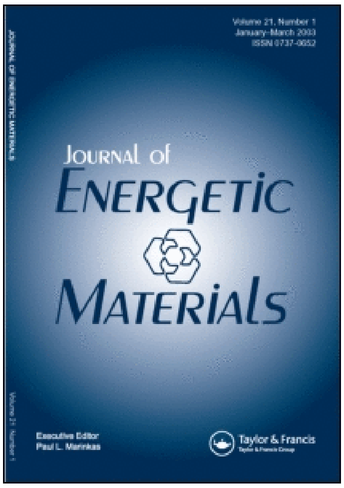

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Accuracy and Calibration of High Explosive Thermodynamic Equations of State

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The Jones-Wilkins-Lee-Baker (JWLB) equation of state (EOS) was developed to more accurately describe overdriven detonation while maintaining an accurate description of high explosive products expansion work output. The increased mathematical complexity of the JWLB high explosive equations of state provides increased accuracy for practical problems of interest. Increased numbers of parameters are often justified based on improved physics descriptions but can also mean increased calibration complexity. A generalized extent of aluminum reaction Jones-Wilkins-Lee (JWL)-based EOS was developed in order to more accurately describe the observed behavior of aluminized explosives detonation products expansion. A calibration method was developed to describe the unreacted, partially reacted, and completely reacted explosive using nonlinear optimization. A reasonable calibration of a generalized extent of aluminum reaction JWLB EOS as a function of aluminum reaction fraction has not yet

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been achieved due to the increased mathematical complexity of the JWLB form.

Keywords: detonation, detonation products, detonation velocity, equation of state

Introduction

Increased mathematical complexity of high explosive equations of state does not guarantee increased accuracy for practical problems of interest. Increased numbers of parameters are often justified based on improved physics descriptions but can also mean increased calibration complexity. This issue is discussed in relationship to the Jones-Wilkins-Lee-Baker (JWLB) thermodynamic equation of state (EOS) and a newly developed generalized extent of aluminum reaction Jones-Wilkins-Lee (JWL)-based EOS. The JWLB thermodynamic EOS was developed to more accurately describe overdriven detonation while maintaining an accurate description of high explosive products expansion work output [1]. The EOS is more mathematically complex than the JWL EOS, because it includes an increased number of parameters to describe the principle isentrope, as well as a Gruneisen parameter formulation that is a function of specific volume. The JWLB mathematical form is

$$P = \sum_{n} A_i\left(1 - \frac{\omega}{R_i V^*}\right)e^{-R_i V^*} + \frac{\lambda E}{V^*} \tag{1}$$

$$\lambda = \sum_{i} (A_{\lambda i} V^* + B_{\lambda i}) e^{-R_{\lambda i} V^*} + \omega \tag{2}$$

where V^* is the relative volume, E is the product of the initial density and specific internal energy, and λ is the Gruneisen parameter. Often it is questioned whether the increased mathematical complexity over JWL is of value, because increased numbers of parameters can mean increased calibration complexity and do not guarantee increased accuracy for practical problems of interest. Two methods of parameter calibration have been used to date: empirical calibration to cylinder test data [1] and formal optimization using JAGUAR thermochemical predictions [2]. This article will only discuss the formal optimization using JAGUAR thermochemical predictions [2].

Analytic Cylinder Model

An analytic cylinder test model that uses JWL and JWLB equations of state has been developed that provides excellent agreement with high rate continuum modeling [3]. Isentropic expansion is assumed for the expanding detonation products from the Chapman-Jouguet state. In addition, constant detonation products are assumed across spherical surfaces that perpendicularly intersect the cylinder inside wall. The products' mass velocities are assumed perpendicular to the spherical surfaces. These assumptions, along with mass, momentum, and energy conservation result in the final model. Figure 1 presents a sketch representation of the analytic cylinder test model.

