of computational problems not associated with pressure-based models. These problems are described in this paper, in particular, (i) in the modelling of explosive impact problems, CREST over-predicts the rate of energy release in an explosive adjacent the impact surface due to the well known Noh error over-prediction of internal energy, and hence entropy, at impact, and (ii) a study of the sensitivity of CREST results to mesh density indicates that an entropy-dependent model requires a finer mesh than a pressure-dependent model to achieve mesh converged results. Additionally, the Snowplough porosity model, which forms part of the CREST model, has been modified to improve the modelling of shocks in low porosity explosives.

## INTRODUCTION

A recent survey[1] has shown that the majority of reactive burn models currently used in hydrocodes to model shock initiation in heterogeneous solid explosives, use pressure-dependent reaction rates. A major deficiency of these pressure-based models is that they fail to describe the explosive response to multiple shock inputs without recourse to an additional 'desensitisation' model.[2-3]

CREST[4] is a new reactive burn model that is able to reproduce a wide range of shock initiation behaviour in explosives, including the response to sustained single and multiple shocks, and thin pulse shock inputs. This has been achieved by utilizing entropy-, rather than pressure-, dependent reaction rates that, importantly, remove the need for an additional 'desensitisation' model for multiple shocks. However, the move to entropy-based reaction rates introduces a number of computational problems, not associated with pressure-based models, which have to be addressed. These problems and other concerns regarding both the hydrocode implementation and use of the CREST reactive burn model are described in this paper.

Although the use of entropy-based models introduces additional numerical complexities, their ability to model a wider range of initiation phenomena when compared with pressure-based models, makes it worthwhile to identify and attempt to solve these additional problems.

## OVERVIEW OF CREST MODEL

The CREST reactive burn model[4] consists of two basic parts: (i) an equation of state (EOS) model for the reacting material, and (ii) a reaction rate model. The reacting material is assumed to be a

mixture of two coexisting phases consisting of unreacted solid explosive and gaseous reaction products. A Mie-Gruneisen form of EOS is used to model the non-reacted explosive[5], where the principal isentrope, written in finite strain form, is taken to be the reference curve, while a JWL EOS is used to model the gaseous reaction products. To yield the EOS of the mixture, the ISE model[6] is used with the assumption that the solid and gaseous phases are in pressure equilibrium. The explosive's initial porosity is included as a parameter in the non-reactive EOS using the Snowplough model.

The key feature of CREST is that it uses an entropy-dependent reaction rate model. Analysis of in-material, particle velocity gauge data for the shock to detonation transition in heterogeneous explosives[7,8] has shown that, in the early stages of the growth to detonation, the reaction rate at any given particle position depends only on the shock strength at that position. This indicates that a function of entropy of the unreacted explosive, $Z_s$, which remains constant between shocks, might be the most appropriate variable representing shock strength for use in a reaction rate model. In CREST, $Z_s$ is evaluated from the solid phase internal energy within the non-reactive EOS for the explosive. The form of the entropy-dependent reaction rate is given in another paper at this conference.[4]

## MODELLING GAS GUN EXPERIMENTS

In-material, particle velocity gauges, which are fielded in one-dimensional explosive gas-gun experiments, help provide valuable insight into the reaction behaviour in impact initiated high explosives. The modelling of these gas-gun experiments is required to help determine the parameters in the CREST reaction rate model by fitting to available particle velocity gauge data. A classical problem in the modelling of such experiments is an over prediction of internal energy, and hence, a function of entropy, $Z_s$, at the impact interface.

To illustrate this problem consider a simple, hypothetical, one-dimensional impact problem where a 30mm long Perspex projectile travelling at a velocity of $u$=0.931mm/μs impacts a stationary PBX-9501 explosive target also 30mm in length. The two materials were assumed to be initially in contact with the mesh nodes of the projectile being given the prescribed velocity $u$, apart form the interface node which had a velocity of $u/2$. On impact a well defined, flat-topped, shock wave should travel into the target material and a similar shock wave travel back into the projectile. Over the timescales considered here, the dimensions of the problem are such that the projectile and the target are affected only by the initial shock wave.

For this hypothetical problem, the magnitude of the shock generated in the explosive would start the initiation process in PBX-9501. However, here the PBX-9501 region was treated as an inert material (no energy release). When developing reactive burn models, non-reactive calculations are performed to ensure that the explosive's unreacted behaviour is accurately modelled before considering calculations with energy release.

