LINKS BETWEEN DETONATION WAVE PROPAGATION AND REACTIVE FLOW MODELS

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The WBL model for detonation wave propagation was extended to allow more general initiation in the context of level set methods. Initiation could then be induced fairly seamlessly from reactive flow simulations. The accuracy of WBL detonation compared favourably with results from full reactive flow, and proved surprisingly robust with respect to changes in numerical parameters used to trigger WBL detonation from the local state in the reactive flow simulation. The level set implementation of WBL detonation was generalised to apply to a Lagrangian mesh rather than the previous Eulerian scheme; the resulting model could then be used to model initially moving explosive and thus to treat scenarios such as reflected-shock initiation. A scheme was developed to model the release of energy behind a curved detonation wave, using the slow tail of the reactive flow model. Reactive flow simulations of the structure of the detonation zone were used to calculate the state at the sonic surface. Reactive flow models were also used to predict the speed of the detonation wave as a function of its curvature, which was compared with experimental data.

INTRODUCTION

A good reactive flow model is necessary to be able to predict the initiation properties of explosives by complicated shock structures, but a very fine spatial resolution is needed in reactive flow to reproduce the detailed dynamics of a detonation wave. However, it is not necessary to use a reactive flow model to simulate the motion of a fully-developed detonation wave in most circumstances. Usually, the same results can be obtained with a coarse computational mesh using "programmed burn" techniques where an eikonal solution is used for the motion of the detonation wave. The simplest type of eikonal solution is a constant speed detonation wave, which is widely used but not adequate for applications requiring a high precision.

In the WBL model [1,2], an eikonal detonation wave propagates through a body of explosive at a speed which depends on the curvature of the wave, and with boundary conditions imposed by inert materials adjacent to the explosive. The WBL model has usually been calibrated directly against measurements of wave curvature and speed rather than through reactive flow, so it is arguably at least as accurate as any reactive flow simulation can be, within the range of conditions used in the calibration.

In some scenarios, such as predictions of the safety of an explosive device, it is necessary to simulate the initiation of reaction in the explosive, followed by the propagation of a detonation wave. These simulations may be 3D, making it particularly desirable to avoid the need for a fine computational mesh. Here we describe extensions to the WBL model which allow it to be linked with reactive

flow so that many problems of this type can be simulated using the best features of reactive flow and of the WBL model.

WBL DETONATION MODEL

The WBL model describes the motion of the leading shock of the detonation wave. As originally formulated [1], the model represented the surface of the detonation wave with a set of connected points, and moved the points through the body of explosive with a speed that depended on the local curvature of the wave. Where the wave meets the interface between the explosive and an inert material, it is constrained to make certain angles with the interface. Equations of motion for the wave were derived by considering the expansion of regions of the wave between "rays" normal to the wave, following Whitham's theory of shock dynamics.

The relation between detonation speed and wave curvature can be justified using the ZND model for finite-rate reaction: in a curved wave, the sonic surface moves towards the leading shock, so some of the energy release occurs behind the sonic surface and is unavailable for driving the wave [2]. Similarly, the boundary conditions can be justified by considering reflected waves from an inert boundary, and deducing angles at which they do not perturb the detonation wave [3]. However, both sets of relations are usually deduced by performing experiments on long rods and slabs of explosive, and measuring the shape of the wave [2,4]. Thus it is not necessary to have a reactive flow model which is accurate at the pressures of full detonation in order to predict the motion of the detonation wave with excellent accuracy, quite apart from having much less stringent requirements for mesh resolution.

Initiation problems

For some problems, it is necessary to calculate both the initiation of detonation (by impact and/or heating) and the subsequent propagation of a detonation wave. An example might be a safety problem, where a projectile strikes a cased charge and initiates a detonation wave in a way which depends strongly on the details of the impact and the charge, and in which it is necessary to calculate the performance of the explosive system following initiation.

Reactive flow is generally necessary to model the initiation process, but it may be very desirable to use programmed burn to model the propagation of the detonation wave. It would be possible in principle to perform the reactive flow simulation, collecting points at which for instance the pressure has exceeded some arbitrary value chosen to indicate detonation, and then to use these points to set up a WBL simulation of detonation in the rest of the explosive. However, the WBL model was developed with reproducible initiation from detonators in mind, and no provision was made in any of the problem generation or simulation schemes for initiation which might vary significantly between problems. Indeed, setting up the initial wavefront has always been one of the more awkward aspects of the WBL model.

