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PORTING INITIATION AND FAILURE INTO LINKED CHEETAH

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Abstract. Linked CHEETAH is a thermo-chemical code coupled to a 2-D hydrocode. Initially, a quadratic-pressure dependent kinetic rate was used, which worked well in modeling prompt detonation of explosives of large size, but does not work on other aspects of explosive behavior. The variable-pressure Tarantula reactive flow rate model was developed with JWL++ in order to also describe failure and initiation, and we have moved this model into Linked CHEETAH. The model works by turning on only above a pressure threshold, where a slow turn-on creates initiation. At a higher pressure, the rate suddenly leaps to a large value over a small pressure range. A slowly failing cylinder will see a rapidly declining rate, which pushes it quickly into failure. At a high pressure, the detonation rate is constant. A sequential validation procedure is used, which includes metal-confined cylinders, rate-sticks, corner-turning, initiation and threshold, gap tests and air gaps. The size (diameter) effect is central to the calibration.

Keywords: size effect, diameter effect, detonation velocity, detonation energy, cylinder test
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INTRODUCTION

To model dead zones with code stability, we developed the Tarantula reactive flow model which uses different rate/pressure relations in different pressure regimes. The model previously used burn fraction/pressure analytic functions [1], but the Piece-Wise Linear Fit does the same with point-by-point input [2]. Both were imbedded in the simple reactive flow model JWL++ [3]. We have converted the model to run in Linked Cheetah [4], which uses a 2-D CALE-type finite difference ALE code, that relaxes its mesh in an Eulerian manner in specific regions away from where the measurements are taken. Cheetah itself is a thermo-chemical code which uses exponential-6 and modified Murnahan models combined with calibration against Hugoniot data [5]. Our modeling was confined to LX-17 and square zones at 4 zones/mm were used throughout.

MODEL DESCRIPTION

The current Tarantula version uses a point-by-point description of the reaction rate versus pressure curve, with linear interpolation between points. An initiation region has now been added. Equation 1

$$\frac{dF}{dt} = G(\tilde{P})(1-F)^{C(\tilde{P})} \tag{1}$$

shows the rate form, where F is the burn fraction, and G and C are functions of the effective pressure, $\tilde{P} = P + Q$, with Q being the numerical artificial viscosity. The G and C functions are determined by calibration through comparison of model detonation results with experiments. In the Piece-Wise Linear Fit implementation, values for G and C are given at specific $\widetilde{P}$ points, with linear interpolation being used to determine other values.

Several effective rate curves, without a 1-F term, are shown in Figure 1. The dotted line is a simple pressure-squared rate with a rate constant of 0.025 (μs GPa^2)$^{-1}$. There is nothing in this simple curve to account for any rate deviation from turning-on to full detonation. The Tarantula curves change abruptly in different pressure regions. At pressure below the 10 GPa in the Threshold region there is no reaction. Above 10 GPa, a slow Initiation reaction region begins with a pressure-squared variation. At about 24 GPa, the rate jumps upward toward in the Failure region. At higher effective pressure above the Failure region is the Detonation region. We found that a constant rate can be used to describe strong detonation propagation. The upper solid Tarantula model curve is the official one used for this report. We recall that the Ignition & Growth reactive flow model also has discontinuous rates, but there the abrupt rate changes occur as a function of burn fraction [6].

In each Tarantula region, the rates take the specific form

$$\frac{dF}{dt} = G_i(\widetilde{P} - P_i^o)^{b_i}(1-F)^{c_i} \qquad (2)$$

where t the time, G_i is the rate constant in region i, P_i^o is the pressure threshold, b_i the pressure exponent and c_i the mass fraction exponent. For the solid curve in Fig. 1 the rate constants are: G_i = (0, 0.025, 0.32, 40), B_i = (0, 10, 10, 10), b_i = (2, 2, 1.75, 0), c_i = (1, 1, 1, 1.5). For the dashed curve the corresponding values are: G_i = (0, 0.025, 0.011, 40), B_i = (0, 10, 10, 10), b_i = (2, 2, 2.7, 0), c_i = (1, 1, 1, 1.5). Units for G_i are in μs^{-1}. The higher exponent value for c_i used in the Detonation regime reduces downward curvature in plots of rate stick size effect curves, resulting in a nearly straight line. By reducing b_i to less than 1 in the Failure regime, the failure curve can be brought lower to make a better looking curve, but the overall agreement with experiment are similar.

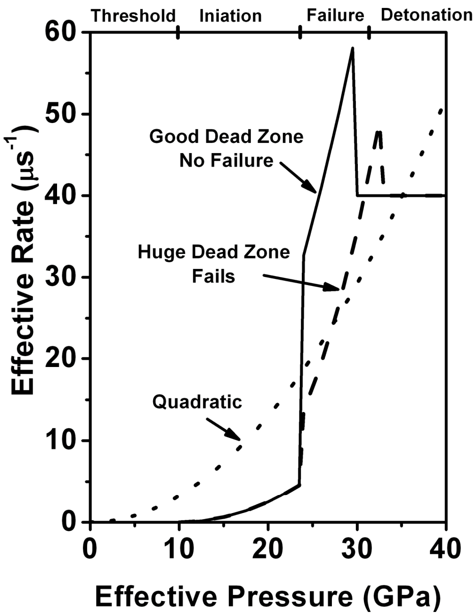

Figure 1. Effective reaction rates for the Tarantula model and a simple quadratic model (dotted). The four rate regions are listed at the top. The higher solid line gives good dead zones but no failure. The lower dashed line gives good failure but too-large dead zones.