The simulations were carried out using the one-dimensional, Lagrangian, multi-material hydrocode PERUSE[9], which is used as a test-bed for model development. A mesh density of 10 zones/mm was defined in both materials, and a monotonically limited artificial viscosity was used to accurately represent the propagating shock discontinuity. The non-reactive calculations are mesh converged at 0.1mm resolution.

The explosive was modelled with its non-reactive EOS[5] only from the CREST model, and was assumed to be non-porous *i.e.* the explosive was at its solid density or theoretical maximum density (TMD). The non-reactive EOS parameters for PBX-9501[10] at TMD are given in Table 1.

**TABLE 1. Non-Reactive EOS Parameters for PBX9501 at TMD.[10]**

| | | |
|---|---|---|
| $\rho_{0s}$ | 1.860 | g/cm$^3$ |
| $K_{0s}$ | 0.1403788 | Mb |
| $A_1$ | 3.489228 | |
| $A_2$ | 5.635034 | |
| $A_3$ | 0.0 | |
| $\Gamma_1$ | 89.40868 | |
| $\Gamma_2$ | 4.929351 | |
| $\gamma_{00}$ | 0.4 | |
| m | 2.0 | |
| $T_{0s}$ | 293.0 | °K |
| $C_{V0s}$ | $1.016\times10^{-5}$ | Mb cm$^3$/g/°K |
| $dC_{Vs}/dT$ | $3.16\times10^{-8}$ | Mb cm$^3$/g/°K$^2$ |

The Perspex impactor was modelled using a Gruneisen EOS of the form,

$$P = P_H(V) + \frac{\Gamma(V)}{V}\left[E - E_H(V)\right] \qquad (1)$$

where P is pressure, V is specific volume, E is specific internal energy, and $P_H$ and $E_H$ are respectively the Hugoniot pressure and energy corresponding to the shock velocity ($U_s$)-particle velocity ($U_p$) relationship,

$$U_s = C_0 + sU_p \quad (2)$$

where $C_0$ is the bulk sound speed, and s is a constant. The Gruneisen gamma, $\Gamma$, is given by,

$$\Gamma(V) = \Gamma_0 + \Gamma_1 \frac{V}{V_{0s}} \quad (3)$$

where $V_{0s}$ is the specific volume at solid density, and $\Gamma_0$ and $\Gamma_1$ are constants. The EOS parameters for Perspex[11] are given in Table 2.

**TABLE 2. EOS parameters for Perspex.[11]**

| | | |
|---|---|---|
| $\rho_{0s}$ | 1.186 | $g/cm^3$ |
| $C_0$ | 0.2598 | cm/μs |
| s | 1.516 | |
| $\Gamma_0$ | 0.0 | |
| $\Gamma_1$ | 0.97 | |

The calculated pressure profiles through the problem at two different times from impact are shown in Figure 1. As the projectile and explosive target are initially in contact, time of impact is t=0.0μs where the material interface is at 30mm. At t=2.0μs and t=4.0μs from impact, the material interface is at 30.8mm and 31.5mm respectively. In the shocked region, pressure is modelled correctly as continuous across the impact interface, and with the correct magnitude as defined by the Rankine-Hugoniot solution to this problem.

For ease of illustration, only the computed internal energy profiles in the unreacted explosive are shown in Figure 2, and are at the same times from impact as in Figure 1. The feature of note here is that the internal energy immediately adjacent to the impact interface is over-predicted as a result of the impact. There is similarly a corresponding over-prediction in the calculated internal energy in the Perspex flyer adjacent to the impact surface. Away from the immediate vicinity of the interface, the internal energies in both the flyer and target materials are correctly modelled. Since the function of entropy, $Z_s$, calculated in the non-reactive explosive is a function of the solid phase internal energy, there is a corresponding over-prediction in this quantity adjacent to the impact surface, as shown in Figure 3.