JWLB EOS

One method of JWLB parameterization is to directly fit the pressure and Gruneisen parameter versus specific volume behaviors predicted by JAGUAR. Formal nonlinear optimization is used for the parameterization procedure. The example presented

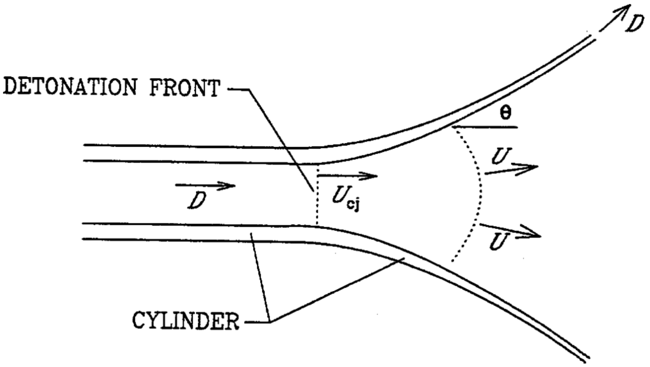

Figure 1. Analytic cylinder test model.

is using the high-energy explosive LX-14. The LX-14 JWL and JWLB relationships were parameterized using the JAGUAR predictions and nonlinear optimization routines. The resulting JWL and JWLB equations of state were then used to model a standard 25.4-mm inside and 30.48-mm outside cylinder test and compared to experimental data using the analytic cylinder test model and the high rate continuum model CALE [4]. Table 1 and Fig. 2 present the resulting outside cylinder velocity results at different inside cylinder cross-sectional areas. The results clearly show the improved agreement to experimental data obtained when using the more mathematically complex JWLB mathematical form, particularly at low area expansions. The improved agreement is attributed to the better representation of the JAGUAR-predicted detonation products' behavior that is achieved using the JWLB form.

Table 1
LX-14 JWL and JWLB cylinder test velocity predictions (km/s) compared to experimental data

	Analytic cylinder			CALE	
A/A0	Avg Exptl	JWL	JWLB	JWL	JWLB
2	1.505	1.562	1.519	1.555	1.527
3	1.664	1.705	1.667	1.682	1.665
4	1.745	1.759	1.738	1.740	1.727
5	1.791	1.790	1.780	1.765	1.761
6	1.817	1.812	1.807	1.781	1.782
7	1.833	1.828	1.826	1.795	1.797
			ABS % Error		
2		3.787	0.930	3.322	1.462
3		2.464	0.180	1.683	0.060
4		0.802	0.401	0.287	1.032
5		0.056	0.614	1.452	1.675
6		0.275	0.550	1.981	1.926
7		0.273	0.382	2.073	1.964
Avg Error		1.276	0.510	1.800	1.353