Here we report new schemes developed to make it easier to define initial waves in the WBL model, and to make it more convenient to couple reactive flow and WBL simulations.

Level set method

We concentrate on the level set (or "propagation of surfaces under curvature", PSC) method for integrating the WBL equations in time [4,5,6,7]. The level set method is attractive because it can treat complicated detonation wave shapes without requiring the relatively exhaustive exercise in computational geometry involved in moving a discretised detonation wave through the explosive.

The level set method works by following the evolution of a space-time field $\psi(\mathbf{r},t)$ so that at any time τ, the detonation wave is the contour

$$\{\mathbf{r} : \psi(\mathbf{r},\tau) = C\}$$

for some constant C (usually zero). This leads to a Hamilton – Jacobi evolution equation for ψ:

$$\partial\psi/\partial t + D|\text{grad } \psi| = 0.$$

The detonation speed D can be a function of the wave curvature K, where

$$K = \tfrac{1}{2} \text{ div } \mathbf{n},$$

and $\mathbf{n}$ is the wave normal,

$$\mathbf{n} = \text{grad}\psi / |\text{grad } \psi|.$$

Examples include the D(K) relations used to date, and also acceleration relations dD(D,K)/dt.

It can be shown that the level set equations reproduce the eikonal equations of motion [8].

INITIATION IN LEVEL SET SIMULATIONS

The natural method for driving a level set calculation from a reactive flow simulation would be to use the reactive flow to define when points in the explosive should be ignited. A new initiation method was devised to do this, based on observations made of the behaviour of reactive flow simulations of the shock-to-detonation transition in high explosives, and of the behaviour of WBL detonation waves when initiated by different methods in a level set scheme.

In our original level set scheme [4], the initial detonation wave was always chosen so that a finite region of explosive was burnt behind it before the level set integration began. This is similar to the wave-tracking solution methods used previously [1], where a curved wave had to be started from a finite radius in order for D to remain positive. In the level set schemes, this also had to be done when starting from a plane wave. This was because the level set field was allowed to evolve freely throughout the explosive, and the region around the ψ=C contour had to be some distance from the boundary of the explosive to avoid spurious edge effects disturbing the evolution of the wave.

The initial field $\psi(\mathbf{r},t_0)$ was set up to be the time from a set of source points $\{\mathbf{r}_i\}$ causing a detonation to start at times t_i,

$$\psi(\mathbf{r},t_0) = \min_i(t_i + |\mathbf{r} - \mathbf{r}_i| / D_i - t_0 + C),$$

where D_i is a reference speed, usually the same for all source points in the same type of explosive.

The use of the shortest distance between $\mathbf{r}$ and $\mathbf{r}_i$ was found to cause problems at the far side of inclusions in the explosive body. grad ψ pointed in the opposite direction to the outward normal to the boundary, which generated instabilities when the boundary conditions were applied. A practical solution was found to be to cut off $\psi(\mathbf{r},t_0)$ at some finite positive value, ψ_{max} say. Doing this, the region of constant $\psi(\mathbf{r}) = \psi_{max}$ remained unchanged until the disturbance from the region of finite grad ψ passed through, whereupon ψ began to evolve at the correct rate. It was found possible to calculate the diffraction of a detonation wave around an inert inclusion to good accuracy, indicating that the accuracy was not compromised in the transition from constant $\psi(\mathbf{r})$ to the profile required of a detonation wave.

Since the evolution of ψ was found to be insensitive to the way in which ψ was initialised at a finite distance from the initial wave, this suggested that a level set calculation could be driven from a reactive flow simulation by setting $\psi(\mathbf{r},t_0) = C_0 \; \forall \mathbf{r}$ at the start of the simulation, where C_0 is greater than C by some finite amount. At some subsequent time $t > t_0$, if the state at a point $\mathbf{r}_i$ in the reactive flow simulation indicates that a detonation wave exists, then $\mathbf{r}_i$ is declared to be a source point with an associated time $t_i = t$. These new source points $\{\mathbf{r}_i\}$ are then used to constrain ψ:

$$\psi(\mathbf{r}_i,t) = \min(C_0,t_i - t + C)$$

where t_i is the initiation time for source i.