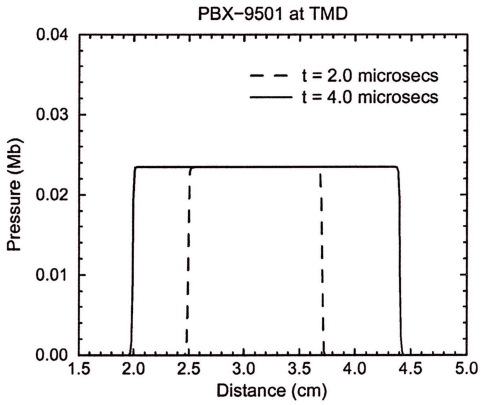


**FIGURE 1. Calculated pressure profiles for impact problem.**

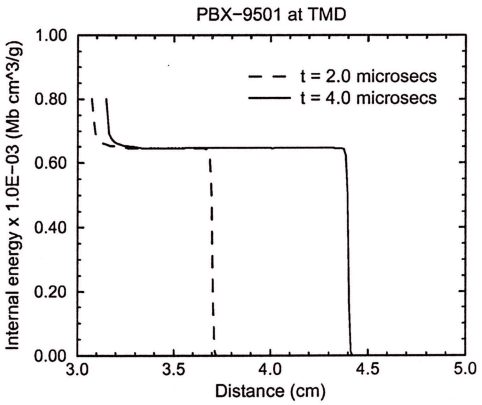


**FIGURE 2. Calculated internal energy profiles in solid PBX-9501 for impact problem.**

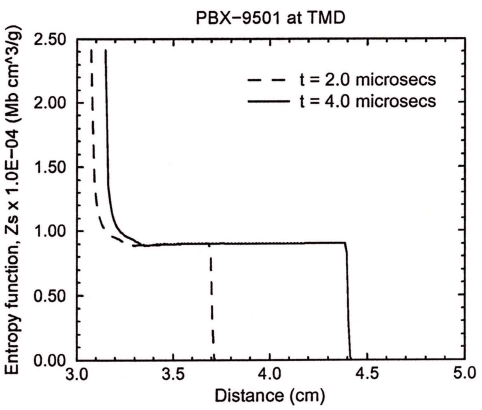


**FIGURE 3. Calculated entropy function profiles in solid PBX-9501 for impact problem.**

The internal energy and function of entropy in the non-reactive explosive material are significantly over-predicted in the first 3-4 meshes adjacent to the impact interface. In CREST, the reaction rate is a function of the current entropy of the unreacted explosive in a mesh. Thus, unlike models that use pressure-dependent reaction rates, CREST will over-predict the extent of reaction in the explosive immediately adjacent to the impact surface since the reaction rate will be artificially too high for the few first zones in the explosive. This could have possible consequences on the modelling, *e.g.* it could affect the selection of parameters in the CREST reaction rate model, which could lead to inaccurate conclusions being made about the reactive behaviour of the explosive.

The over calculation in internal energy, and hence function of entropy, at the impact interface is analogous to the calculational errors described by Noh[12], and is a result of a numerical start up error due to excess 'wall heating' on shock formation. Artificial viscosity based codes typically spread shocks over a fixed number of meshes (~3 or 4). Upon impact, it thus takes a finite time for the shock to be formed, and during this time excessive shock heating occurs in the first few zones adjacent to the impact surface, which then propagates as an error over the time frame of the calculation. Since evaluation of temperature within hydrocodes is based on internal energy calculations, then temperature-based reactive burn models will also suffer from the same ('wall heating') problem.

The effect of the error in the function of entropy at an impact interface has been examined[13] in reactive gas-gun calculations of the HMX-based explosive EDC37. To prevent an over-prediction in reaction rate occurring, the entropy function in the 'wall heated' zones was scaled locally to remove the 'wall heating' effect. Comparing CREST energy release calculations, both with and without entropy scaling factors, showed that the over-prediction in the entropy function at the impact surface made little difference to calculated particle velocity histories. This suggests that the 'wall heating' effect may not be problematic in modelling EDC37 explosive. However, this may not be the case for other explosives of interest. Methods therefore need to be sought to minimize the effect of this long standing problem, *e.g.* use of an adaptive mesh shock capturing procedure.[14]

## SNOWPLOUGH SHOCKS

All heterogeneous solid explosives of interest contain some degree of porosity, and it is well known that this has an important influence on an explosive material's non-reactive Hugoniot. Recently, a methodology for determining the EOS of unreacted explosives as a function of porosity has been developed[5]. This involves extrapolating available experimental Hugoniot data for the porous explosive to a best estimate of the fully dense Hugoniot. The EOS for the fully dense material used in conjunction with an appropriate porosity model then allows the unreacted Hugoniot at any porosity to be recovered.

CREST employs a porosity-dependent unreacted EOS. To take account of porosity in determining a porous explosive's non-reactive Hugoniot, CREST currently uses the Snowplough porosity model. In this model, the porous material is assumed to compact to close to its solid density at zero pressure, until its state lies on the EOS surface of the fully dense material for the rest of the calculation. In addition, it is assumed that the sound speed is zero during the compaction process.

