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<b>Report title (In translation)</b> On calibrating reaction rate laws using detonation shock dynamics		
<b>Abstract (not more than 200 words)</b> A computer code has been developed that solves the flow equations in the reaction zone between the leading shock front and the sonic plane for a detonating high explosive. The code is based on the Detonation Shock Dynamic theory, which is valid for weakly curved self-sustained detonations. From measured relations between the detonation velocity and shock curvature, a reaction rate law can be calibrated in an efficient way.		
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<b>Rapportens titel</b> Kalibrering av brinnekvationer för fasta explosivämnen med detonationsstötdynamik.		
<b>Sammanfattning (högst 200 ord)</b> <p>En datorkod för beräkning av flödet i reaktionszonen i ett detonerande sprängämne har utvecklats. Koden baseras på teorin för svagt krökta detonationer. Från uppmätta relationer mellan detonationshastigheten och detonationsfrontens krökning kan en brinnekvation kalibreras på ett effektivt sätt.</p> <p>En kalibrerad brinnekvation är av vikt vid simuleringar av vapenverkan och ammunitionssäkerhet för vapensystem som innehåller okänsliga sprängämnen. Dessa uppträder ofta icke-idealt, vilket innebär att reaktionszonens storlek påverkar sprängämnets uppträdande. Detta gör att enklare modeller som förutsätter en omedelbar omsättning av sprängämne till spränggaser ej kan användas. Genom att inkludera en brinnekvation i detonationsmodellen kan inverkan av reaktionszonens ändliga utbredning beskrivas på ett fysikalisk sätt, t.ex. kan funktionssäkerhet och ammunitionssäkerhet simuleras med avseende på beskjutning och liknande mekaniska stötförlopp.</p>		
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# 1 Introduction

Insensitive high explosives have become increasingly more important due to the stricter requirements for ammunition safety. They are non-ideal in the sense that the reaction zone is so broad that initiation and size effects can't be neglected. To accurately simulate the propagation of a detonation in a non-ideal explosive, the physics in the reaction zone must be properly described. This can be accomplished by incorporating a reaction rate law, which describes the conversion of explosive to reaction products, in the hydrodynamic equations. Thus, to predict performance and safety aspects for weapons containing insensitive explosives, a carefully calibrated reaction rate law is needed.

To directly measure reaction rates is very difficult, which suggests that an indirect method should be used. A well-established method relies on the fact that the detonation velocity for a cylindrical charge depends on the charge diameter. For finite charges, radial flows will curve the detonation front, which leads to incomplete reaction in the reaction zone. A lower reaction rate implies a larger curvature and lower detonation velocity. By measuring the curvature and velocity of the detonation front for several different charge diameters, a reaction rate law can be constructed. In a direct method, the detonation process is simulated in a hydrodynamic computer code where the reaction rate law contains a number of parameters. The parameters are adjusted until agreement with measurements is reached. Such a method is very time consuming, considering the large amount of simulation that must be done and output files which must be analyzed to completely parameterize a reaction rate law. In this work, a one-dimensional code will be presented that calculates the flow in the reaction zone for a weakly curved self-sustained steady detonation. The code is based on the Detonation Shock Dynamics (DSD) theory [1], which has its origins in the pioneering works by Wood & Kirkwood [2] and Bdzil [3] who extended the ZND theory for plane detonations to weakly curved detonations. The advantage with this code is that a large number of simulations can be performed in a short time. A typical run for thousands of different parameter values and ten different charge diameters only takes a few minutes.

In section 2, the governing equations for steady two-dimensional flow in the reaction zone are presented and it is shown how these can be rewritten as a system of ordinary differential equations. In section 3 follows a discussion on the equation of state for a reacting media. In section 4 the one-dimensional code for calibrating reaction rate laws to experimental curvature-velocity measurements are presented. In section 5 the results from the one-dimensional code are compared with results from a full two-dimensional simulation using the hydrodynamic computer code DYNA2D [4]. Finally, the results are summarized in section 6.