This scheme has many potential applications and advantages. The initial detonation wave can be a point, or could start at $t > t_0$ – neither of which was possible with our previous level set schemes. The scheme could also be extended to do even more, such as applying a limit or a statistical constraint to ψ, for example in order to encourage the level set simulation to reproduce experimentally-measured detonation arrival times

Ideally, it would be possible to choose C_0 arbitrarily far from or close to C, and to set $\psi(\mathbf{r}_i)$ instantaneously to C when the reactive flow simulation indicates that a detonation wave is present at $\mathbf{r}_i$. However, if C_0 is too close to C then the solution becomes sensitive to noise and truncation errors in the numerical scheme. It was also found that, for the predictor-corrector schemes developed to integrate $d\psi/dt$, changing an individual value instantaneously from C_0 to C generated a numerical instability. Instead, it was found necessary to integrate $\psi(\mathbf{r}_i,t)$ smoothly from the time at which $t - t_i + C = C_0$, i.e. the time at which the constrained solution passed through C_0. In practice, this means that the information required from the reactive flow simulation is a warning that a detonation wave *will be present* at $\mathbf{r}_i$ at a time C_0 in the future.

The performance of this scheme was investigated in some detail. The speed of the detonation wave was slightly incorrect to begin with, but it approached the correct value with time. Various options were considered whereby the necessity for $C_0 > 0$ and the associated mistiming between the WBL detonation and the reactive flow detonation could be minimised. These options included adding a model of "numerical superdetonation" so the WBL detonation could catch up, or initiating the WBL simulation at a slightly different position.

Despite some limitations associated with the finite value of C_0, this new initiation scheme for the WBL model provides the basis of a link with reactive flow simulations, and can be used directly by performing the reactive flow simulation, collecting a list of initiation points, using these for the WBL simulation, then using the WBL burn times for accurate detonation with a coarse mesh. A convention is needed for choosing states which indicate detonation or incipient detonation during the reactive flow simulation. The choice of these "trigger states" is not straightforward, and is discussed further below.

In general the reactive flow simulation should not be terminated when the first trigger state occurs before performing the WBL calculation. In many problems, detonation may start elsewhere shortly afterwards. For example, if a shock generated by a projectile impact is too weak to run to detonation, but on reflection from a case it becomes strong enough to initiate promptly, a whole sequence of trigger states may be produced as the shock sweeps across the case at a phase speed which is much faster than D. In this case it would be incorrect to take only the first trigger state produced.

However, if care is taken to include trigger states generated over a reasonable period of the reactive flow simulation, then a WBL calculation could usefully be driven from a reactive flow simulation. A full reactive flow simulation would be performed from the initial impetus imparted to the system until the occurrence of large-scale reactions, recording trigger states during the simulation. These trigger states would then be used to initiate a WBL calculation, running from at least C_0 before the first trigger state until all the explosive had been consumed. The WBL burn times would then be used to program the burn in a reactive flow simulation starting at the same (simulation) time as the WBL calculation, and running for as long as necessary to predict the performance of the device.

The reactive flow simulations need a mesh fine enough to model initiation with adequate accuracy; this is generally far less severe than that needed to model curvature effects in full detonation.

INTIMATE LINK WITH REACTIVE FLOW

For general problems, it is desirable to integrate the reactive flow and WBL equations in parallel. The main difficulty is that C_0 is finite, so the WBL calculation requires a degree of foreknowledge of trigger states from the reactive flow simulation. We have developed an initial trial implementation of coupled reactive flow and WBL solutions [9,10].

If the level set equations are to be integrated in parallel with the reactive flow, then in principle the materials in the level set calculation must evolve as they move according to the reactive flow simulation. For example, preshocked but undetonated explosive is in motion and has a distorted shape compared with the virgin material.