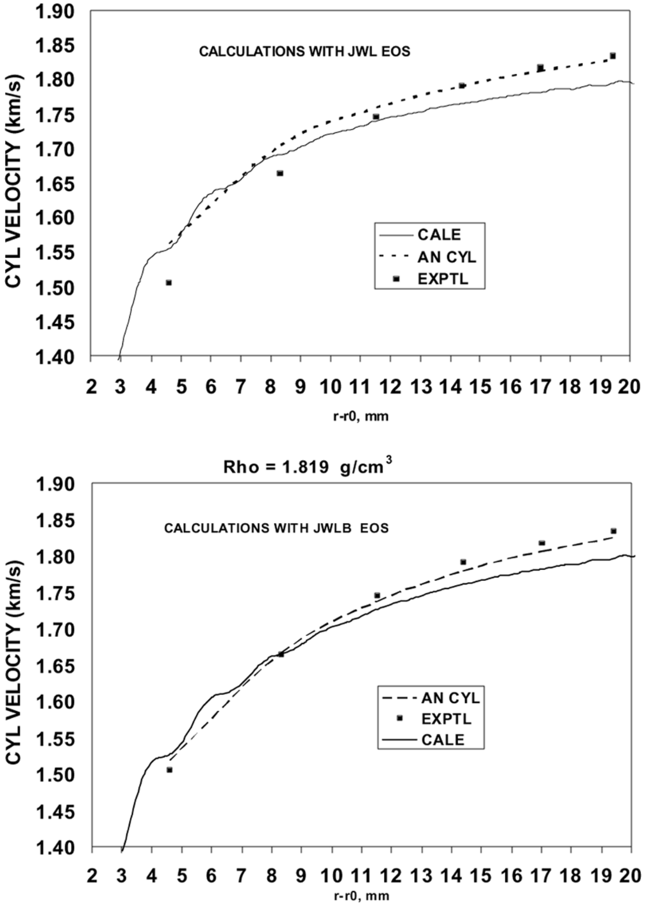

Figure 2. LX-14 JWL and JWLB cylinder test predictions compared to experiments.

Eigenvalue Detonation

Previous studies have shown that traditional Chapman-Jouguet detonation theory does not explain the observed detonation states and expansion behavior achieved by aluminized explosives. The detonation behavior of these explosives has been studied using both experimental data and JAGUAR thermochemical calculations [5]. In order to account for the observed behavior of the aluminized explosives investigated, a model was postulated in which the explosive expands through a reaction zone at a detonation velocity often controlled by the Hugoniot for zero aluminum reaction [6,7]. At the zero aluminum reaction Hugoniot, the aluminum is unreacted and the other gaseous and solid C-H-N-O products are in equilibrium. For the partially reacted aluminum Hugoniots, the reacted aluminum fraction detonation product (aluminum oxide) is in equilibrium with the other C-H-N-O products. For the reaction zone, the necessary Hugoniot and Rayleigh line relationships must be satisfied. However, for the aluminized explosives investigated to date, the unreacted aluminum Hugoniot curves actually fall above the reacted aluminum Hugoniots in P-V space. Therefore, the minimum detonation velocity solution occurs with the Rayleigh line intersecting the zero aluminum reaction Hugoniot at the tangency point. The associated eigenvalue detonation velocity is the velocity that would be measured experimentally. Two associated thermodynamic equation of state representations have been developed. For relatively fast aluminum reaction, an eigenvalue JWLB EOS and calibration methodology has been developed. The resulting eigenvalue JWLB EOS is more accurate at early detonation products expansion compared to an eigenvalue JWL EOS. For a relatively slower aluminum reaction rate, a partial reaction JWL thermodynamic EOS and calibration method were developed to describe the unreacted, partially reacted, and completely reacted explosive.

Eigenvalue JWLB EOS

The same JWLB parameterization was used to directly fit the pressure and Gruneisen parameter versus specific volume behaviors predicted by JAGUAR. The examples presented used the new aluminized combined effects explosives PAX-30 and PAX-29. PAX-30 and PAX-29 are 15% by weight aluminum based on HMX and CL-20, respectively. Because the PAX-30 and PAX-29 explosives produce eigenvalue, rather than traditional, Chapman-Jouguet detonations, a modified analytic cylinder test model was developed that assumes isentropic expansion from the eigenvalue detonation produced weak point (WPT) [8,9]. Table 2 and Fig. 3 present the resulting outside cylinder velocity results at different inside cylinder cross-sectional areas for PAX-30. Table 3 and Fig. 4 present the results for PAX-29. The results clearly show the improved agreement to experimental data obtained when using the more mathematically complex JWLB mathematical form. Again, the improved agreement is attributed to the better representation of the JAGUAR-predicted detonation products' behavior that is achieved using the JWLB form.