The modelling of shocks in porous materials in conjunction with the Snowplough porosity model has been shown to be an area of concern regarding the use of the CREST model. To illustrate this, the simple impact problem described previously was re-run with porous PBX-9501 explosive in place of the explosive at TMD. The initial density of the PBX-9501 region was taken to be 1.825 g/cm$^3$, corresponding to an initial porosity of ~2%, with the explosive material again being assumed inert, and hence modelled with its non-reactive EOS taken from the CREST model.

The EOS constants for the Perspex impactor, and unreacted PBX-9501 target at TMD, were as given in Tables 1 and 2 respectively. The non-reactive EOS for the porous explosive was evaluated from the EOS at solid density using the Snowplough model. The calculated pressure-distance profiles at t=2.0μs and t=4.0μs from impact are shown in Figure 4. With the introduction of porosity into the explosive, small numerical oscillations in the pressure profiles are now observed behind the propagating shock wave.

The calculated internal energy profiles through the explosive region only are shown in Figure 5. When the explosive was assumed to be at its TMD,

the calculated internal energy, away from the immediate vicinity of the impact interface, gave a flat-topped profile behind the shock front. With the porous explosive, the calculated internal energy oscillates about the correct value throughout that part of the explosive that has been traversed by the shock giving a 'sawtooth'-like profile. Again, the calculated internal energy adjacent to the impact surface in the unreacted explosive is over-predicted. However, with the introduction of porosity, the magnitude of this error has been reduced in comparison to the calculation where the explosive was at its TMD. As the function of entropy calculated in the non-reactive explosive is a function of the solid phase internal energy, then the observed 'sawtooth'-like behaviour behind the shock front is repeated in the calculated profiles of this quantity, as shown in Figure 6.

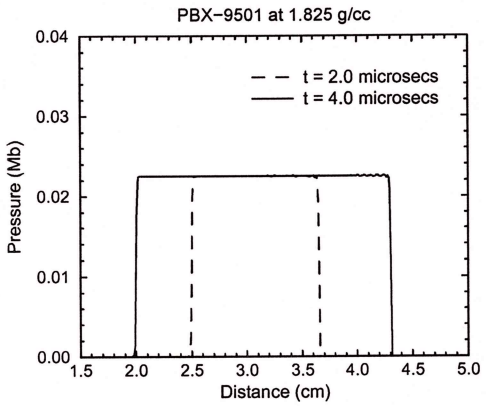


**FIGURE 4. Calculated pressure profiles impact problem.**

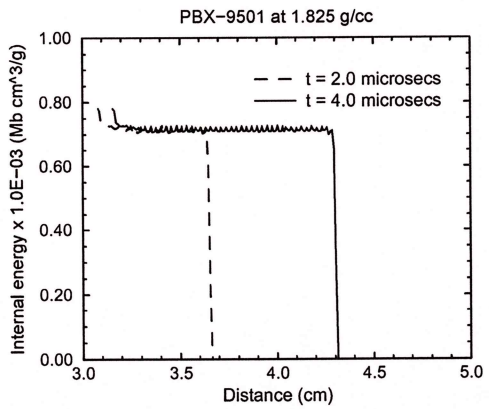


**FIGURE 5. Calculated internal energy profiles in porous PBX-9501 for impact problem.**

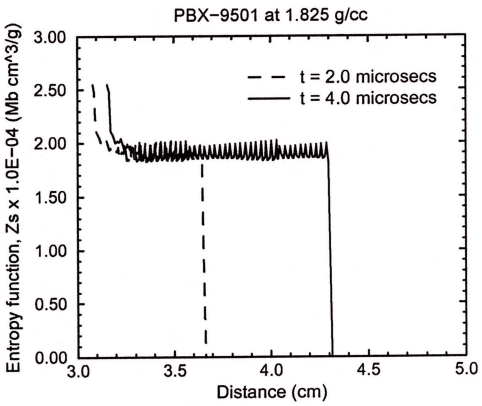


**FIGURE 6. Calculated entropy function profiles in porous PBX-9501 for impact problem.**

The 'sawtooth'-like behaviour seen in the computed internal energy and function of entropy profiles in the explosive region is clearly an undesirable feature when using a reaction rate model dependent on the function of solid phase entropy, $Z_s$, in a mesh. These oscillations, which interestingly are not damped out at some distance behind the shock front, unlike the pressure, could give rise to numerical instabilities when considering calculations with energy release.