The level set equations developed previously [4] were expressed using a computational mesh that is stationary with respect to the material into which the detonation wave propagates, actually a Lagrangian mesh frozen in time. In order to solve the general case, the equations must be modified to take account of the initial motion of the explosive. This can be done with respect to Eulerian or Lagrangian meshes; here we concentrate on the latter.

The level set scheme used previously was generalised slightly to take account of motion of the material behind the detonation wave, essentially adding an advection term for ψ in the region where it is negative. For a detonation wave running into undisturbed material, these modifications should reproduce the results of the original level set equations. The modifications are introduced in converting $d\psi/dt$ to a Lagrangian derivative, $d\psi_R/dt$ say, where the subscript R denotes differentiation along a trajectory following an element of the explosive material, as opposed to a constant spatial position:

$$d\psi_R/dt = d\psi/dt + \mathbf{u} \,.\, \text{grad}\, \psi$$

where $\mathbf{u}$ is the local material velocity. Thus the evolution equation becomes

$$d\psi_R/dt - \Delta\mathbf{u} \,.\, \text{grad}\, \psi + D\, |\text{grad}\, \psi| = 0$$

where $\Delta\mathbf{u} = \mathbf{u} - \mathbf{u}_0$ is the local material velocity relative to its initial velocity $\mathbf{u}_0$. The use of an explicit initial state generalises the equation to apply to situations where the explosive is moving with respect to the coordinate system before it detonates, such as a preshock or an explosive projectile.

If the explosive is accelerated dynamically during the simulation, such as by the passage of a weak shock, then $\mathbf{u}_0$ should be taken just before each element of explosive detonates, i.e. as $\psi \rightarrow C$ for the first time. However, if artificial viscosity is used to stabilise hydrodynamic shocks in the reactive flow scheme, the leading shock of the detonation wave is smeared over a few computational cells. A safer method is to take $\mathbf{u}_0$ as the particle velocity when $\psi \rightarrow C'$ for the first time, where C' is some small amount to the unburnt size of C. In either case, it is necessary to store $\mathbf{u}_0(\mathbf{r})$ as a state parameter in the explosive.

If the WBL and reactive flow equations are integrated simultaneously, then cross-terms are needed to link the equations. Contributions in $d\psi/dt$ from the reactive flow state, and in the reactive flow state from ψ, were investigated. The cross-terms can be expressed in terms of formal sources in the continuum equations; in the present work we adopted more direct constraints on the field values, as described below.

Trigger states

A key element of the link between reactive flow simulations and the WBL model is the choice of "trigger states" in the reactive flow field which can be used to signal to the WBL calculation that detonation waves should be initiated. Many states or combinations could be used; the choice depends on the class of problem.

One choice of trigger state is that the reaction progress variable λ tends to 1. It could be argued that anywhere that the explosive has reacted, it would make sense to treat as reacted in the ψ field. However, it is possible for a region of explosive to react gradually beside a region which does not react at all, such as in shock desensitisation or when a failing detonation wave drills through a block of insensitive explosive. If simulations of these situations were triggered using λ then grad ψ would be large (infinite) across the boundary between unreacted and reacted material, giving unphysical (or numerically unstable) terms in the WBL equations.

Other choices include combinations of the hydrodynamic state variables ρ and p (pressure); however, it is quite easy to contrive situations where these can reach values comparable to those in a detonation wave without detonation occurring. Shock desensitisation is again an example.

Another type of trigger is to use the reaction rate $d\lambda/dt$. We could define the trigger state when $d\lambda/dt$ is "reasonably large" (exceeds some value $d\lambda_1/dt$), so as to give a short run to detonation. As an additional constraint, λ should exceed some minimum value λ_1. This allows greater control over shock desensitisation, where reaction might occur rapidly up to some threshold where it is suppressed by the desensitising processes. Ideally, we would choose $d\lambda_1/dt$ and λ_1 such that the time to detonation at that point is C_0, the "psychic" trigger state. Further work is needed to investigate how accurately the WBL detonation can be made consistent with detonation in the reactive flow simulation for real explosives, but results so far indicate that C_0 can be made quite small, as demonstrated later.