JAGUAR has the capability to allow specified temperature differences between the gaseous products and unreacted aluminum. This procedure enables aluminum melting to be suppressed initially. Only slight differences result with this procedure for

Table 2

PAX-30 JWL and JWLB cylinder test predictions compared to experiments

	Analytic cylinder				CALE	
A/A0	Avg Exptl	JWL	JWLB	JWLB WPT	JWL	JWLB
2	1.499	1.599	1.550	1.541	1.582	1.531
3	1.682	1.759	1.702	1.703	1.741	1.685
4	1.774	1.823	1.780	1.779	1.801	1.762
5	1.827	1.862	1.831	1.825	1.837	1.811
6	1.859	1.890	1.868	1.856	1.862	1.845
7	1.883	1.911	1.897	1.879	1.883	1.872
			ABS % Error			
2		6.671	3.402	2.802	5.537	2.135
3		4.578	1.189	1.249	3.508	0.178
4		2.762	0.316	0.282	1.522	0.676
5		1.916	0.219	0.109	0.547	0.876
6		1.668	0.484	0.161	0.161	0.753
7		1.487	0.744	0.212	0.000	0.584
Avg Error		3.180	1.059	0.803	1.879	0.867

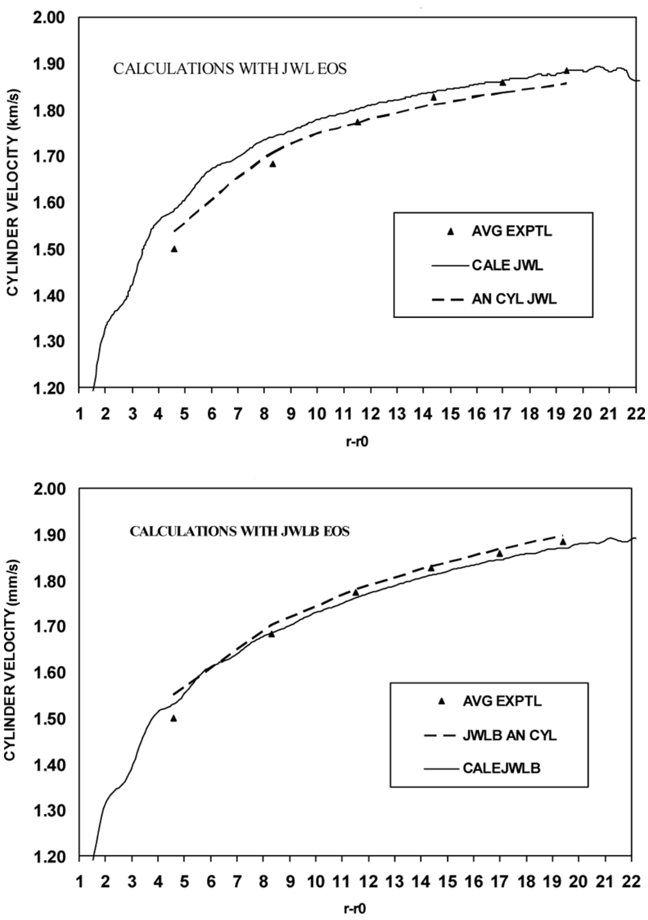

Figure 3. PAX-30 JWL and JWLB cylinder test predictions compared to experiments.

the calculated detonation velocities, and thermal equilibrium should be attained rapidly on subsequent reaction and expansion.

Generalized JWL EOS

In order to aid in the effective determination and representation of the behavior of aluminized explosives with a slower aluminum reaction, a calibration optimization procedure has been developed

Table 3
PAX-29 JWL and JWLB cylinder test predictions compared to experiments

	Analytic cylinder				CALE	
A^*	Avg Exptl	JWL	JWLB	JWLB WPT	JWL	JWLB
2	1.601	1.678	1.636	1.617	1.663	1.614
3	1.777	1.843	1.792	1.781	1.822	1.772
4	1.868	1.908	1.869	1.859	1.883	1.844
5	1.919	1.948	1.920	1.907	1.922	1.896
6	1.950	1.976	1.957	1.941	1.947	1.930
7	1.970	1.998	1.985	1.965	1.966	1.957
			ABS % Error			
2		4.809	2.186	0.999	3.873	0.812
3		3.714	0.844	0.225	2.532	0.281
4		2.141	0.054	0.482	0.803	1.285
5		1.511	0.052	0.625	0.156	1.199
6		1.333	0.359	0.462	0.154	1.026
7		1.421	0.761	0.254	0.203	0.660
Avg Error		2.488	0.709	0.508	1.287	0.877