The observed numerical oscillations in the computed profiles in the explosive region are as a result of the assumption made in the Snowplough model that the sound speed is zero while the material is in its porous state. This assumption affects the calculation of artificial viscosity. The form of artificial viscosity, Q, used in hydrocodes to represent a shock discontinuity is generally defined as a combination of linear and quadratic viscosities (*e.g.* monotonic Q),

$$Q = C_l \rho c |\Delta u| + C_q \rho (\Delta u)^2 \qquad (4)$$

where $\rho$ is density, c is sound speed, $\Delta u$ is the velocity jump across a mesh, and $C_l$ and $C_q$ are constants. For a shock wave propagating into a porous material using the Snowplough model, the artificial viscosity is defined by only the quadratic viscosity term during compaction. The linear viscosity term is only non-zero once the porosity has been removed. From past experience of modelling inert solid materials, use of only a quadratic viscosity term results in numerical oscillations behind the shock front. The purpose of

the linear term is to damp out these undesirable oscillations

By the particular method that the hydrocode uses to evaluate the sound speed, examination of the squares of the sound speed ($c^2$) calculated from the non-reacted EOS for the explosive material in its porous state has shown that, at low porosities (~few %), a realistic sound speed is returned. At higher porosities, $c^2$ is non-physically negative, a state that cannot be tolerated in a hydrocode. Thus, for only slightly porous explosive materials, the calculated sound speed from the non-reactive explosive's EOS could be used in the calculation of the artificial viscosity while the material is in its porous state.

In the PBX-9501 explosive at a density of 1.825 g/cm$^3$ (~2% porosity), the unreacted EOS returns realistic values for $c^2$ while the material is being compressed up to solid density. Thus, the Snowplough model was modified by removing the assumption that the sound speed is zero during compaction process, and using the sound speed as evaluated from the non-reactive EOS. The impact calculation with porous PBX-9501 was repeated using the modified model, and the calculated internal energy and function of entropy profiles through the explosive region are shown respectively in Figures 7 and 8.

These figures show that using a realistic sound speed in the calculation of artificial viscosity while the material is in its porous state, all but removes the numerical oscillations and 'sawtooth'-like behaviour previously seen when assuming that the sound speed was zero. However, the modified Snowplough model is not suitable for highly porous explosives, *e.g.* Non-Ideal explosives, since the $c^2$ values evaluated from the non-reactive EOS will be non-physically negative.

In this case, a P-$\alpha$ porosity model[15] will be required. The main difference between a P-$\alpha$ porosity model and the Snowplough model is that a P-$\alpha$ type model aims to provide a realistic description of the compaction process at low stress levels which is absent from the Snowplough model. Thus, it allows the calculation of a realistic pressure and sound speed while the material is being compressed up to its solid density, and hence use of a P-$\alpha$ porosity model, in place of the Snowplough model, should help improve the modelling of shocks in porous explosives using CREST.

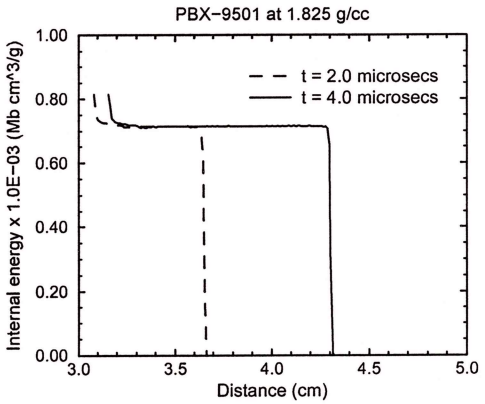


**FIGURE 7. Calculated internal energy profiles in porous PBX-9501 (using sound speed as calculated from EOS).**

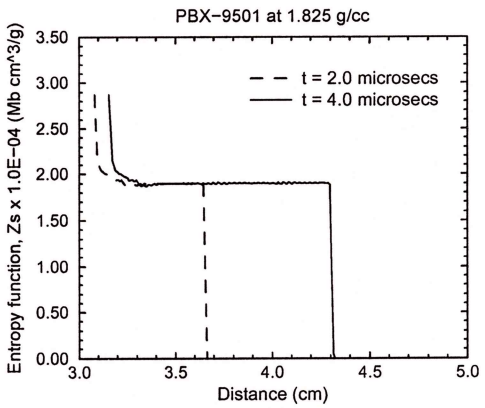


**FIGURE 8. Calculated entropy function profiles in porous PBX-9501 (using sound speed as calculated from EOS).**

## MESH SENSITIVITY

In developing reactive burn models, fine zoning is usually required to ensure adequate phenomenon resolution. A study of the sensitivity of CREST calculations (with energy release) to mesh density has been performed by modelling gas-gun experiments on the HMX-based explosive EDC37[16]. By fitting to embedded particle velocity gauge data from these experiments, a CREST model for EDC37 explosive was developed by Handley[4]. The CREST model parameters for EDC37 are given in Table 3.

