

COMPARISON OF WILLIAMSBURG AND JWL EQUATIONS OF STATE FOR NITROMETHANE

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The Williamsburg is a thermodynamically complete equation of state for detonation products. Williamsburg parameters have been obtained for nitromethane by fitting to the results of chemical equilibrium calculations. The resulting equation of state was evaluated by simulating cylinder tests with a hydrocode. Plane Chapman-Jouguet detonation and a partial form of the WBL model were used to programme the motion of the detonation wave. Using the Williamsburg, the expansion history of the cylinder wall was predicted with a similar accuracy as using the JWL.

INTRODUCTION

Analytic equations of state (EOS) are often constructed so as to give the best representation of some set of experimental data. A problem with this approach is that if equal care is not taken over the general form of the EOS - e.g. from theoretical considerations - then the accuracy of the EOS is liable to be poor away from the range of the data. The effect can be insidious, as hydrocode users (important 'customers' of such EOS) often require a black box which is robust for arbitrary design calculations, and may have no time to worry about the accuracy of individual hydrocode models so long as the results look plausible.

The Jones-Wilkins-Lee (JWL) is an example of an EOS whose physical validity is limited outwith the range of the data to which it is fitted. The JWL consists of additive corrections to a perfect gas EOS, which is the simplest physical EOS. Parameters may be found by fitting to a relatively narrow range of states, e.g. the region of a single expansion adiabat in a cylinder test. However, the JWL is computationally efficient, and relates the pressure p to the density ρ (or specific volume v) and specific internal energy e - the most convenient representation for calculations of continuum mechanics.

The Williamsburg^{1, 2, 3}(WB) is an EOS whose general form can be justified on theoretical grounds for molecules interacting via inverse power potentials. Of course, this form of interaction is only a model, but inverse powers have been used with reasonable success for a range of applications, and the WB EOS has the potential to be accurate further from the region where it is normalised to data. The WB is thermodynamically complete - a valuable

characteristic for reactive flow investigations, when the temperature may dominate the reaction rate. On the other hand, the WB relates e to v and the specific entropy s , which means that further manipulation is necessary to use this EOS in continuum mechanics calculations.

At a more fundamental level, theoretical techniques (or the computer power to support them) have developed to a point where more detailed calculations of material behaviour at the microscopic level are becoming feasible. Reactive media are typically more difficult to treat than inerts, but chemical equilibrium calculations based on interatomic potentials are a reasonable means of predicting thermodynamic properties. In principle, interpolation between the ordinates of tabulated states allows an EOS to be represented as accurately as the individual states can be calculated. Indeed, tabular EOS are used widely, particularly for inert materials⁴. However, it is still advantageous to choose a computationally efficient analytic form, and the results obtained from tabular EOS can depend on the form of interpolation function used.

In the present work, discrete thermodynamic states were generated for the detonation products of nitromethane (NM) by performing chemical equilibrium calculations in the region of the Chapman-Jouguet (CJ) adiabat. Parameters were calculated for the WB EOS to match these states. The EOS was made available for continuum mechanical calculations either by direct implementation (requiring a numerical root-finding process) or by tabulating the WB EOS itself. In the latter case, the WB was being used as a physically justified form of extrapolation function outwith the range of the chemical equilibrium calculations.

Comparisons are made with an empirical JWL EOS along representative trajectories in state space and using continuum mechanical simulations of a cylinder test.

CHEMICAL EQUILIBRIUM CALCULATIONS

Chemical equilibrium calculations were performed by one of the authors (MB) to predict the thermodynamic state of NM in the region of the CJ isentrope. The detonation code 'IDeX'⁷ was employed, which uses a constrained minimisation method to obtain chemical equilibrium for a non-ideal multi-phase system. A Weeks-Chandler-Anderson (WCA) EOS with Kang Lee Ree and Ree extensions was used for fluids, and a Birch-Murnaghan treatment for graphite and diamond. For computational efficiency the WCA intermolecular potential EOS was fitted to Tchebychev polynomials⁸. The only data required for these calculations were the initial chemical composition (CH₃NO₂), heat of formation and density (1.13 Mg/m³)⁵, and the thermodynamics of the product molecules.