## 2 Flow equations for steady weakly curved detonations

If viscosity and heat transfer are neglected, the flow in the reaction zone is given by the Euler equations, which follows from the laws of mass conservation

$$\frac{d\rho}{dt} + \rho \nabla \cdot \vec{u} = 0, \quad (1)$$

momentum conservation

$$\rho \frac{d\vec{u}}{dt} + \nabla P = 0, \quad (2)$$

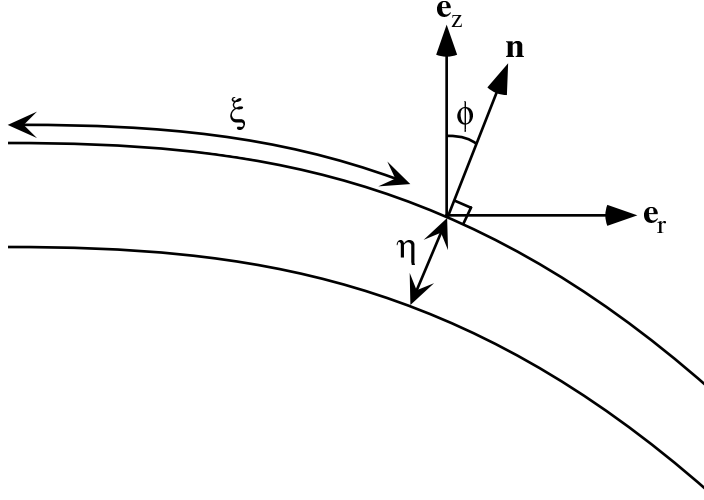


Figure 1: The shock attached coordinates.

and energy conservation

$$\frac{dE}{dt} - \frac{P}{\rho^2} \frac{d\rho}{dt} = 0. \quad (3)$$

Here  $\rho$  is the density,  $P$  is the pressure,  $\vec{u}$  is the flow velocity,  $E$  is the specific internal energy and  $d/dt = \partial/\partial t + \vec{u} \cdot \nabla$  denotes the total time derivative. In the present work it is assumed that the reaction is described by a single variable  $\lambda$ , the burn fraction, which is the mass fraction of the explosive that has reacted. The decomposition of explosives is governed by a rate law

$$\frac{d\lambda}{dt} = R(\rho, P, \lambda), \quad (4)$$

and the equation of state is expressed as

$$E = E(\rho, P, \lambda). \quad (5)$$

Now consider a detonation wave moving in a cylindrical charge with constant velocity  $D_0$  along the  $z$ -axes and introduce a shock-attached coordinate system  $(\xi, \eta)$  moving with the front. Here  $\xi$  is the arc-length along the shock and  $\eta$  is the distance behind the shock measured along the extension of the local shock normal, see Fig. (1). It is also convenient to define the angle  $\phi$  that the shock normal makes with the  $z$ -axis and the total curvature defined by

$$\kappa = \frac{d\phi}{d\xi} + \frac{\sin \phi}{r} = \frac{z_s''}{[1 + (z_s')^2]^{3/2}} + \frac{z_s'}{r\sqrt{1 + (z_s')^2}}, \quad (6)$$

where  $z_s(r)$  is the position of the front as function of the radius.

When the flow in the reaction-zone is steady and the radius of curvature is much larger than the reaction-zone length, the Euler equations reduce to a set of ordinary differential equations in one variable [1]

$$(D_n - u_\eta)\rho_{,\eta} - \rho u_{\eta,\eta} + \rho \kappa u_\eta = 0, \quad (7)$$

$$\rho(D_n - u_\eta)u_{\eta,\eta} - P_{,\eta} = 0, \quad (8)$$

$$(D_n - u_\eta)E_{,\eta} - \frac{P}{\rho^2}(D_n - u_\eta)\rho_{,\eta} = 0, \quad (9)$$

$$(D_n - u_\eta)\lambda_{,\eta} = R, \quad (10)$$

where terms of order  $\kappa^2$  have been dropped. Here

$$D_n = D_0 \cos \phi, \quad (11)$$

is the normal component of the detonation velocity.

