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Abstract. For non-ideal explosives a wide range of behavior is observed in experiments dealing with differing sizes and geometries. A predictive detonation model must be able to reproduce many phenomena including such effects as: variations in the detonation velocity with the radial diameter of rate sticks; slowing of the detonation velocity around gentle corners; production of dead zones for abrupt corner turning; failure of small diameter rate sticks; and failure for rate sticks with sufficiently wide cracks. Most models have been developed to explain one effect at a time. Often, changes are made in the input parameters used to fit each succeeding case with the implication that this is sufficient for the model to be valid over differing regimes. We feel that it is important to develop a model that is able to fit experiments with one set of parameters. To address this we are creating a new generation of models that are able to produce better fitting to individual data sets than prior models and to simultaneous fit distinctly different regimes of experiments. Presented here are details of our new Piece Wise Linear reactive flow model applied to LX-17.

Keywords: Detonation modeling, reactive flow
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INTRO

Non-ideal explosives experiments dealing with differing sizes and geometries exhibit a wide range of behavior [ref??? 1-2]. The cause behind this is that the experiments sample different regions of the phase space of detonation waves. Most applied detonation modeling is done using program burn models with phenomenological equations of state or simple reactive flow models [3-5]. These models have been developed to explain one effect at a time. Often, changes are made in the input parameters used to fit each succeeding case, with the implication that this is sufficient for the model to be valid over differing regimes. For predictive capabilities we feel that it is important to develop detonation models that are able to fit all experiments with one set of parameters. Such a model should be able to reproduce the many observed phenomena including: variations in the detonation velocity with the radial diameter of rate sticks, slowing of the detonation velocity around gentle corners, production of dead zones for abrupt corner turning, failure of small diameter rate sticks, failure for rate sticks with sufficiently wide cracks, and initiation.

The JWL++ model [3] was developed in order to model prompt detonation with a Reactive Flow model that would produce satisfactory answers while minimizing the number of coefficients. JWL++ added kinetics to prompt detonation, i.e. the time-dependence of the explosive's chemical reaction, while retaining a very simple format. In JWL++ two species (reactant and product) were treated. These were related through one rate equation, which gave the rate of change in the product species. The rate equation used had the form

$$\frac{dF}{dt} = G_O (P+Q)^B F^A (1-F)^C , \quad (1)$$

where F is the product species mass fraction, P is the pressure, and Q is the numerical artificial viscosity. The constants G_O, A, B, and C are model parameters. For typical usage, A = 0 and C = 1 were used. For the reactant species a Murnahan equation of state (EOS) was used. The EOS for the product species was taken to be in the JWL ABC format which is purely density dependent.

This simple model was found to be able to roughly describe a wide range of explosive phenomena. It was applied to a variety of experiments that explore different detonation wave regimes, such as size effect detonation velocity variations for rate sticks, rate stick failure, crack failure, detonation wave corner turning dead zone production, and corner turning surface breakout timing. What was found was that different model parameters were needed for the same explosive to accurately describe different experiments or possible even different aspects of the same experiment. Additionally we found that rate stick size effect curves suffered excessive downward curvature unless the pressure power-law dependence was nearly linear. From examinations of simulations with JWL++ of experimental conditions we concluded that the assumptions that the rate law varies with pressure as a simple power law and that the mass fraction form factor parameter C should be ≤ 1 needed to be re-examined.

We present here an extension of the JWL++ model that we call the Piece Wise Linear (PWL) model that replaces the pressure power law dependence with a general piecewise-liner functional form calibrated using experimental data. A mass fraction term of the factor $(1 - F)^{3/2}$ was found to strongly remove downward curvature effects for rate stick modeling. For LX-17 we demonstrate the high accuracy this rate model exhibits in reproducing a wide range of explosive data