WILLIAMSBURG EOS

The Williamsburg (WB) EOS expresses the specific internal energy e in terms of the specific entropy s and specific volume v :

$$e(s, v) = \frac{e_0}{v^{g_\infty - 1}} \prod_{j=1}^m \left(\frac{1 + b_j v s^{\bar{a}_j}}{1 + b_j} \right)^{g_j}$$

where

$$\bar{a}_j \equiv a_j + d_j \ln s$$

$$v \equiv v/v_0$$

$$g_\infty \equiv g_0 + \sum_{j=1}^m g_j$$

$$g_0 = 1 + \sum_{j=1}^m a_j g_j$$

and

$$s \equiv \exp[(s - s_0)/nk_B]$$

is the reduced entropy. Quantities with a subscript 0 specify a reference state, e.g. the CJ. The α , β , δ and γ are complex parameters.

Parameters for NM were obtained by a least squares optimisation procedure to match the CJ isentrope plus one isentrope (shifted by 0.5% in reduced entropy) above and below. The order of the approximation in the fit, m , was chosen such that increasing the order further (up to $m=4$)

made little difference. A complication in this procedure was the formation of solid carbon at some point on each isentrope, leading to discontinuities in the states. Carbon condensation was modelled in the chemical equilibrium calculations, but could not be modelled accurately by the smooth form of the WB.

The WB is a thermodynamically complete EOS, since expressing e in terms of v and s allows any other thermodynamic quantity to be found without further state information. However, $e(s, v)$ is an inconvenient form for many continuum mechanics problems, where the EOS is normally required in the form $p(e, v)$. It is straightforward to solve for $p(e, v)$ from $e(s, v)$ numerically as required for a continuum mechanics problem, but the obvious solution schemes are iterative and thus impose a significant computational burden on such calculations. Nevertheless, the WB was implemented in this way within an EOS package for use with hydrocodes, to provide a slow but robust reference method.

An approach which is computationally more efficient is to tabulate the WB EOS 'off-line' and use the tabular EOS for continuum mechanics calculations. The EOS can be tabulated to give $p(v, e)$ (and the sound speed $c(v, e)$, also required for hydrocodes), but this type of table is not naturally rectangular, being bounded at the lower end by the cold curve (OK isotherm). An EOS of this form was however produced, by tabulating along a series of isochores (lines of constant v), without requiring that the k^{th} value of e should be the same for all isochores. To calculate $p(v, e)$, the isochores bounding v were found, then the bounding values of e on each of the bounding isochores, and p could then be found by interpolation. $c(v, e)$ is found in the same way.

In the present work, isochores were generated over the range $0.005 \text{ g/cm}^3 \leq \rho \leq 2.5 \text{ g/cm}^3$, each isochore spanning the (reduced) entropy range $0.01 \leq \sigma \leq 10$. For ideal (CJ) detonation, the products should never explore states with (reduced) entropy less than at the CJ point ($\sigma_{\text{CJ}}=1$ in our formulation). In practice, numerical schemes may allow states to stray into the region $\sigma < \sigma_{\text{CJ}}$ (e.g. in the predictor step of a predictor-corrector scheme) when expanding down the CJ isentrope. It is therefore necessary to extend the table below σ_{CJ} even for calculating ideal detonation. In addition, extending the table below σ_{CJ} makes it possible to investigate non-ideal detonations such as over-driving, where σ may really be below σ_{CJ} .

The WB can also be tabulated in the manner used in the SESAME library⁴, by calculating $p(\rho, T)$ and $e(\rho, T)$ over a rectangular array of (ρ, T) ordinates. The same software mechanics can be used if the WB is instead tabulated over ordinates of ρ and σ , except that no meaningful temperatures can be obtained without a little extra work.

JWL EOS

The JWL EOS has the form

$$p = we/v + \sum_i A_i \left(1 - \frac{wv_{os}}{R_i v} \right) \exp(-R_i v / v_{os})$$

where it is usual to use two exponential terms. It can be seen that the JWL takes the form of a modified perfect gas EOS, with the exponential terms acting to stiffen the EOS at high densities. Since the exponentials are functions of p only and not e or T , it can be shown that the JWL is not an accurate representation of the non-ideal interaction of real product molecules at the densities occurring in detonation. The JWL is therefore expected to have a limited validity away from the data - usually an isentrope - to which it is fitted.