to obtain relationships for the variation of JWL constants with reaction fraction of aluminum, X. This new thermodynamic EOS is parameterized using the JAGUAR thermochemical potential computer program [10]. This P-V-E EOS has the advantage for continuum modeling that it is parameterized directly using partially reacted states rather than balanced between unreacted and fully reacted relationships. This parameterization methodology insures that the P-V-E behavior of the partially reacted materials EOS agrees appropriately (and precisely) for Hugoniots and isentropes and enables accurate calculations at nonisentropic conditions. The partial reaction JWL EOS is

$$P = \sum_{1}^{2} A_i \left(1 - \frac{\omega}{R_i V^*}\right) e^{-R_i V^*} + \frac{\omega E}{V^*} \qquad (3)$$

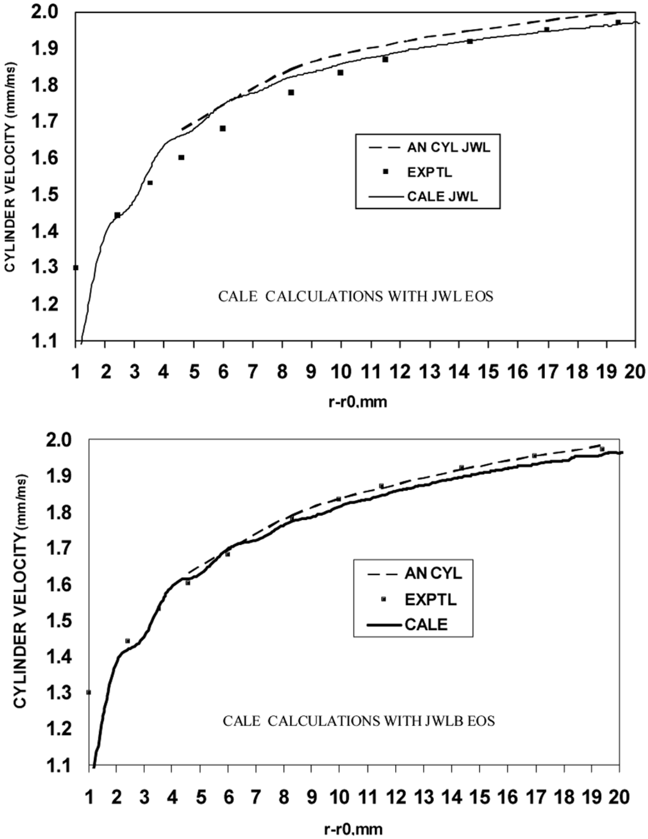

Figure 4. PAX-29 JWL and JWLB cylinder test predictions compared to experiments.

where V^* is the relative volume and E is the the product of the initial density and specific internal energy. The constants A_i and R_i of Eq. (3) are assumed to vary linearly with fraction aluminum reaction as

$$A_i = a_{i1} + a_{i2}X \tag{4}$$

$$R_i = r_{i1} + r_{i2}X \tag{5}$$

In order to find the eight optimum parameters a_{i1}, a_{i2}, r_{i1}, and r_{i2} of Eqs. (4) and (5), the objective function is to minimize the sum of the squares of the deviations between pressures calculated with Eq. (3) and the JAGUAR pressures for the isentropes at 0, 50, and 100% aluminum reaction. The C-J velocities and energies at 7 volume expansions are constrained to be equal to the JAGUAR-predicted values. The constants of the generalized JWL relationships for several aluminized explosives are presented in Table 4.