The PWL Model

As with the JWL++ model, we desire to keep the form of the PWL rate model as simple as possible. The simplest form for the reaction rates is that of a single step decomposition rate. In PWL the form used is that of a piecewise linear depend pressure

$$\frac{dF}{dt} = G(P+Q)(1-F)^C . \quad (2)$$

The function G(P+Q) is the piece-wise linear function

$$G(x) = \sum_{i=1..N} \Gamma_i , \quad (3$$

where

$$\Gamma_i = G_{i+1} \frac{(x - x_i)}{(x_{i+1} - x_i)} + G_i \frac{(x_{i+1} - x)}{(x_{i+1} - x_i)} . \quad (4)$$

for $x_i < x < xi_{+1}$ and is zero otherwise. Here x represents P + Q. The coefficients G_i are determined by calibration with experiments. We again use the sum of the physical pressure P plus the numerical artificial viscosity stability term Q in the rate as this the actual pressure applied. The artificial viscosity term is significant only in one or two spatial zones in front of the detonation wave. For a very fine mesh the artificial viscosity term is insignificant and its inclusion aids in making the rate model less mesh dependent.

What greatly aided the G_i calibration process was the observation that as a detonation wave front weakens there is a corresponding decrease in both the peak pressure and the pressure at the end of the reaction zone. Detonation wave properties were found to be very weakly dependent upon the rate value at pressures significantly lower those within the reaction zone. A given strength detonation wave thus is sensitive only to a narrow range of pressures in our rate law. Rate stick and corner turning experiments were used to cover conditions from pure shock waves in the unreacted material to near planar detonation waves.

Calibration was started using steady state rate stick size effect detonation velocity data. We started using the smallest radii data for cases just above failure. This represents the weakest rate stick detonation wave. We started with a P^3 variance for G(P+Q) up to the first G_i corresponding to a P + Q value slightly lower than the weakest rate stick reaction zone value. Results for steady detonations were weakly dependent upon this pressure regime. G_i values for P + Q spanning the reaction zone range were then adjusted to fit the experimental detonation velocity. G_i values for higher P + Q were set to a constant value equal to the highest G_i used in the fitting. Increasingly larger rate sticks were used to calibrate sequentially larger G_i. The low pressure portion of the rate law was calibrated using breakout timing data from the CTX corner turning experiment [6]. In this experiment the detonation wave from a hemispherical TATB booster tries to turn around an air well and a permanent dead zone of unreacted explosive forms that can be seen by X-ray transmission. Simulations show that the break-out timing data covers regions consisting of strong detonation waves through transient detonation waves and weak shock waves. The corner turning calibration led to a low pressure cut-off, below which the burn rate is zero. We used this cur-off pressure as ignition trigger to start the burn process transforming the reactant into the product species.

Weak shocks are known to desensitize energetic materials making them more difficult to ignite. To account for the unburned dead zone observed in corner turning experiments we added a second rate of the form,

$$\frac{dF_I}{dt} = G_D F_R \tag{5}$$

which converts the unreacted explosive to an inert material. Here the parameter G_D is taken to be constant below a specified pressure P_0, and zero above this pressure Thus, the two processes are mutually exclusive. In Eq. 5, F_I is the inert species mass fraction and $F_R = 1 - F_I - F$ is the reactant species mass fraction.

In the mass fraction dependence in the PWL model, $(1\text{-}F)^C$, we have dropped the F^A term which corresponds to the assumption of the formation of many hot spots covering the whole surface of each grain. Typically the C parameter in the mass fraction form factor is chosen to be between 2/3 – 1. The value of 2/3 corresponds to inward burning of grains from hot-spots. The value of unity would be expected for a simple first order chemical reaction. However, when applied to cylindrical rate sticks, this rate of C can lead significant downward curvature for the size effect. Values of C greater than unity lead to an enhanced reduction in the rate as most of the explosive is consumed. This simulates the effect of a multi-step chemical rate model with the late time rate time scale longer that the initial rate time scale. LX-17 does appear to have a longer time scale phase behind the detonation front due to carbon kinetic effects [7]. In our modeling here we therefore fix C = 3/2.

As was the case for the JWL++ model, the PWL model uses a separate equation of state for each species and combines the resulting partial pressures using mass fraction weighting. The three species used correspond to the initial reactant species, an inert version of the reactant species, and a product species. The transformation of the reactant to the inert material is initiated by a weak shock, and lessens the ability for a second stock to develop into a detonation wave.

The equations of state models used in PWL are of the same form as those used in JWL++. For the reactant we used a Murnahan EOS. The EOS pressure for the inert species is assumed to be the same as for the reactant. For the product a JWL EOS in the C-term density only form was used.