Empirical JWL parameters for NM, optimised to reproduce cylinder expansion data, were obtained from the literature⁵. An inconsistency was found in the parameters - they did not give a CJ state - so an adjustment was made to remove the most likely source of error (Table 1).

TABLE 1: JWL PARAMETERS FOR NITROMETHANE

ρ_s	1128 kg/m ³
E_0	4.5212765 MJ/kg
A_1	209.2 GPa
R_1	4.40
A_2	5.689 GPa
R_2	1.20
w	0.30
D_{cj}	6.282 km/s
p_{cj}	125 GPa

The pure JWL EOS is generally acknowledged to be too soft at high compressions. It may be improved by adding a Pike extension, so above some critical compression v_{crit} (often taken as v_{CJ}) the EOS takes the form

$$p = \frac{we}{v} + Cv^{-\gamma}$$

where C and γ are chosen to keep p and the first differential with respect to volume continuous at $v=v_{crit}$. Taking $v_{crit}=v_{CJ}$ for the nitromethane JWL data gives $C=0.029377$ (Mb, cm, μ s units) and $\gamma=2.6124$.

The WB and JWL/Pike EOS were in fair agreement (Figure 1). In absolute terms, the major disagreement is in the high density, low entropy region, which may be reached only by a strong isentropic compression - unlikely

in shock wave scenarios. Comparing relative differences, the EOS agree reasonably well between the initial state and the CJ point, but the fractional discrepancy increases rapidly at low densities (Figure 2).

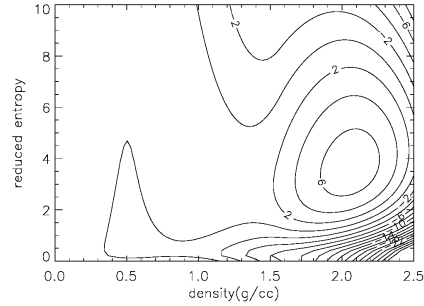


FIGURE 1: DIFFERENCE IN PRESSURE (WB MINUS JWL/PIKE) - CONTOUR 0.5 GPa APART

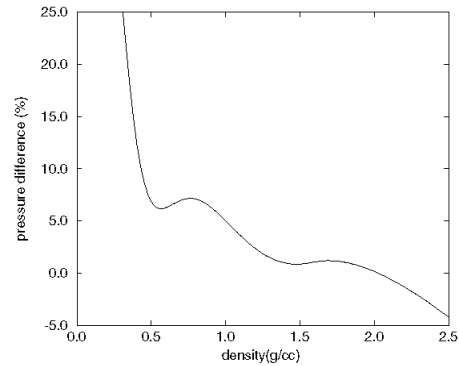


FIGURE 2: RELATIVE (%) DIFFERENCE BETWEEN WB AND JWL ON CJ ISENTROPE

STATE TRAJECTORIES

During the evolution of an initial value problem in continuum mechanics, each element of material follows some path through state space. When explosives are used to drive inert materials, the significant part of the path for elements of the explosive is usually along the lines of:

1. When detonated, start at the CJ state (or nearby, for non-ideal detonation).
2. Expand along the CJ isentrope.
3. At some point, re-shock along a secondary Hugoniot (e.g. when a reflected shock passes).
4. Expand along secondary isentrope.

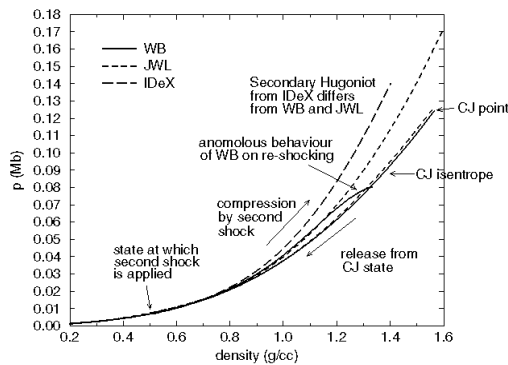


FIGURE 3: STATE TRAJECTORIES FOR RE-SHOCKING FROM CJ ISENTROPE.