Calculations using the partial reaction JWL EOS have been used to accurately reproduce observed cylinder test data of several aluminized explosives. One of the initial kinetic models considered for the aluminum reaction behavior of the zones is a pseudo first-order model,

$$X = 1 - \exp(-DEC(t - t_0)) \tag{6}$$

Table 4
Parameters of generalized JWL relationships for aluminized explosives

	PAX-3 HMX	PAX-29 CL-20	PAX-30 HMX	PAX-42 RDX
Al (wt%)	18	15	15	15
ρ_0 (g/cm^3)	1.866	1.999	1.909	1.834
a_{11} (Mbar)	9.5342	15.9932	9.6294	9.9872
a_{12} (Mbar)	6.6006	14.8808	−0.63196	4.9768
a_{21} (Mbar)	0.22167	0.46824	0.10453	0.27971
a_{22} (Mbar)	0.35652	0.50294	0.11400	0.33391
r_{11}	5.0215	5.5721	4.7231	5.1757
r_{12}	1.7141	2.0922	0.33447	1.4267
r_{21}	1.52630	1.74214	1.07379	1.5569
r_{22}	0.24991	0.24618	0.16594	0.25709
C_1 (Mbar)	7.6510E-3	9.5806E-3	8.2921E-3	8.7711E-3
C_2 (Mbar)	5.8150E-3	5.0455E-3	5.2828E-3	5.2673E-3
W_1	0.2802	0.3407	0.30711	0.31326
W_2	−6.8399E-2	−9.7833E-2	−7.2446E-2	−7.2722E-2

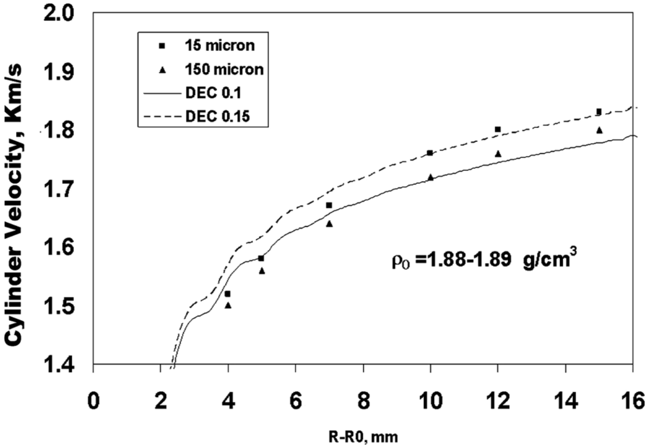

Figure 5. Experiment and modeling comparisons for HMX/Al 85/15.

Figure 5 presents a comparison of experimental and computed cylinder velocities for two 85% HMX and 15% Al by weight compositions with different aluminum particle sizes [11,12].

Although the JWLB EOS provides a more accurate prediction of the early products' expansion, a reasonable calibration of the JWLB parameters as a function of aluminum reaction fraction has not yet been achieved due to the mathematical complexity of the JWLB form.

Conclusions

The results clearly show that the JWLB EOS produces improved accuracy for overdriven detonation while maintaining or increasing the prediction accuracy of the detonation products expansion work output. However, for many practical applications when overdriven detonation or early products expansion phenomenon are not important, the JWL EOS provides adequate accuracy. The generalized JWL EOS as a function of aluminum reaction fraction that has been developed for slower aluminum reactions has been shown to provide improved modeling capability and increased insight for some aluminized explosive compositions. Although the JWLB EOS provides a more accurate prediction of the early products expansion, a reasonable calibration of the JWLB parameters as a function of aluminum reaction fraction has not yet been achieved due to the mathematical complexity of the JWLB form. Implementations of the JWLB thermodynamic equations of state have been completed in the DYNA [13], CALE [4], CTH [14], and ALE3D [15] hydrocode applications. These thermodynamic equations of state enable the improved continuum modeling of overdriven detonation, early detonation products expansion, and aluminized explosives.

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