Consistency of initial WBL wave with reactive flow

As discussed above, in principle the level set scheme needs advance notice by some finite time C_0 of when a detonation wave is to pass a point. One way to arrange this is to use the trigger state from the reactive flow calculation at a position $\mathbf{r}$ to control $d\psi/dt$ at a different position $\mathbf{r}' = \mathbf{r} + DC_0\mathbf{n}$, where $\mathbf{n}$ is the predicted normal to the detonation wave. However, $|\mathbf{r}'-\mathbf{r}|$ may span several computational cells, so this approach involves relatively complicated nonlocal geometry.

Another approach is to allow D to exceed its value in the D(K) relation, to allow a numerical "superdetonation" to compensate for the time delay. This can be implemented through the use of an acceleration relation dD(D,K)/dt: in principle all that is required is to choose a suitable relation and to pick a higher initial value of D when the WBL calculation starts. This method was investigated briefly, but was found to be unnecessary for the trial problems considered here.

PROTOTYPE IMLEMENTATION

A prototype version of the modified level set scheme described above was implemented in a 1D Lagrangian testbed hydrocode, using a predictor-corrector integration scheme with artificial viscosity to stabilise shock waves.

Reactions were operator-split from the hydrodynamics – the code could operate with time-accurate integration, but this reduced the time-step dramatically for high explosives. No effort was devoted to controlling the higher rates in detonation for maximum stability as this was not the main thrust of this work. As a result, the peak pressure in a detonation wave tended to exhibit periodic variations which were preserved in the rarefaction, since the positive velocity divergence reduced the ability of the compressive artificial viscosity to damp out oscillations. Smooth rarefactions have been obtained using the same models for similar explosives, with a moderate amount of effort to resolve the reaction adequately while retaining computational efficiency.

Trigger states were chosen to satisfy a pressure – temperature condition,

$$p > p_{min}(T).$$

p_{min} could be any functional form, but the for present work was taken to be a constant value typically around 20 GPa. Triggering was suppressed if ψ had already fallen below some finite value, indicating that a detonation wave was nearby. When the trigger condition was satisfied by the state at a point (and triggering was not suppressed by a value of ψ which had already started to evolve), then a new source point for applying a $\psi(t)$ history was added to the previous set $\{\mathbf{r}_i\}$. To keep the solution stable, the initiation time t_i for the new source point was set a little later than the time at which the trigger condition was reached, by the "trigger delay time". This was typically equal to the initial (constant) value given to ψ across the whole mesh, C_0.

If the computational cells can move with respect to their position just before the passage of a detonation wave, then for any points at which $\psi(t)$ is constrained by a source point, the ψ history should be corrected for the motion of the cells. This modification was not implemented in the present work, since the key elements of the scheme developed here can be tested completely by calculations with no source points at the outset.

The "applied ψ history" constraint was weakened slightly to be used only if ψ from the constraint was less than the value obtained by integrating the PSC equation. This is necessary if the simulation is to be able to detonate regions earlier than predicted from any given initial (or intermediate) set of detonation centres, which is the whole point of investigating the intimate link between WBL and hydrodynamics.

The local particle velocity $\mathbf{u}$ was stored for use in calculating $\Delta\mathbf{u}$ when ψ fell below a certain value ψ_s. ψ_s was chosen to be sufficiently close to C such that no significant flow occurred between the time at which ψ fell to ψ_s and the time at which ψ reached C (i.e. between the time that $\mathbf{u}_0$ was stored and the time that the detonation wave passed), but far enough from C that any influence of the leading shock broadened by artificial viscosity was negligible.

When $\psi(\mathbf{r}) - C$ changed sign in any time step, a "reacted" state was imposed on the flow field at $\mathbf{r}$, but only if the "fraction reacted" of this state was greater than that already present. This inhibited the PSC integration from proceeding into regions which had already reacted. Reacted states were allowed to vary in principle with the local wave curvature. However, all simulations were performed in plane geometry in the present work, so only a single reacted state was necessary. This scheme provides a link to energy release modelling in WBL simulations. Parameters could be found from detailed reactive flow simulations, in the form of the state at the end of the detonation zone as a function of curvature.