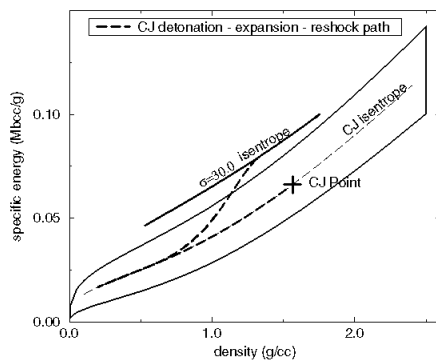


FIGURE 4: SECONDARY HUGONIOT COMPARED WITH (DENSITY, ENERGY) RANGE OF TABULATED EOS.

Re-shocking and subsequent expansion can result in thermodynamic states far enough from the CJ isentrope for physical inadequacies in simple products EOS to matter. Comparing CJ isentropes and Hugoniots for a re-shock from $\rho = 0.5 \text{ g/cm}^3$ on the CJ isentrope, the secondary Hugoniots diverge for shock pressures over about 5 GPa (Figure 3). There appears to be an anomaly in the WB curve (computed in this case by iterative solution of the WB equations), which actually intersects the CJ isentrope. Comparing with the tabulation (Figure 4), we find that the secondary Hugoniot samples states far outwith the original range. If we attempt to re-tabulate over this wider range, we find that the WB predicts unphysical states (p decreasing with increasing σ along isochores) for $\sigma > 5$ or so (Figure 5). It appears therefore that the extrapolation used to construct the WB EOS only remains physical up to $\sigma \sim 5$.

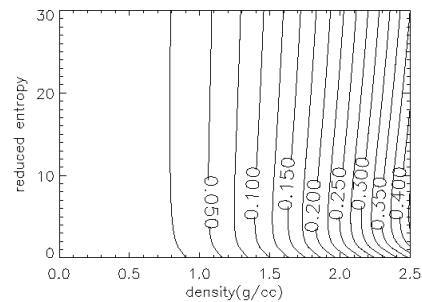


FIGURE 5: TABULATED WILLIAMSBURG EOS OVER EXTENDED RANGE OF REDUCED ENTROPY (PRESSURE IN Mb).

CYLINDER TESTS

The cylinder test is a standard experiment for measuring explosive performance. The experimental geometry consists of a cylindrical charge, 12" long by 1" diameter, encased in a precisely-machined cylinder of copper, typically 2mm thick. The charge is initiated at one end, usually with a plane wave generator, and the expansion history of the cylinder wall is measured using a variety of techniques including Fabry-Perot interferometry, the extinction of total internal reflection in an inclined glass block, and the triggering of electrical probes along the edge of an angled PCB.

JWL EOS are routinely obtained from cylinder tests by simulating the experiment in a hydrocode and varying parameters in the EOS until the measured expansion is adequately matched. In order for this procedure to work well, the simulation must include sufficient relevant physics. It is common practice to use programmed burn to model the propagation of the detonation wave, assuming a plane wave travelling at the CJ speed, and to ignore the stress in the copper; reasonable assumptions in the case of an ideal high explosive. The effect is to make the simulations independent of scale. Data for NM⁶ include cylinder tests of 1" and 2" diameter, but with different relative thicknesses of the copper cylinder (1.359mm for the 1" shot, 5.20mm for the 2")[†]. This may mask any scaling effect in NM, so the WBL detonation model^{9,10} was used as an alternative to the CJ model in simulating the cylinder tests.

WBL DETONATION MODEL FOR NM

The WBL detonation model⁹ describes the propagation of a detonation wave through a body of explosive,

[†] This was wrongly attributed in our paper in the Oxford Shock-wave Workshop in Sep. 1997 to an anomalous scaling effect in NM. The relative wall thickness explains much of the difference.

assuming that the speed D of the wave at any instant is a function of its local curvature K . The properties of a given explosive are defined by its $D(K)$ relation and a boundary condition constraining the angle which the wave can make with an adjacent inert material. $D(K)$ relations have been deduced for a range of solid explosives from observations of the shape of a steady detonation wave in a long rod or slab of explosive¹⁰. The boundary angles may be measured from the wave-shapes or the smooth functions used to fit them, or predicted from an analysis of the waves reflected from the inert material¹¹.