We will now show that Eqs. (7-10) only permits a continuous solution for certain combinations of  $D_n$  and  $\kappa$ . If the relation

$$E_{,\eta} = E_{,P}P_{,\eta} + E_{,\rho}\rho_{,\eta} + E_{,\lambda}\lambda_{,\eta},$$

is substituted into Eq. (9), the energy conservation law can be written

$$(D_n - u_\eta)P_{,\eta} - c^2(D_n - u_\eta)\rho_{,\eta} + \frac{RE_{,\lambda}}{E_{,P}} = 0, \quad (12)$$

where  $c$  is the frozen sound speed defined by

$$c^2 = \left( \frac{\partial P}{\partial \rho} \right)_{s,\lambda} = \frac{1}{E_{,P}} \left( \frac{P}{\rho^2} - E_{,\rho} \right). \quad (13)$$

Using Eqs. (7) and (8) to eliminate  $\rho_{,\eta}$  and  $P_{,\eta}$  in Eq. (12), a relation called the master equation is achieved:

$$\left[ (D_n - u_\eta)^2 - c^2 \right] u_{\eta,\eta} = -c^2 \kappa u_\eta - \frac{RE_{,\lambda}}{\rho E_{,P}}. \quad (14)$$

At the sonic point where  $c + u_\eta = D_n$ , the left hand in Eq. (14) vanishes and thus we impose the condition

$$\kappa u_\eta + R\chi = 0 \quad \text{when} \quad c + u_\eta = D_n, \quad (15)$$

where we have defined the thermicity coefficient

$$\chi = E_{,\lambda}/\rho c^2 E_{,P}. \quad (16)$$

For given value on  $D_n$  the condition (15) can only be satisfied for an unique value of  $\kappa$ , i. e. Eq. (15) predicts a universal relation  $\kappa = \kappa(D_n)$ , independent of the charge size. The relation is valid not only on the charge axis as in Ref. [2], but along the whole shock front where the assumption of small curvature is valid. The solution which satisfies Eq. (15) is called an eigenvalue solution.

When the relation between the normal detonation velocity and local curvature is known, the shock front shape can be calculated from Eq. (6),

$$r_s(\phi) = \int \cos \phi d\xi = \int \frac{\cos \phi d\phi}{\kappa(D_0 \cos \phi) - \sin \phi/r_s}, \quad (17)$$



$$z_s(\phi) = z_0 + \int \sin \phi d\xi = z_0 + \int \frac{\sin \phi d\phi}{\kappa(D_0 \cos \phi) - \sin \phi / r_s}. \quad (18)$$

If the angle  $\phi_{\text{edge}}$  that the shock normal makes with the  $z$ -axis at the charge edge is known, Eq. (17) results in a relation between the detonation velocity at the charge axis  $D_0$  and the charge diameter  $d = 2r_s(\phi_{\text{edge}})$ . For a bare charge, the edge angle is determined by the condition that the flow behind the shock must be sonic [5],

$$c^2 = (u_{n,\text{edge}} - D_0 \cos \phi_{\text{edge}})^2 + D_0^2 \sin^2 \phi_{\text{edge}}.$$

### 3 Equation of state for reacting systems

The unreacted explosive and the reaction products are described by two separate equation of states (EOS)

$$E(\text{explosive}) = E_e(v_e, P_e), \quad E(\text{products}) = E_p(v_p, P_p),$$

where indices  $e$  and  $p$  denotes the unreacted explosive and the reaction products respectively. We assume that the two phases are in mechanical and thermal equilibrium,

$$T_e(v_e, P) = T_p(v_p, P), \quad (19)$$

and that the specific energy and volume are given by,

$$E(v, P, \lambda) = (1 - \lambda)E_e(v_e(v, P, \lambda), P) + \lambda E_p(v_p(v, P, \lambda), P), \quad (20)$$

$$v = (1 - \lambda)v_e + \lambda v_p, \quad (21)$$

where  $v_e$  and  $v_p$  are given by Eqs. (19) and (21).

Our primary interest here is to calculate various energy derivatives to get the frozen sound speed  $c$  and the thermicity coefficient  $\chi$ , given by Eqs. (13) and (16). Using the chain rule the energy derivatives can be written

$$\frac{\partial E}{\partial v} = (1 - \lambda) \frac{\partial E_e}{\partial v_e} \frac{\partial v_e}{\partial v} + \lambda \frac{\partial E_p}{\partial v_p} \frac{\partial v_p}{\partial v}, \quad (22)$$

$$\frac{\partial E}{\partial P} = (1 - \lambda) \left[ \frac{\partial E_e}{\partial v_e} \frac{\partial v_e}{\partial P} + \frac{\partial E_e}{\partial P} \right] + \lambda \left[ \frac{\partial E_p}{\partial v_p} \frac{\partial v_p}{\partial P} + \frac{\partial E_p}{\partial P} \right], \quad (23)$$

$$\frac{\partial E}{\partial \lambda} = (1 - \lambda) \frac{\partial E_e}{\partial v_e} \frac{\partial v_e}{\partial \lambda} + \lambda \frac{\partial E_p}{\partial v_p} \frac{\partial v_p}{\partial \lambda} - (E_e - E_p). \quad (24)$$

In equations (22-24), the derivatives of  $v_e$  and  $v_p$  appears, which can be obtained by differentiating Eqs. (19) and (21).

