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JWL Calculating

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The following is a list of JWL properties to be sent to Sedat Esen, who is an explosive analyst for a Swedish industrial institute at

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The JWL is a standard equation of state used worldwide to describe the pressure-volume-energy behavior of a detonating explosive. Even so, not many people are very good at working with it. So I list all the various equations that describe how it works, then give one way that the solution can be obtained in an iterative manner.

I have collaborated with Sedat Esen for several years. I am indebted to him for supplying almost all of our collection of dynamite data. He now works with ammonium nitrate/fuel oil, which is another area of interest to us.

2.1.1. Arithmetic of the JWL

Two forms of the JWL

The three-coefficient JWL equation is

$$P = A\exp(-R_1 v) + B\exp(-R_2 v) + \frac{C}{v^{1+\omega}}. \tag{1}$$

The integral is the internal energy

$$E_S = \frac{A}{R_1}\exp(-R_1 v) + \frac{B}{R_2}\exp(-R_2 v) + \frac{C}{\omega v^{\omega}}. \tag{2}$$

In our codes, E_S is positive and at its maximum at the C-J point (there is no spike with the pure JWL). As the products expand, E_S declines toward zero. From Eq. 2

$$C = \omega v^{\omega}\left[E_s - \frac{A}{R_1}\exp(-R_1 v) + \frac{B}{R_2}\exp(-R_2 v)\right]. \tag{3}$$

If we substitute Eq. 3 into Eq. 1, we get

$$P = A\left[1 - \frac{\omega}{R_1 v}\right]\exp(-R_1 v) + B\left[1 - \frac{\omega}{R_2 v}\right]\exp(-R_2 v) + \frac{\omega E_s}{v}. \tag{4}$$

This is the form hydrocode people like at out Lab, because both energy and pressure enter into it. They like having all three variables confirmed at each step.

Γ at the C-J Point

At the C-j Point, the Rayleigh Line equation is

$$P_{cj} = \rho_o U_s^2 (1 - v_{cj}) \tag{5}$$

so that

$$\frac{dP_{cj}}{dv} = -\rho_o U_s^2. \tag{6}$$

Then,

$$\Gamma_{cj} = -\frac{vdP}{Pdv} = \frac{v_{cj}}{1 - v_{cj}}. \tag{7}$$

Our Lab's current codes use the C-J parameter of

$$bhe = \Gamma_{cj} + 1 = \frac{1}{1 - v_{cj}}. \tag{8}$$

This is used as a rate constant in Program Burn. So that the rate goes as bhe(1-v).

Another Form of the C-J Pressure

At the C-J point, the internal energy is the sum of the chemical energy E_o and the energy of compression, E_c, which is

$$E_c(cj) = \frac{1}{2} P_{cj}(1 - v_{cj}) \tag{9}$$

so that

$$E_s(cj) = E_o + E_c(cj) \,. \tag{10}$$

We now take Eq. 4 and substitute for E_s to get

$$P_{cj} = A\left[1 - \frac{\omega}{R_1 v_{cj}}\right]\exp(-R_1 v_{cj}) + B\left[1 - \frac{\omega}{R_2 v_{cj}}\right]\exp(-R_2 v_{cj}) + \frac{\omega}{v_{cj}}\left[E_o + \frac{1}{2}P_{cj}(1 - v_{cj})\right] \tag{11}$$

We solve for P_{cj} to get

$$P_{cj} = \frac{A\left[1 - \frac{\omega}{R_1 v_{cj}}\right]\exp(-R_1 v_{cj}) + B\left[1 - \frac{\omega}{R_2 v_{cj}}\right]\exp(-R_2 v_{cj}) + \frac{\omega E_o}{v_{cj}}}{1 - \frac{\omega(1 - v_{cj})}{2 v_{cj}}} \tag{12}$$

On the Adiabat

E_o is the total chemical energy present in the explosive but it only comes out in the detonation after the products expand to infinite volume. Along the way, we get out some of the energy at the relative Cylinder test volumes of 2.2, 4.4 and 7.2. So, at some volume v larger than C-J, we have

$$E_d(v) = \left[E_s(v_{cj}) - E_s(v)\right] - E_c(cj) \,. \tag{13}$$

At the C-J point, E_d equals $-E_c$ and is negative in our codes. At infinite volume, $E_s(v)$ is zero and $E_d(\infty) = E_o$, the largest positive number. At somewhere around v ~ 0.91, the crossover from negative to positive detonation energy occurs. We substitute the C-J quantities in Eq. 10 into Eq. 13 to get

$$E_d(v) = E_o - E_s(v). \tag{14}$$

We substitute Eq. 2 to get

$$E_d(v) = E_o - \left[\frac{A}{R_1}\exp(-R_1 v) + \frac{B}{R_2}\exp(-R_2 v) + \frac{C}{\omega v^{\omega}}\right]. \tag{15}$$