WBL detonation waves travel with a different speed in different regions of the explosive. From a detailed consideration of states within and behind the detonation zone¹⁰, it is found that the energy release should be modified to be consistent with variations in detonation speed. This modification was beyond the scope of the present work; the WBL model used was a partial implementation.

D(K) RELATIONS

The phase speed D_0 and shape $z(r)$ of detonation waves in NM have been measured in Pyrex tubes of different internal diameters¹². Sample points were estimated at a range of positions across each wave.

Given a $D(K)$ relation and D_0 for a particular charge, $z(r)$ can be deduced easily by integration⁹. Given D_0 and $z(r)$ for each wave, a $D(K)$ relation was deduced by assuming a functional form, and varying the parameters according to a Gauss-Newton minimisation scheme until the experimental $z(r)$ was reproduced to an acceptable accuracy. This procedure was followed with a linear $D(K)$ relation,

$$D = D_{CJ} (1 - AK)$$

where D_{CJ} and A are explosive-dependent parameters (Figure 6).

A linear $D(K)$ relation was found to be adequate to model each of the experiments in isolation, but as was found with the TATB-based explosive EDC35, the $D(K)$ relations were different (Figure 7). The relations from the rounds of larger diameter were in reasonable agreement, the differences probably reflecting the uncertainty in D_0 . The relation from the smallest experiment had a higher intercept and greater slope than the other relations. This is the opposite trend to that found for EDC35.

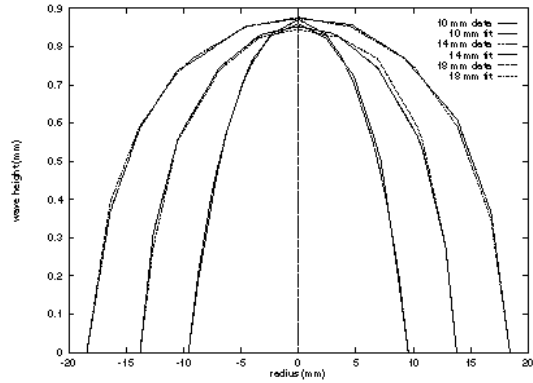


FIGURE 6: SAMPLED EXPERIMENTAL WAVE-SHAPE AND A FIT FROM A LINEAR $D(K)$ RELATION TO NM CHARGES OF DIFFERENT RADIUS

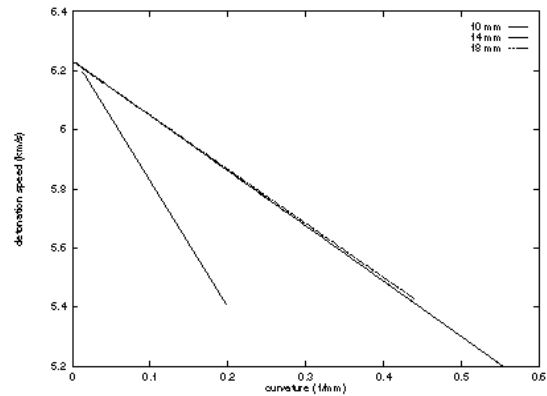


FIGURE 7: COMPARISON BETWEEN $D(K)$ RELATIONS FROM DIFFERENT ROUNDS.

The similarity between the $D(K)$ relations from the larger rounds suggests that even larger rounds are likely to obey the same relation. Accordingly, an averaged relation was calculated for use in analysing experiments of greater diameter (Table 2). The boundary angle ϕ_a was estimated from the slope of the fitting function at the edges of each charge.