Trial calculations were performed of initiation and detonation in the TATB-based explosive LX-17. Material properties for LX-17 were taken from Tarver's three-term ignition and growth model [11], but the parameters were used in a more general reactive flow model with finite mechanical and thermal equilibrium between any pair of equations of state [12,13]. This model has been found to give similar initiation properties to those obtained with other implementations of Tarver's model, while allowing more accurate models to be substituted easily in order to simulate complicated problems such as multiple-shock initiation. The Lee-Tarver model imposes complete pressure and temperature equilibrium, so the equilibration times

were set to a small number (10^{-12} μs). The mesh size was 0.5 mm for all the calculations of LX-17.

CJ detonation by programmed burn

A CJ detonation was simulated in order to verify that the modified PSC algorithm operated correctly. Detonation was calculated against a rigid wall at x=0. C_0 was taken to be 1.0 μs and the simulation was started at a time of -1.0 μs in order to allow the point at x=0 to detonate at t=0. The post-reaction state was taken to be the CJ state. The simulation exhibited a self-similar Taylor wave behind the initial CJ shock. The detonation speed, calculated by finding the best-fitting straight line to the shock front (maximum of q/ρ), was 7.579 km/s, compared with a nominal 7.596 km/s for the set of Tarver parameters – a satisfactory accuracy.

It should be emphasised that in contrast to simple implementations of programmed burn, the unreacted explosive was represented here by a complete reactive flow model. Programmed burn, determined by the WBL/PSC calculation, was used to alter the state in the material. (This is in contrast to for example the use of a pressure multiplier, where the unreacted material typically cannot transmit stress waves, and deformations or shocks short of detonation cannot be modelled.)

Single shock initiation

As a test of the ability of the scheme to hand-over from reactive flow to programmed burn, we simulated the shock-to-detonation transition followed by a sustained detonation.

To avoid any confusion caused by the finite trigger delay, the explosive was split into two regions. The first region was thick enough for a detonation wave to develop. In the second region, the ignition and growth rates were set to zero, so reaction could progress only by the WBL simulation. Both regions were 5 cm wide; pressure being applied to the fully reactive region to drive the initial shock wave

The best results were achieved with a trigger pressure of 0.25 Mb and a trigger delay of ~0.2 μs.

Simulations were repeated using reactive flow only. The position – time history of the leading shock was in excellent agreement. The pressure profiles were similar but not identical, because of the difference in material properties behind the WBL wave and the omission of the von Neumann spike from the WBL profiles (Fig. 1).

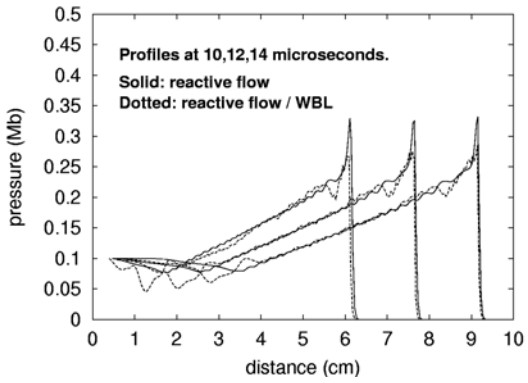

FIGURE 1: PRESSURE PROFILES FOR SINGLE-SHOCK INITIATION WITH FULL REACTIVE FLOW AND WITH THE WBL LINK.

The calculation ran with the first set of parameters tried, but the programmed burn portion of the detonation was found to be sensitive to the trigger delay, and could run stably ~10% slower than the CJ speed, accelerating only very gradually, for a wide range of parameter values. This happened even though a CJ detonation had been established in the region of full reactive flow. It was found that the trigger delay could be significantly smaller than C_0; in fact this seemed necessary in order to minimise the perturbation to the flow induced by the transition from a detonation dominated by reactive flow to one dominated by programmed burn but with a mismatch in arrival time. A value ~0.1 μs worked well and the detonation speed matched the CJ speed accurately over a fairly wide range of trigger delays of the same order.

Reflected shock initiation

As a more interesting test, we simulated the shock-to-detonation transition on reflection of a weak shock from a rigid boundary.

As with the single-shock initiation, programmed burn should not be expected to take over from reactive flow significantly in plane geometry. The hand-off was enforced as before by modifying the ignition and growth rates in part of the explosive so

inhibit reaction. In this case, it was the region nearer to the rigid wall which was fully reactive.