#### Constant $P$ and $\lambda$ .

Differentiating Eqs. (19) and (21) for constant  $P$  and  $\lambda$  gives

$$\begin{cases} \frac{\partial T_e}{\partial v_e} \frac{\partial v_e}{\partial v} - \frac{\partial T_p}{\partial v_p} \frac{\partial v_p}{\partial v} = 0, \\ (1 - \lambda) \frac{\partial v_e}{\partial v} + \lambda \frac{\partial v_p}{\partial v} = 1, \end{cases} \quad (25)$$

from which  $\partial v_e / \partial v$  and  $\partial v_p / \partial v$  can be obtained.

### Constant $v$ and $\lambda$ .

Differentiating Eqs. (19) and (21) for constant  $v$  and  $\lambda$  gives

$$\begin{cases} \frac{\partial T_e}{\partial v_e} \frac{\partial v_e}{\partial P} - \frac{\partial T_p}{\partial v_p} \frac{\partial v_p}{\partial P} = \frac{\partial T_p}{\partial P} - \frac{\partial T_e}{\partial P}, \\ (1 - \lambda) \frac{\partial v_e}{\partial P} + \lambda \frac{\partial v_p}{\partial P} = 0, \end{cases} \quad (26)$$

from which  $\partial v_e / \partial P$  and  $\partial v_p / \partial P$  can be obtained.

### Constant $v$ and $P$ .

Differentiating Eqs. (19) and (21) for constant  $v$  and  $P$  gives

$$\begin{cases} \frac{\partial T_e}{\partial v_e} \frac{\partial v_e}{\partial \lambda} - \frac{\partial T_p}{\partial v_p} \frac{\partial v_p}{\partial \lambda} = 0, \\ (1 - \lambda) \frac{\partial v_e}{\partial \lambda} + \lambda \frac{\partial v_p}{\partial \lambda} = v_e - v_p, \end{cases} \quad (27)$$

from which  $\partial v_e / \partial \lambda$  and  $\partial v_p / \partial \lambda$  can be obtained.

## 4 The one-dimensional computer code

A computer code that solves the flow equations in the reaction zone has been developed. The code requires as input a table of experimentally measured  $D_n - \kappa$  values and two equation of states, one for the unreacted explosive and one for the reaction products. The reaction rate  $R$  is assumed to be on the form

$$R = Af(\rho, P, \lambda; \vec{\sigma}), \quad (28)$$

where  $A$  is a rate multiplier and  $f$  is a function which describes the burn model, normalized to some suitable value.  $\vec{\sigma}$  is a parameter vector of rank  $n$  which will be varied to reproduce the measured  $D_n - \kappa$  relation.

If we denote the particle velocity in the shock attached frame by  $w = D_n - u_\eta$  and introduce the burn fraction as the independent variable, the flow equations (7), (8) and (14) can be written in conservative form as

$$\begin{aligned} \frac{d}{d\lambda}(\rho w) &= -\frac{\kappa u_\eta}{R} \rho w, \\ \frac{d}{d\lambda}(P + \rho w^2) &= -\frac{\kappa u_\eta}{R} \rho w^2, \\ \frac{dw}{d\lambda} &= -w \frac{\chi + \kappa u_\eta / R}{1 - (w/c)^2}, \end{aligned} \quad (29)$$

with initial conditions given by the Rankine-Hugoniot relations [6]

$$\begin{aligned} \rho_s w_s &= \rho_0 D_n, \\ P_s + \rho_s w_s^2 &= \rho_0 D_n^2, \\ E(\rho_s, P_s, 0) - E_0 &= \frac{1}{2}(D_n - w_s)^2, \end{aligned} \quad (30)$$

where the subscript  $s$  denotes the value just behind the shock front. Two auxiliary functions  $\psi$  and  $\Phi$  are defined as

$$\psi = 1 - w^2/c^2,$$

and

$$\Phi = \chi + \kappa u_\eta / R,$$

to examine the sonic condition (15). In the reaction zone,  $\psi > 0$  (the flow is sub-sonic) and  $\Phi < 0$  (the chemical energy release is greater than the transverse energy flow), and at the sonic point where  $\psi = 0$  we have the constraint  $\Phi = 0$ .