TABLE 2: $D(K)$ RELATIONS AND BOUNDARY ANGLES FROM NM IN PYREX CYLINDERS

Radius(mm)	D_{CJ} (km/s)	A (mm)	ϕ_a (degrees)
9.57	6.253	0.683	74.1
13.78	6.236	0.300	65.0
18.42	6.231	0.293	68.5
(average)	6.234	0.296	66.7

BOUNDARY ANGLES

It has been postulated¹³ that the chemical reactions and hence the velocity of a detonation wave at an inert interface alter until the angle is such that no wave is reflected into the reaction zone. If a rarefaction is reflected, the reaction rates, pressure and shock speed are decelerated near the interface, and ϕ decreases. Conversely, if a shock is reflected then ϕ increases. The stable state is that where no wave, shock or rarefaction, is reflected into the reaction zone. The re-orientation of the detonation wave requires a finite time, corresponding to a distance of perhaps a few lengths of the detonation zone. On the scale of typical explosives engineering calculations this is likely to be negligible. In recognition of the existence of time scales for the detonation velocity to change, the angle at which no wave is reflected is termed 'asymptotic', ϕ_a .

The boundary angles inferred from functional fits to the shape of NM detonation waves in Pyrex tubes were compared with theoretical calculations, and predictions were made of the angles to use in simulations of cylinder tests with a copper case. Boundary angles were required between NM and each of Pyrex and copper, so Hugoniot EOS were obtained for each of these materials using published relations^{5,14} and shock wave data^{15,16}.

Following a method similar to that used previously¹¹, angles were predicted using either the von Neumann (vN, unreacted) or CJ (fully reacted) states in the NM. There was some uncertainty in the EOS to use for Pyrex, but the effect of the different NM state was greater. (Table 3).

TABLE 3: BOUNDARY ANGLES FOR NITROMETHANE

NM model	ϕ_a (degrees)	
	Pyrex	copper
CJ products	52.9±2.0	84.2
unreacted	66.2±2.0	85.5

The angle deduced for Pyrex from experimental wave shapes (Table 2) lay closer to the prediction using unreacted NM. This is in contrast to previous experience on a solid explosive and brass, where the products EOS gave better agreement¹¹. However, the difficulty in measuring the slope of the wave shape near the edge of the charge and the variation in results from different models of the Pyrex mean that no firm conclusion can be drawn about the relative accuracy of the predictions.

CYLINDER TEST SIMULATIONS

NM cylinder tests were simulated using a 2D Eulerian multi-material hydrocode. The expansion history of the case was monitored roughly halfway along. The sensitivity to mesh size was investigated, and converged results obtained with cells 0.25mm square.

Once a steady detonation wave has developed in the cylinder, all elements of the explosive products should expand down the CJ isentrope, because only rarefactions are reflected from the case and free surface. Thus the cylinder test should not be regarded as a suitable technique for determining a complete products EOS - other geometries, such as reflected shocks from the interface with a dense material, should be employed to investigate the behaviour of an EOS away from the CJ isentrope. The differences observed between the WB and JWL in the present work reflect the sensitivity of the cylinder expansion history to the difference in CJ isentrope calculated above.

Although the products should explore the same range of thermodynamic states in cylinder tests of any scale, it was felt useful to simulate both the 1" and 2" experiments anyway. This allowed the importance of any scaling effect to be assessed (after accounting for the difference in wall thickness), and allowed more experimental data to be included in the evaluation.

The NM was detonated according to programmed times obtained from the CJ and WBL models. Comparing with CJ detonation, the WBL model gave a slightly faster expansion in both cases. This is because the shock in the explosive is curved, and delivers an impulse with a radial component to the cylinder wall. The shock wave thus imparts a slightly greater radial velocity component.

In accordance with accepted practice for comparing the calculations with experimental data, a smooth curve was fitted to the data and both simulated and measured expansion histories were presented as deviations from the curve. In the present work, the fitting function was an 8th order polynomial.

It is a tricky calculational problem to define the precise instant at which the cylinder surface begins to expand, especially when the shock wave is smeared out over a few cells with an artificial viscosity. (At the CJ pressure in NM, the shock in the copper travels at ~0.5km/s, so each cell over which the shock is smeared represents ~0.5 μ s.) It can be similarly difficult to identify the time of first motion in an experiment. Thus there is some uncertainty in the absolute difference between the simulated and measured expansion histories. No adjustments were made to improve the apparent match.