For initiation from a reflected shock, the value of ψ_s was of course important. Reasonable results were obtained for $\psi_s \sim 0.8$ μs.

The position – time history of the leading shock was in good agreement (Fig. 2). The pressure profiles varied much more than in the single-shock case. This is probably because the WBL calculation imposed the same state at the end of the detonation zone as was used in the single-shock simulation. The solution would be to allow this imposed state to vary with the state of the material into which the detonation is running, which could be calibrated by careful reactive flow simulations. (Fig. 3.)

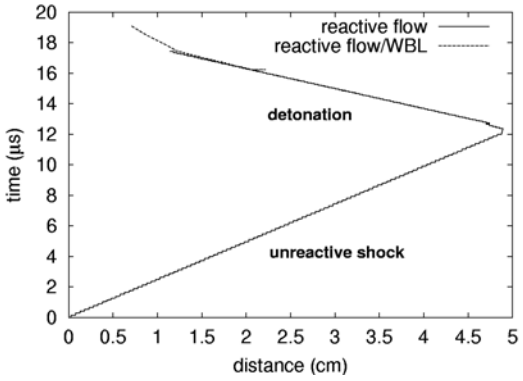

FIGURE 2: SHOCK LOCATION FOR REFLECTED SHOCK INITIATION.

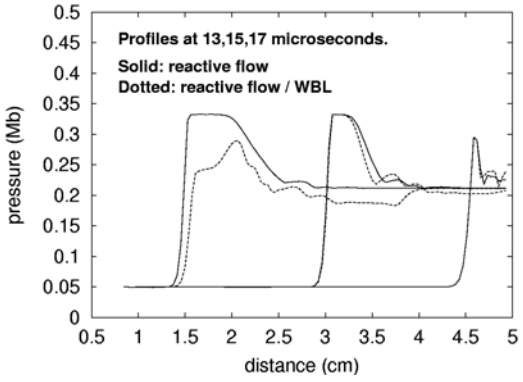

FIGURE 3: PRESSURE PROFILES FOR REFLECTED SHOCK INITIATION WITH FULL REACTIVE FLOW AND WITH THE WBL LINK.

It should be noted that the Tarver form of ignition and growth model is not suitable for multiple-shock initiation. The calculations described here are intended only to demonstrate the calculational principle, not to provide accurate simulations for any particular explosive.

APPLICATION TO EDC37

Here we present a preliminary application of the WBL/reactive flow link applied to the HMX-based explosive EDC37.

The "coarse mesoscale" temperature-dependent reactive flow model [12,13] was used to predict a D(K) relation by a variant of the quasisteady curved-geometry technique previously used with simpler reaction rates [2]. For a steady flow, the conservation equations in 1D curved geometry are

$$\rho w' + w\rho' + \rho\sigma = 0$$
$$\rho w w' + p' = 0$$
$$p w' + \rho w e' + p\sigma = 0$$

where w is the particle speed relative to the leading shock, σ is a curvature term,

$$\sigma = \alpha(D - w) / (Dt - y),$$

D is the detonation speed, t the time since the wave set out from the origin, α is a curvature switch (0 for plane, 1 for cylindrical, 2 for spherical), and priming denotes differentiation with respect to distance behind the leading shock. These equations can be closed with the addition of the material model, by substituting

$$p' = \partial p/\partial e|_\rho e' + \partial p/\partial \rho|_e \rho'.$$

Given a value for the detonation speed, the Rankine-Hugoniot equations were solved to find the von Neumann state in the explosive, then the steady flow equations were solved to find the curvature which gave a stable sonic state as described previously [2] – a shooting problem.

D(K) relations for EDC37 have been deduced from the steady shape of waves in rods and slabs of the explosive [4,14]. By comparison, the relations predicted using the reactive flow model exhibited similar features, but did not follow the empirical relations closely (Fig. 4). This might reflect inaccuracy in the reaction rates at the states generated in full detonation, or it could indicate

that acceleration terms should be included in the WBL parametrisation for EDC37 – these issues will be addressed in future studies. The broad agreement is nevertheless quite encouraging.