The rate model was implemented in a 2D ALE hydrodynamics code used to simulate experiments.

Results

We give here an example for the PWL model calibrated to LX-17 data. Figure 1 shows G(P+Q). The sharp drop in G below 0.35 Mbar corresponds to the onset of failure for small diameter rate sticks. The very low pressure behavior is roughly proportional to P^3 below 0.2 Mbar. The G function has a cut-off at 0.08 Mbar below which the burn rate in Equation (2) is zero and desensitization takes place. We found the use of $G_D = 1$ to reproduce long time dead zone densities found in the CTX experiment.

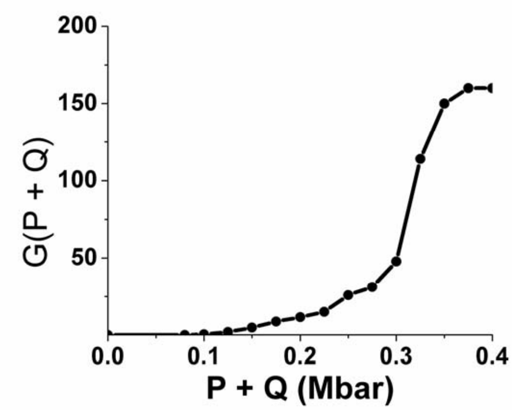

Figure 1. Piece Wise Linear calibrated rate function for LX-17. The burn rate is zero below the cut-off pressure of 0.08. The desensitization rate has a value of $G_D = 1$ and is applied below the cut-off.

In Figure 2 we compare the calibrated detonation velocities for LX-17 with experimental data [8]. Calibration was done using data only for the confined cases. Excellent agreement is given for the unconfined results. Note the abrupt failure achieved for both confined and unconfined systems. The results for simulations of the CTX experiment are given in Figure 3. Very good agreement is seen between data and the PWL results calibrated for the CTX configuration without a steel liner surrounding the air gap. CTX data for LX-17 however does not show any significant sensitivity to the presence of the liner. The PWL model predicts that a faster corner turning with the steel liner.. Further work needs to be done to determine if this is a model deficiency or due to a problem with the experimental data analysis.

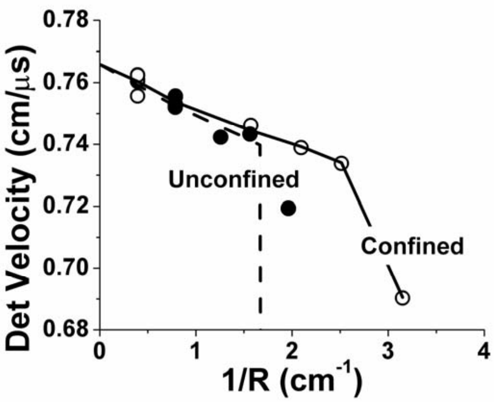

Figure 2. Rate stick detonation velocities for LX-17 comparing the PWL model (solid and dashed curves) with data (circles).

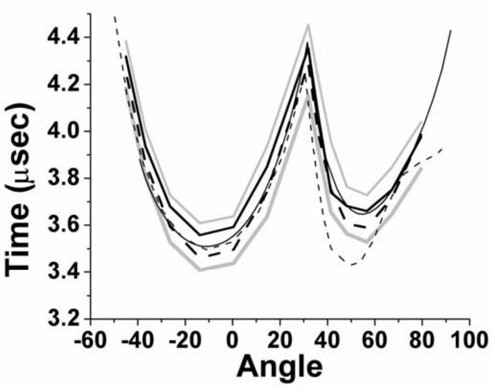

Figure 3. Break out timing for CTX experiment for LX-17. PWL results for the cases without steel (thin solid line) and with steel (thin dashed line). Experimental data are shown as thick lines.

CONSLUSIONS

Early calibration results of the Piece Wise Linear reactive flow model have shown that it gives very accurate agreement with data over a broad range of detonation wave strengths. Calibration of the pressure variation of the rate shows the non-linear structure of the detonation burn rate. Abrupt failure of small rate sticks is shown to be a feature caused by the rapid decrease in burn rate with decreasing pressure. Transient corner turning behavior is determined by the low pressure component of our rate model which includes a pressure cut-off below which the explosive is desensitized.

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