**TABLE 3. CREST parameters for EDC37.[4]**

| | | |
|---|---|---|
| $\rho_{0s}$ | 1.8445 | g/cm$^3$ |
| Reaction products equation of state | | |
| A | 6.642021 | Mb |
| B | 0.2282927 | Mb |
| $R_1$ | 4.25 | |
| $R_2$ | 1.825 | |
| $\omega$ | 0.25 | |
| Unreacted equation of state | | |
| Q | 0.0719557 | Mb cm$^3$/g |
| $K_{0s}$ | 0.1424525 | Mb |
| $A_1$ | 2.417494 | |
| $A_2$ | 2.208027 | |
| $A_3$ | 0 | |
| $\Gamma_1$ | 32.33557 | |
| $\Gamma_2$ | 3.596933 | |
| $\gamma_{00}$ | 0.4 | |
| m | 2.0 | |
| $T_{0s}$ | 293.0 | °K |
| $C_{V0s}$ | $9.17\times10^{-6}$ | Mb cm$^3$/g/°K |
| $dC_{Vs}/dT$ | 0.0 | Mb cm$^3$/g/°K$^2$ |
| Reaction rate parameters | | |
| $c_0$ | $2.0\times10^8$ | $\mu s^{-2}$(Mb cm$^3$/g)$^{-c1}$ |
| $c_1$ | 2.0 | |
| $c_2$ | $2.2\times10^8$ | $\mu s^{-2}$(Mb cm$^3$/g)$^{-c3}$ |
| $c_3$ | 2.5 | |
| $c_6$ | 0.0 | $\mu s^{-1}$ |
| $c_8$ | $1.6\times10^{-4}$ | $\mu s^{-1}$(Mb cm$^3$/g)$^{c9}$ |
| $c_9$ | 1.0 | |
| $c_{10}$ | $4.0\times10^5$ | $\mu s^{-1}$(Mb cm$^3$/g)$^{-c11}$ |
| $c_{11}$ | 1.8 | |

The PERUSE hydrocode was used to perform the mesh sensitivity study where the mesh resolutions used ranged from 5-100 zones/mm. For each calculation, a monotonically limited artificial viscosity was used. Since the porosity of EDC37 is small (~0.2%), for the purposes of this study it has been treated as a fully dense material. In addition, the effect of the over-prediction in the entropy function, $Z_s$, due to the 'wall heating' effect has been shown to be small in EDC37 explosive.[13]

Figure 9 shows the calculated particle velocity results at a number of different gauge locations for EDC37 Shot 1159. For ease of illustration, only the results at 2.9mm, 6.0mm, and 9.0mm gauge locations are shown which correspond roughly to the early, middle, and late stages respectively of the growth to detonation process. In the calculations, reaction is allowed to proceed as the function of entropy rises with the arriving shock, *i.e.* there is reaction through the shock front. The computed CREST results show that mesh resolution has a significant effect on the calculated particle velocity histories. There is increased reaction at the 2.9mm and 6.0mm gauge locations with decreasing mesh density, which in turn results in earlier shock time of arrival at the gauge locations since the shock wave is accelerating faster. Correspondingly, there is a shortening of the computed run distance and time to detonation with decreasing mesh density. Overall, the results indicate that a mesh density of 50 zones/mm is required for mesh convergence.

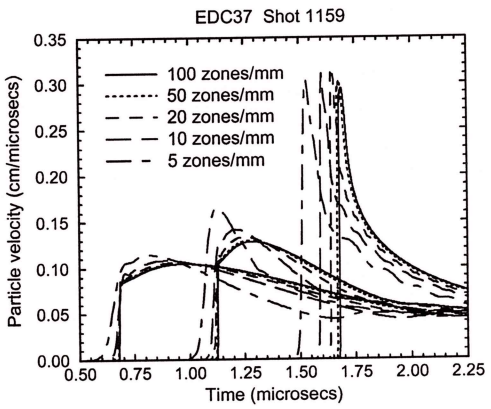


**FIGURE 9. Calculated CREST profiles at 2.9, 6.0, and 9.0mm gauges for Shot 1159.**

The CREST mesh sensitivity results are to be compared with the corresponding calculations of Shot 1159 using a pressure-dependent reactive burn model. The pressure-based Lee and Tarver[17] model is probably the most widely used reactive burn model for simulating shock initiation in heterogeneous explosives, and has been implemented in the PERUSE hydrocode. A Lee and Tarver model for EDC37 explosive was previously developed by Winter et al.[18] by attempting to fit to a number of the EDC37, sustained single shock, gas-gun experiments. The Lee and Tarver model parameters for EDC37 are given in Table 4.