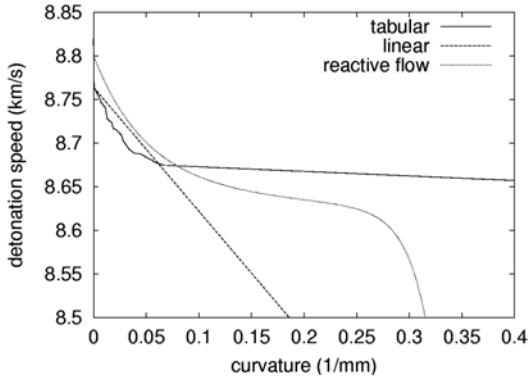

FIGURE 4: DETONATION SPEED -- CURVATURE RELATIONS FROM WAVESHAPE MEASUREMENTS AND FROM REACTIVE FLOW MODEL

The 1D reactive flow simulations allowed us to tabulate the state of the reacting EDC37 as a function of distance behind the leading shock, and as a function of curvature. This data – which can be approximated with smooth functions for convenience if desired – was used to supply the states imposed on the reactive flow field by the passage of the detonation wave in the WBL simulation, and hence to make the programmed burn consistent with a detonation wave moving with variable speed. The state imposed on the flow field was that at the sonic surface, where for a curved wave reaction was incomplete. The reactive flow equations were then used to integrate the last portion of the reaction. If significant, rarefactions could quench this part of the reaction, leading to a lower amount of work from the explosive. The tabulation of states with curvature and position within the reaction zone should allow us to perform calculations with meshes smaller than the detonation zone seamlessly, i.e. with no need to adjust the model.

DISCUSSION

Used correctly, the WBL model can provide both computational efficiency and greater accuracy than pure reactive flow simulations. For the simplest reactive flow models, where the explosive is not modelled as a mixture of species and where no mechanical or thermal equilibrium is required, coupled WBL calculations may not save much time compared with a well-optimised reactive flow calculation. The reaction rate in the hydrocode should be limited so that the detonation wave takes more than one timestep to cross a computational cell. However, if the reactive flow model includes sub-cell processes then it is probably more efficient to calculate the propagation of the detonation wave using the WBL model, and convert explosive to detonation products without the need to consider intermediate states of mixed composition.

Unless the reactive flow simulation has a resolution of at least several computational cells across the detonation zone, it is likely to overpredict the effect of curvature on the speed of the detonation wave. The WBL model can provide significantly greater accuracy in simulating the propagation of detonation waves of changing curvature.

The WBL model does not necessarily provide the same level of accuracy in predicting mechanical forces. As implemented here, it omits the von Neumann spike and thus underpredicts the impulse delivered by the detonation zone. "Traditional" programmed burn at constant speed also omits the details of the detonation zone. It would be possible to extend the WBL model even further to include a pressure – distance relation inside the detonation zone, as a function of wave curvature.

CONCLUSIONS

Modifications to the level set method were developed to allow a level set calculation to be performed in parallel with a hydrocode simulation, using the same computational mesh. We concentrated on methods appropriate for Lagrangian hydrocodes, where it was necessary to introduce an advection term in the level set equation.

A modified level set scheme was implemented in a 1D Lagrangian hydrocode in order to investigate the coupled solution of reactive flow and WBL equations. The implementation included a prototype model of energy release in a WBL simulation.

Simulations of CJ detonation from a pre-defined initiation point were at least as accurate as achieved by previous WBL/PSC codes. Simulations of detonation following single-shock initiation matched the corresponding full reactive flow simulations extremely well in terms of shock

arrival time and reasonably well in terms of pressure profile. Simulations of initiation from a reflected shock were similar to the full reactive flow calculation in terms of shock arrival time, but varied more significantly in terms of pressure profile. The discrepancy was probably because the WBL simulations imposed the same state at the end of the detonation zone in the reflected shock case as was used in the CJ case.

Programmed burn with a detonation of variable speed was made consistent with the flow behind, using reactive flow to treat reactions occurring behind the sonic surface. A reactive flow model for the HMX-based explosive EDC37 was used to calibrate this "energy release" model. Predictions of the relation between detonation speed and curvature indicated that some further work is desirable to improve the reactive flow model at high pressures.

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