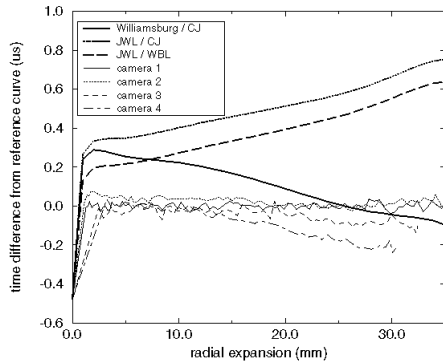


FIGURE 8: COMPARISON BETWEEN CALCULATED AND MEASURED EXPANSION HISTORIES (RELATIVE TO REFERENCE CURVE), 1" CYLINDER TEST.

Because the effect of a non-ideal WBL detonation on the reaction history was ignored, the speed of expansion quickly became the same as the CJ; ~2% slower than the data in both experiments. Because of the faster early motion, the WBL predictions were closer to the data. The WB EOS (with CJ detonation) was ~2% faster than the data in both experiments. There is some evidence of a residual scaling effect not modelled in the simulations (Figures 8 and 9).

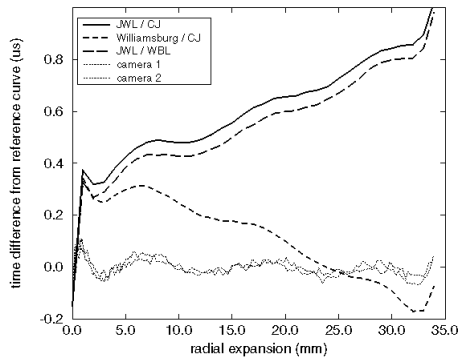


FIGURE 9: COMPARISON BETWEEN CALCULATED AND MEASURED EXPANSION HISTORIES (RELATIVE TO REFERENCE CURVE), 2" CYLINDER TEST.

CONCLUSIONS

Chemical equilibrium calculations predicted an EOS for NM which was in reasonable agreement with an empirical (JWL) EOS near the CJ point. Expanding down the CJ isentrope, the agreement gradually deteriorated. Off-isentrope, the WB produced unphysical results once the reduced entropy exceeded about 5, equivalent to a

shock of about 5GPa from an expanded state of density $\sim 0.5\text{g/cm}^3$.

The WB was successfully implemented in a way which is convenient for traditional continuum mechanics calculations by tabulating it against density and either energy or reduced entropy. In this instance, the WB provided a physically-based functional form for interpolation and extrapolation from the chemical equilibrium calculations.

Future development of the WB may include an extended range of validity (including the use of data covering a wider range of states) and measures to cope with the discontinuity caused by a phase change. It may be desirable to develop more efficient and robust algorithms for employing the WB form of EOS in a mechanical $(p(\rho, e))$ hydrocode.

Linear relations were deduced between the speed of a detonation wave in nitromethane and its curvature. The relations appeared to vary with the charge diameter, but a compromise relation was proposed for large charges. Future work might include the derivation of a non-linear or acceleration relation by considering wave shapes from rounds of several different diameters simultaneously.

Equations of state were obtained for the Hugoniot states of nitromethane and Pyrex from shock wave experiments. Boundary conditions were then deduced for the angle between a detonation wave in nitromethane and the shock waves induced in Pyrex and copper. Treating the nitromethane as unreacted or fully reacted gave significantly different results in both cases. Variation in the modelling of Pyrex had a smaller effect. The angle from the unreacted model was closer to that measured for Pyrex.

Comparing with data from cylinder tests of 1" and 2" diameter and different relative wall thicknesses, the JWL EOS gave an expansion ~2% slow and the WB ~2% fast. There was some evidence of a scaling effect in the data, but it was smaller than the difference between calculation and experiment. Since the WB was not optimised to match these experiments, this should be considered as fairly good agreement.

The results obtained here underwrite the use of chemical equilibrium calculations in predicting the equations of state of detonation products, and the use of the Williamsburg form for interpolating between and extrapolating from the states calculated with equilibrium chemistry. In extrapolation, the Williamsburg gave physical states well away from the range where it was fitted, though it drifted away from the states predicted using equilibrium chemistry. When extrapolating far enough, it did eventually predict unphysical states.

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