For given values of  $D_n$  and  $\kappa$ , the code searches for the rate multiplier which permits an eigenvalue solution. Starting with an initial guess  $A = A_0$ , the flow equations (29) are integrated from the shock with initial values given by Eq. (30), using a fourth order Runge-Kutta method. After each integration step the functions  $\psi$  and  $\Phi$  are inspected to check if either  $\psi \leq 0$  or  $\Phi \geq 0$ . If both conditions are satisfied, the rate multiplier is accepted; otherwise the rate multiplier is changed according to the following rule:

1. decrease  $A$  if  $\psi \leq 0$  and  $\Phi < 0$ :  $A_{\max} = A_i$ ,  $A_{i+1} = \frac{1}{2}(A_i + A_{\min})$ ;
2. increase  $A$  if  $\Phi \geq 0$  and  $\psi > 0$ :  $A_{\min} = A_i$ ,  $A_{i+1} = \frac{1}{2}(A_i + A_{\max})$ ;

and a new calculation is performed. Using this scheme for a set of  $M$  different experimentally measured pairs  $\{(D_n, \kappa)\}_k$  gives a set of rate multipliers  $\{A\}_k$ . For a correct reaction rate law the rate multipliers should all take the same value. Hence we define the merit function

$$\Pi = \sum_{k=1}^M \left( \frac{A_k - \langle A \rangle}{\langle A \rangle} \right)^2$$

as a measure of deviation from a constant rate multiplier. A Levenberg-Marquardt algorithm is used to find the parameters  $\vec{\sigma}$  which minimize the merit function.

## 5 Comparison between a full two dimensional simulation and the DSD-code

To test if the one-dimensional DSD-code can be used instead of a full two-dimensional simulation to calibrate reaction rate laws, a numerical experiment has been performed with DYNA2D where the detonation velocity and shock curvature were calculated for a number of different sized cylindrical charges (rate sticks) of the explosive TNT. For the simulations, the DYNA2D equation of state 7 (Ignition and growth of reaction in HE) was used, which contains the JWL EOS described in Appendix A for both the unreacted explosive and the reaction products, and the two-term Ignition and Growth reaction rate law described in Appendix B. The parameters for cast TNT were taken from Ref. [7] and are listed in Table 1. A very fine mesh with 10 elements/mm was used to resolve the reaction zone. The detonation was initiated at one end with a TNT-booster described by a simple programmed burn model. The length of the charge was extended long enough for flow to be stationary at the opposite end, where the arrival times were tracked at eight different points, equidistantly placed along a constant  $z$ -plane. The position of the shock front,  $z_s(r)$ , was fitted to a polynomial in  $r^2$  and the normal component of the detonation velocity and the local curvature was then calculated from Eqs. (6) and (11). The results for five rate sticks with charge radius 30 mm, 15 mm, 10 mm, 6 mm and 5 mm are presented in Fig. 2, together with the

Table 1: Data for cast TNT.

Performance				
$\rho_0$ (cm/cc)	$E_0/v_0$ (Mbar)	$D$ (cm/ $\mu$ s)	$p_{CJ}$ (Mbar)	
1.61	0.07	0.6972	0.21	
Unreacted JWJ				
$A$ (Mbar)	$B$ (Mbar)	$\alpha v_0$	$\beta v_0$	$\omega$
17.98	-0.931	6.2	3.1	0.8926
Reacted JWJ				
$A$ (Mbar)	$B$ (Mbar)	$\alpha v_0$	$\beta v_0$	$\omega$
3.712	0.0323	4.15	0.95	0.3
Specific heat				
$c_v(\text{explosive})/v_0$ (Mbar/K)		$c_v(\text{products})/v_0$ (Mbar/K)		
$2.05 \times 10^{-5}$		$1.0 \times 10^{-5}$		
Ignition term				
$I$ ( $\mu$ s $^{-1}$ )	$a$	$x$	$\mu_c$	$f_{\text{max,ig}}$
50	0.2222	4.0	0.0	1.0
Growth term				
$G_1$ ( $\mu$ s $^{-1}$ Mbar $^{-y}$ )	$b$	$c$	$y$	$f_{\text{max,gr}}$
40	0.222	0.667	1.2	1.0

prediction from the DSD-code. For charges with radius less than 5 mm the detonation failed to propagate. It is clear from these simulations that for  $\kappa \leq 1.5 \text{ cm}^{-1}$ , the points closely follow a single curve in agreement with the DSD prediction. For points close to the critical radius there is a small deviation from the DSD-prediction, but the agreement is still quite good.