The use of a multi-pressure rate model is not new, and this model was inspired but differs from the CpeX model of Leiper and Cooper [7, 8]. What makes the process different here, besides the emphasis in failure, is the extensive use of calibration experiments with the basic ones being listed in Table 1. It is important to list the results obtained for all tests without changing any coefficients. All runs are done at 4 zones/mm with square zones. Care should be taken to make sure these mesh resolution conditions are met, because zoning below 2.5 zones/mm will cause the model to fail.

In JWL++, the JWL is so constructed that the Cylinder test energies and the infinite-radius detonation velocity are automatically incorporated. This does not happen in Cheetah, where 12.7 mm-radius cylinders must be run to set the starting calibration. Because of the symmetry of the TATB molecule, Cheetah predicts reaction products that pass through a mythical CHNO radical phase, which is highly sensitive to the molecular size. Also, our kinetic model contains a carbon reaction, which slowly reacts from small carbon clusters to large ones [9]. Because small carbon is a primary product in the model, the value of the heat of formation of this soot-like material is critical. For a detonation G_4 of 40 μs^{-1}, a CHNO size of 42.8 nm and a small carbon heat of 60 kJ/mol are used for the initial calibration. In Table 1, the top set of basic tests contains the cylinder detonation velocity and energy as a necessary start.

Once this is done, the settings can be found with only a few more of the Table 1 basic tests. G_2 is quickly set by running the 12.5 GPa time-to-detonation. The rest of the size effect curve in is set using G_3 determined by the detonation velocity of the 4 mm copper cylinder, which is the closest to failure. If failure occurs, then the 3 mm cylinder should not propagate. The corner-turn calibration is done using the double cylinder with the steel backing plate. Once the value of G_3 is obtained, the G_2 value must be rechecked for small changes. The requirement that all these experiments fit as much as possible constrains the model so that the answer is about as closed as a hydrocode ever gets. The result is an absence of "knobs" for further adjusting the model.

As a detail, the double cylinder model is initialized using either program burn or a simple JWL++ booster of LX-14 at 1.78 g/cm^3. Clearly, the new detail used for the main charge will require better modeling of the booster.

Not everything works. A breakdown occurs with the 17.5 GPa time-to-detonation, where the model jumps too quickly out of initiation. There is some evidence that this may improve with increased zoning. The worst problem is that cylinder failure and dead zone formation cannot be optimized together with the same setting. Previously, we assumed that both occurred because of failure, but it appears that different mechanisms may be involved. As seen in Figure 1, the upper curve does dead zones well but cylinder failure does not occur. The lower curve does cylinder failure perfectly, but the dead zones are too large. It is possible to go in-between and not do either one well. Changing parameters produces the same outcome. It appears that the conditions for dead zones are weaker than for cylinder failure. It also seems that the entire failure region causes either dead zones or failure, and they cannot be allocated to specific pressures inside Failure region.

The Tarantula model is zone-dependent. In going to 8 zones/mm with P_i^o fixed, G_2 and G_4 stay the same but G_3 drops from 0.12 to 0.092. The zoning at which G_3 becomes a true constant is unknown.

Table 1. Basic validation experiments for calibration of the Tarantula model. The regions are: 2. initiation, 3. failure, and 4. detonation. The upper curve in Fig. 1 is used and the tests are graded.

Region	Experiment	Measured Result	Grade
2	12.5 GPa run-to-detonation time	1.7-2.2 μs	A
3	3 mm, 2 mm copper cylinder	fails	C
3	double cylinder with steel corner turn	cf. breakout times	A
4	4 mm, 2.25 mm copper cylinder, det velocity	7.33-7.35 mm/μs	A
4	12.7 mm FW Cu cylinder, det velocity	7.54-7.56 mm/μs	A
4	12.7 mm FW Cu cyl., wall velocity @ 10 μs	1.37-1.43 mm/μs	A
4	12.7 mm FW Cu cyl., wall velocity @ 20 μs	1.44-1.50 mm/μs	A

JUSTIFICATION OF THE COEFFICIENTS

We now consider where some of the input numbers come from. The pressure threshold, determining the range of the Threshold region, is the asymptotic pressure threshold measured in flyer experiments, run-to-detonation and gap tests, which arrive at a value somewhere between

7.5 and 9 GPa [10]. Our choice of 10 GPa is set to get code agreement at our zoning, with a lower value being possible at increased zoning. The quadratic power of the pressure in the initiation region comes the critical energy E_{cr} equation

$$E_{cr} = \frac{\left(P - P^{o}\right)^{2}\tau}{\rho_{o} U_{S}} \qquad (3)$$

used for initiation, where τ is the pulse length.

P_3 is the pressure boundary between the Failure and Detonation regions, and we expect it to be roughly the failure pressure. If we use the rule-of-thumb [11],

$$P_{3} \approx \left(\frac{U_{S}(fail)}{D}\right)^{2} P_{m}^{o} \ , \qquad (4)$$

where we have 7.66 mm/μs for the infinite-radius detonation velocity, D, and about 7.3 mm/μs at failure. The infinite radius spike pressure, $P_m{}^o$, which is calculated from Cheetah, is perhaps 1.4 times 26 GPa or 36 GPa, so that P_3 here is about 33 GPa.

The initiation rate constant, G_4, can be estimated from size effect data [11]. Assuming that the pure detonation rate is pressure-independent

$$G_{4} = <\nu> \approx \frac{-D^{2}}{\partial U_{S} / \partial (1/R_{o})} \ , \qquad (5)$$

Which results from model calculations to a rate of ~40 μs^{-1}. The failure rate constant, the most sensitive of all parameters, is found by adjustment, mostly from the 4 mm copper-confined cylinder. This is the closest size to failure that detonates, so that locking this in sets the rest of the size effect curve. The pressure that borders between the Initiation and Failure regions is guessed at, but a value may come someday from run-to-detonation gauge records.

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