The calculated particle velocity profiles for Shot 1159 at 2.9mm, 6.0mm, and 9.0mm gauge locations using the Lee and Tarver model are shown in Figure 10. As with the CREST simulations, reaction was allowed to proceed through the arriving shock front in each computational mesh.

**TABLE 4. Lee-Tarver constants for EDC37.[18]**

| | | |
|---|---|---|
| $\rho_0$ | 1.842 | g/cm$^3$ |
| Reaction products equation of state | | |
| A | 8.524 | Mb |
| B | 0.1802 | Mb |
| $R_1$ | 4.60 | |
| $R_2$ | 1.30 | |
| $R_3$ | $3.8\times10^{-6}$ | |
| $C_V$ | $1.0\times10^{-5}$ | Mb/°K |
| E | 0.102 | Mb |
| Unreacted equation of state | | |
| A | 69.69 | Mb |
| B | -1.727 | Mb |
| $R_1$ | 7.80 | |
| $R_2$ | 3.90 | |
| $R_3$ | $2.148789\times10^{-5}$ | |
| $C_V$ | $2.505\times10^{-5}$ | Mb/°K |
| E | 0.00205 | Mb |
| Reaction rate parameters | | |
| I | $3.0\times10^{10}$ | $\mu s^{-1}$ |
| b | 0.667 | |
| a | 0.0 | |
| x | 20.0 | |
| $G_1$ | 90 | $Mb^{-y}\mu s^{-1}$ |
| c | 0.667 | |
| d | 0.333 | |
| y | 2.0 | |
| $G_2$ | 200 | |
| e | 0.333 | |
| g | 1.0 | |
| z | 2.0 | |
| $F_{ig\ max}$ | 0.3 | |
| $F_{G1\ max}$ | 0.5 | |
| $F_{G2\ max}$ | 0.0 | |

Using the Lee and Tarver model, there is only minimal effect on the calculated results with decreasing mesh resolution over the range of mesh densities used. It is only at the coarsest resolution tested (5 zones/mm) that the resolution used starts to have some noticeable effect on the calculated particle velocity histories. The trend is to slightly delay the growth of reaction with increasing mesh size, rather than to increase it as observed with CREST. Using Lee and Tarver, there are only very small differences in the run distances and times to detonation over the range of mesh densities used. The Lee and Tarver calculated results show that mesh convergence occurs at a mesh density of 10 zones/mm. Thus, it would appear that an entropy-dependent model requires a finer mesh than a pressure-dependent model in order to achieve mesh converged results.

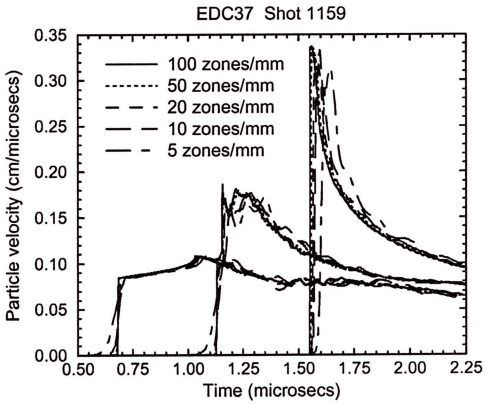


**FIGURE 10. Calculated Lee and Tarver profiles at 2.9, 6.0, and 9.0mm gauges for Shot 1159.**

The CREST mesh sensitivity study was repeated using two alternative approaches, termed 'Q-switching', for turning on the reaction in a computational mesh, namely; (i) reaction turned on when $dQ/dt<0$, which occurs approximately half way through the rise time of the arriving shock front, and (ii) the reaction was supressed until the artificial viscosity, Q, dropped below a specified threshold ($10^{-6}$ Mb) *i.e.* no reaction throughout the rise time of the shock front. The computed results for Shot 1159 using 'Q-switching' method (i) for the onset of reaction in a cell gave very similar profiles to those shown in Figure 9, showing only a very small improvement in mesh convergence properties compared to the results where reaction was allowed to proceed through the arriving shock wave.