## 6 Summary

A computer code has been developed to facilitate the calibration of reaction rate laws using detonation front curvature experiments. The code searches for the functional form of a reaction rate law that best fits the experimental relation between the normal detonation velocity and the local shock front curvature. By using the asymptotic behavior of the flow equations for small curvature, a very fast method to parameterize a reaction rate law is achieved. The present method was inspired by the work in Ref. [8].

With the computing power available today, usage of direct numerical simulations (DNS) is extremely time consuming. To get convergent results with a DNS a very fine mesh is required to resolve the reaction zone, and the simulation must proceed long enough for a steady detonation to be established. If a large number of simulations must be performed, this is not a viable alternative. We think that DNS is mainly useful for verifying a calibrated reaction rate law.

The universal relation between  $D_n$  and  $\kappa$  is only valid to first order in  $\kappa$ . If higher order terms are included in the analysis, a more complex relation exist between  $D_n$  and  $\kappa$ , which also involves the detonation velocity at the charge axis [9],  $\kappa = \kappa(D_n, D_0)$ .

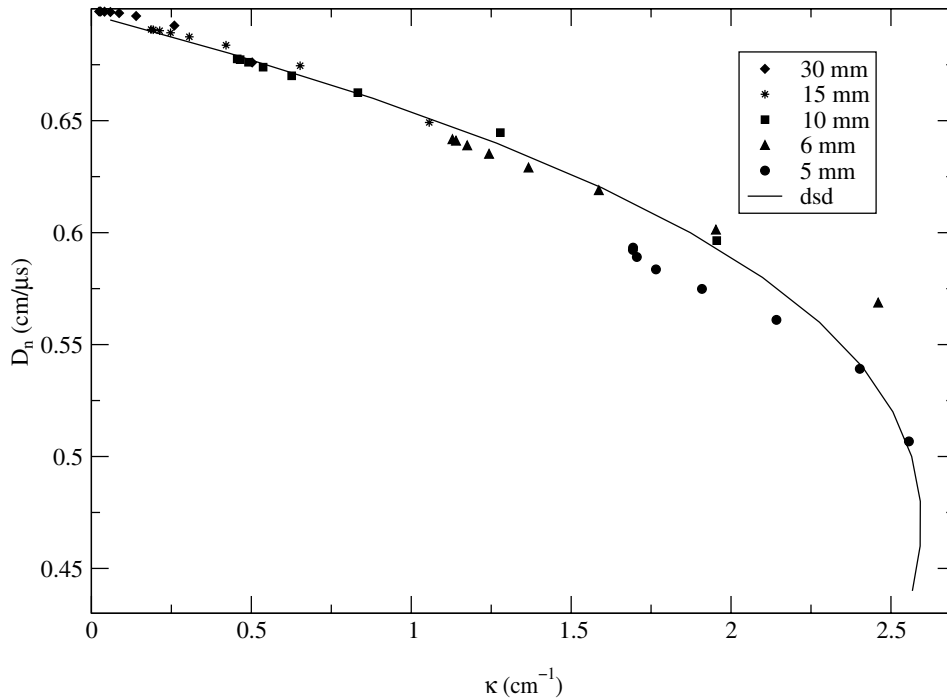


Figure 2: Calculated detonation velocity and curvature for 5 rate-sticks of different radius.

From the numerical experiment in Sec. 5 we found that the different curves almost coincide for TNT. Considering the errors in calculating curvatures from experimental data and the differences from batch to batch, it is doubtful if the more advanced method is more appropriate. We conclude that the described code is a valuable tool to calibrate reaction rate laws.