Rayleigh Line

If we differentiate Eq. 1 we have

$$\frac{dP}{dv} = -AR_1 \exp(-R_1 v) - BR_2 \exp(-R_2 v) - \frac{(1+\omega)C}{v^{2+\omega}}. \tag{16}$$

We combine this with Eq. 6 to get the detonation velocity

$$U_s = \left\{\frac{1}{\rho_o}\left[AR_1 \exp(-R_1 v) + BR_2 \exp(-R_2 v) + \frac{(1+\omega)C}{v^{2+\omega}}\right]\right\}^{1/2}. \tag{17}$$

2.1.2. New Calculation Method

Start with ρ_o, R_2, R_1, ω, and E_o which stay constant. Also, we start with initial values of U_s, $E_d(2.2)$, $E_d(4.4)$ and $E_d(7.2)$ which should not change much during the calculation. Add rough values for A, B and bhe, which will be calculated and could change considerably. Then we go through these 7 steps.

$$v_{cj} = 1 - \frac{1}{bhe} \tag{8}$$

$$P_{cj} = \frac{A\left[1-\frac{\omega}{R_1 v_{cj}}\right]\exp(-R_1 v_{cj}) + B\left[1-\frac{\omega}{R_2 v_{cj}}\right]\exp(-R_2 v_{cj}) + \frac{\omega E_o}{v_{cj}}}{1-\frac{\omega(1-v_{cj})}{2v_{cj}}} \qquad (12)$$

$$C = \omega v^{\omega}\left[E_s - \frac{A}{R_1}\exp(-R_1 v) + \frac{B}{R_2}\exp(-R_2 v)\right] \qquad (3)$$

$$E_d(v) = E_o - \left[\frac{A}{R_1}\exp(-R_1 v) + \frac{B}{R_2}\exp(-R_2 v) + \frac{C}{\omega v^{\omega}}\right] \text{ at v = 2.2, 4.4 and 7.2} \qquad (15)$$

$$U_s = \left\{\frac{1}{\rho_o}\left[AR_1\exp(-R_1 v) + BR_2\exp(-R_2 v) + \frac{(1+\omega)C}{v^{2+\omega}}\right]\right\}^{1/2} \qquad (17)$$

$$P_{cj}(a) = \rho_o U_s^2(1-v_{cj}) \qquad (5)$$

$$P_{cj}(b) = A\exp(-R_1 v_{cj}) + B\exp(-R_2 v_{cj}) + \frac{C}{v_{cj}^{1+\omega}} \qquad (1)$$

We define these %-change comparisons

$$\alpha = \frac{100\left[U_s - U_s(\text{inital})\right]}{U_s(\text{inital})} \qquad (18)$$

$$\beta = \frac{100\left[P_{cj}(a) - P_{cj}(b)\right]}{P_{cj}(b)} \qquad (19)$$

$$\delta(v) = \frac{100\left[E_d(v) - E_d(v,\text{inital})\right]}{E_d(v,\text{initial})} \text{ at v = 2.2, 4.4 and 7.2} \tag{20}$$

$$\delta = \frac{\delta(2.2) + \delta(4.4) + \delta(7.2)}{3} \tag{21}$$

We now enter a loop of repetitive calculations, in which we change the three variables one after another using these algorithms

$$\text{bhe(new)} = \text{bhe(old)} + 0.01\delta \tag{22}$$

$$A(\text{new}) = \left(1 - 0.03\alpha\right)A(\text{old}) \tag{23}$$

$$B(\text{new}) = (1 + 0.05\beta)B(\text{old}) \tag{24}$$

We go through the 7-steps again that we listed above after each variable change so we have three complete calculations on each loop. The process is repeated for 50 cycles or until

$$\alpha,\beta \leq 0.0002\,, \tag{25}$$

where these limits are arbitrary. The new JWL is balanced within the errors of Eq. 25. Like all non-linear fitters, the initial guesses have to reasonably close to the final answer. It is also possible to get an unphysical result, which usually appears in the form of a negative value for B. Because of this, it is usually best to make a large change in small increments.

People are getting fussier with their JWL's and are starting not to like the round-off errors. To reproduce exactly a JWL, we really need to save the three adiabat energies. In saving all these numbers, it inconvenient to have numbers calculated out to a huge number of decimal places. An improvement may be made by rounding off the $E_d(v)$ values to 5 decimal places and recalculating.