The calculated results for EDC37 Shot 1159 using 'Q-switching' method (ii) for the onset of reaction in a computational cell are shown in Figure 11. Delaying the onset of reaction to start at approximately the top of the rise time of the arriving shock front, has improved the mesh convergence. There is now only a small effect on the calculated particle velocity results, and hence run distances and times to detonation, with decreasing mesh resolution over the range of mesh densities used. It is only the 5 zones/mm results at late times that show any significant differences. Results are mesh converged at 10 zones/mm giving comparable mesh convergence properties to the

pressure-based Lee and Tarver model. Comparing the CREST results in Figure 11 with the Lee and Tarver results in Figure 10, and ignoring the differences in the shape of the calculated profiles, there is a remarkable similarity, in terms of the mesh size effect, between the two sets of calculations.

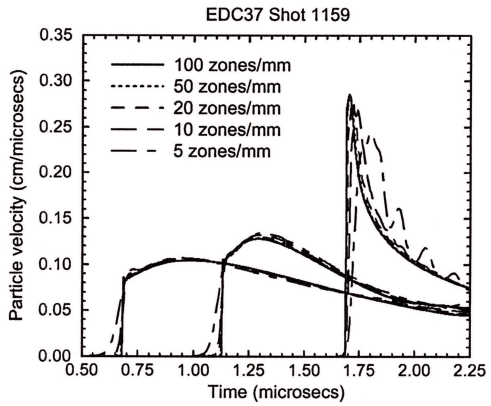


**FIGURE 11. Calculated CREST profiles at 2.9, 6.0, and 9.0mm gauges for Shot 1159.**

Comparing all three approaches in CREST for turning reaction on in a cell, the same results are essentially obtained at the highest mesh densities (100 and 50 zones/mm) irrespective of where the reaction is turned on in respect of the arriving shock front. However, at coarser resolutions significantly different results are obtained between the different approaches. Least variation in the calculated results with mesh size is observed where reaction is supressed throughout the arriving shock front.

It is not clear why one particular method for reaction commencement in a computational cell should be preferred over any other of the approaches tried here. However, to implement the 'Q-switching' methods described required additional modifications to be made to the hydrocode, and hence the more natural approach is to allow reaction to proceed through the arriving shock wave. The mesh sensitivity study has shown that using this approach the entropy-dependent CREST model requires a finer mesh (50 zones/mm) than a pressure-based model (10 zones/mm), to achieve mesh converged results.

To overcome the more restrictive mesh size requirements of an entropy-dependent model, CREST has been implemented into a 2D Eulerian adaptive mesh refinement (AMR) hydrocode[19] with an appropriate refinement criteria defined for the model. This will enable large, two-dimensional, shock initiation problems of interest to be simulated at the size of mesh required by CREST to obtain mesh converged results.

## CONCLUSIONS

The entropy-dependent CREST reactive burn model suffers from a number of computational problems not associated with pressure-dependent models. The classical 'wall heating' problem at an impact interface could affect the selection of parameters in CREST's reaction rate model when fitting to data from explosive gas-gun experiments. This in turn could have possible consequences on the modelling of a range of shock initiation problems, and could lead to inaccurate conclusions being made about the reactive behaviour of an explosive. Consequently, appropriate methods are to be sought to try to minimize the effect of this long standing problem. It is noted that temperature-based models will also suffer from the same ('wall heating') problem.

Application of the Snowplough porosity model in CREST to determine the EOS of the non-reacted porous explosive produces undesirable numerical oscillations in the calculated function of entropy of the solid phase explosive, the variable upon which the CREST reaction rate model is dependent. This could give rise to numerical instabilities in energy release calculations. To improve the modelling of shocks in low porosity explosives, the Snowplough model was modified by removing the assumption that the sound speed is zero during the compaction process. Although this modification removes unwanted numerical oscillations, it is only applicable to low porosity materials. In future, to enable explosives with a larger range of initial porosities to be modelled using CREST, the Snowplough model will be replaced by a P-$\alpha$ porosity model.

A study of the sensitivity of CREST calculations to mesh density indicates that, where reaction is allowed to proceed through the arriving shock front, an entropy-dependent model requires a finer mesh than a pressure-based model to obtain mesh converged results. This has led to the implementation of the model in a 2D Eulerian AMR hydrocode to enable real problems of interest to be calculated at appropriate mesh resolutions.

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