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## A The JWL equation of state

The JWL is a constant Grunisen gamma equation of state and has the form

$$P = A \left(1 - \frac{\omega}{\alpha v}\right) e^{-\alpha v} + B \left(1 - \frac{\omega}{\beta v}\right) e^{-\beta v} + \frac{\omega}{v}(E - E_0). \quad (31)$$

The pressure can also be written as a function of specific volume and temperature. From the thermodynamic relation

$$\left(\frac{\partial E}{\partial v}\right)_T = T \left(\frac{\partial P}{\partial T}\right)_v - P,$$

and the identity

$$\left(\frac{\partial E}{\partial v}\right)_T = \left(\frac{\partial E}{\partial P}\right)_v \left(\frac{\partial P}{\partial v}\right)_T + \left(\frac{\partial E}{\partial v}\right)_P,$$

it follows that

$$\left(\frac{\partial E}{\partial P}\right)_v \left(\frac{\partial P}{\partial v}\right)_T + \left(\frac{\partial E}{\partial v}\right)_P = T \left(\frac{\partial P}{\partial T}\right)_v - P.$$

Using Eq. (31) to evaluate the energy derivatives we get

$$v \left(\frac{\partial P}{\partial v}\right)_T - \omega T \left(\frac{\partial P}{\partial T}\right)_v + (1 + \omega)P = A(1 + \omega - \alpha v)e^{-\alpha v} + B(1 + \omega - \beta v)e^{-\beta v}.$$

This is a hyperbolic partial differential equation, which can be solved with the method of characteristics. The general solution is

$$P(v, T) = Ae^{-\alpha v} + Be^{-\beta v} + f(v^\omega T)/v^{1+\omega},$$

where the function  $f$  is related to the specific heat at constant volume  $c_v$  through the relation

$$c_v = \left(\frac{\partial E}{\partial T}\right)_v = \left(\frac{\partial E}{\partial P}\right)_v \left(\frac{\partial P}{\partial T}\right)_v = f'(v^\omega T)/\omega.$$

Assuming a constant  $c_v$  we get

$$f = \omega c_v T v^\omega + C,$$

where  $C$  is an integration constant. The pressure and energy can now be written as functions of  $v$  and  $T$  as

$$P = \frac{\omega c_v T}{v} + A e^{-\alpha v} + B e^{-\beta v} + \frac{C}{v^{1+\omega}},$$

$$E = E_0 + c_v T + \frac{A}{\alpha} e^{-\alpha v} + \frac{B}{\beta} e^{-\beta v} + \frac{C}{\omega v^\omega},$$

which, with  $C = 0$ , is the form used in DYNA2D.

## B The ignition and growth model

The reaction rate model used in DYNA2D was suggested by Tarver et. al. [10], which is an extension to the model proposed by Lee & Tarver [7] to model the ignition and growth of reaction in high explosives. The reaction rate law has the form

$$R = R_1 + R_2 + R_3, \quad (32)$$

where  $R_1$  is an ignition term which describes the reaction of a small amount of explosive soon after the shock wave compresses it,  $R_2$  is a slow growth of reaction term which models the spread of this initial reaction and  $R_3$  is a rapid completion of reaction term which dominates at large pressure and temperature. The form of the ignition term is

$$R_1 = I(1 - \lambda)^a (\mu_e - \mu_c)^x,$$

where  $\mu_e = \rho_e/\rho_0 - 1$  is the compression of the unreacted explosive and  $\mu_c$  is the minimum compression required to start the reaction. The ignition term is set to zero when  $\lambda \geq \lambda_{\max,ig}$ . The form of the growth and completion terms are

$$R_2 = G_1(1 - \lambda)^b \lambda^c P^y,$$

$$R_3 = G_2(1 - \lambda)^d \lambda^e P^z.$$

The growth term is set to zero when  $\lambda \geq \lambda_{\max,gr}$  and the completion term is set to zero when  $\lambda \leq \lambda_{\min,gr}$ .

In the original work of Lee & Tarver, only the two first terms in Eq. (32) were present and this form is called the two-term model. The third term was added to accurately simulate short pulse duration shock initiation. The burn fraction exponents  $a$  and  $b$  are usually set to 2/9 in the two-term model and to 2/3 in the three-term model. The burn fraction exponent  $c$  is usually set to 2/3 in the two-term model and to 1/9 in the three-term model. The compression exponent  $x$  is usually set to 4, or with  $\lambda_{\max,ig} < 1$  to a higher value. The pressure exponents  $y$  and  $z$  are usually in the range  $1 \leq y \leq z \leq 3$ .