JCZS3—An Improved Database for EOS Calculations

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Abstract. At Sandia National Laboratories, we have created several large equation of state (EOS) databases used to calculate detonation states. These include the BKWS, JCZS, JCZS2, and a new JCZS3 database, which is the subject of the current work. The JCZS3 database provides exponential-6,13 (Exp-6,13) potential parameters for the JCZ3-EOS, which has been criticized for not matching Monte Carlo data well. We address perceived problems with the JCZ3-EOS and show that this EOS meets preliminary *sine qua non* tests of matching Monte Carlo simulations and various "acid" tests that include matching 1) experimental liquid Hugoniot tests, 2) overdriven detonation of condensed explosives, and 3) detonation performance of a variety of explosives. Our older databases, JCZS and JCZS2, used both Hugoniot data and detonation velocity to obtain EOS parameters. These older databases give accurate detonation predictions at the expense of the original Hugoniot fits. The new JCZS3 database is composed of potential parameters obtained from Hugoniot data without fine tuning to match the detonation velocity measurements. We show that this new database, adequately fits both Hugoniot data as well as detonation performance.

Introduction

An accurate equation of state (EOS) of detonation products is required to determine explosive performance of condensed phase explosives that can have detonation velocities ranging from 2-10 km/s and pressure ranging from a few bars to almost 0.5 Mbar. The most accurate equations of state (EOS) for condensed-phase detonation calculations are based on Exp-6,α:

$$\varphi(r) = \varepsilon\left[\left(\frac{6}{\alpha-6}\right)\exp\left[\alpha\left(1-\frac{r}{r^*}\right)\right]-\left(\frac{\alpha}{\alpha-6}\right)\left(\frac{r^*}{r}\right)^6\right], \qquad (1)$$

where $\varphi(r)$, r, r^*, ε, and α represent the spherically symmetric intermolecular potential function, intermolecular separation distance, value of "r" at the energy minimum, depth of the potential at the minimum, and the stiffness of the potential. The stiffness, α, determines the slope of the potential in the repulsion region at small values of r. Ree[1]

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provides a mixture model for the stiffness, α, and suggests that variable stiffness is necessary for accurately calculating detonation performance of condensed explosives.

The emphasis of the current work is on an Exp-6,13 database that supports the Jacobs, Cowperthwaite, Zwisler EOS[2] (JCZ3-EOS). The "3" in the JCZ3-EOS refers to the JCZ-EOS that incorporates the exp-6 potential. The other JCZ-EOS's (JCZ1, and JCZ2) are based on less accurate potentials and are no longer used. The database in the current work has a similar acronym (JCZS3) with the "S" referring to our laboratory and the "3" referring to the third version of this library. More information about the JCZS[3] and JCZS2[4] databases can be found in the references.

Table 1 shows the JCZ3-EOS one-fluid mixture rules used in the TIGER and JAGUAR codes. Mixture rules for other Byers-Brown exp-6 EOS models[5,6,7] used in codes such as THEOSTAR, TDS, and CHEETAH are also given in Table 1. The Lorentz-Berthelot approximation was used to generate the interaction between unlike species, and a van der Waals one fluid mixture rule (vdW1f) was used for the intermolecular separation distance, r_m. The mixture rule for the depth of the potential minimum, ε_m, is simpler in the JCZ3-EOS than the vdW1f approximation used in the other Exp-6 EOS. Also, the stiffness parameter, α, is constant in the JCZ3-EOS. The mixture rule for α used in the other Exp-6 models was proposed by Ree[1].

Table 1. Mixture rules used in JCZ3 and Exp-6

Both	$r_{ij} = \frac{r_{ii}+r_{jj}}{2}$	$\varepsilon_{ij} = \sqrt{\varepsilon_{ii}\varepsilon_{jj}}$	$\alpha_{ij} = \sqrt{\alpha_{ii}\alpha_{jj}}$
JCZ3	$r_m^3 = \sum_{i,j} x_i x_j r_{ij}^3$	$\varepsilon_m = \sum_{i,j} x_i x_j \varepsilon_{ij}$	$\alpha_m = 13$
Exp-6	$r_m^3 = \sum_{i,j} x_i x_j r_{ij}^3$	$\varepsilon_m = \frac{\sum_{i,j} x_i x_j \varepsilon_{ij} r_{ij}^3}{r_m^3}$	$\alpha_m = \frac{\sum_{i,j} x_i x_j \alpha_{ij} \varepsilon_{ij} r_{ij}^3}{\varepsilon_m r_m^3}$

Brown and Amaee critically reviewed the JCZ3-EOS and stated that "…Jacobs EOS is a rather complicated semi-empirical equation, and its agreement with Monte Carlo computer simulation results is poor…The same is true of the JCZ3-EOS for mixtures, which might be slightly improved by using the vdW1f mixing rule…Were it not for the fact that the mixture version…(JCZ3) has been incorporated into the well-known TIGER ideal detonation code, the Jacobs EOS, …, would only be of historic interest."[8]

Brown and Amaee's tough review was made before large databases were created. Furthermore, additional Monte Carlo numerical data[9,10,11] are available to determine if the claim of "poor" agreement with Monte Carlo simulations is true or not. Thus, part of the current work will show that the JCZ3-EOS is a good EOS by replicating Monte Carlo data, which is Brown's[5] *sine qua non* test.

The exp-6 potential parameters, r_{ii} and ε_{ii}, for the JCZS3 database discussed in the current work were obtained from pure liquid Hugoniot data. These parameters were then used with the JCZ3-EOS to predict the overdriven detonation Hugoniots of condensed explosives, detonation performance for a large number of condensed explosives, and detonation of gases at high initial pressures. These predictions are compared to experiments to determine whether Brown's[5] "acid" test is satisfied by the JCZ3-EOS.

Monte Carlo Calculations

Ross and Adler[9] performed Monte Carlo (MC) calculations for shock compression of Argon using an Exp-6,13.5 potential. The method generated a sequence of configurations by a Markov process with averages corresponding to a canonical ensemble with up to 300,000 configurations to determine average pressure and energy for the given potential. Fried et al.[11] extended Ross and Adler's MC calculations by using an Exp-6,11.5 and an Exp-6,15.5 potential.

Figure 1 presents the MC calculations as symbols and model calculations as lines. The thick solid line represents the JCZ3-EOS calculation. The exp-6 EOS using integral theory is represented by a thin solid line. The exp-6 EOS using variational perturbation theory is represented by the a dashed-line. The JCZ3-EOS is as good as integral theory and better than the variational perturbation theory in matching the Monte Carlo results using the same Exp-6,α potential. These results satisfy Brown's *sine qua non* test.

The Exp6-EOS used in subsequent sections in the current work are included for comparison to predictions using the JCZ3-EOS with the new

JCZS3 database. The Exp-6 predictions were made using Brown's method[5] applied to solutions of

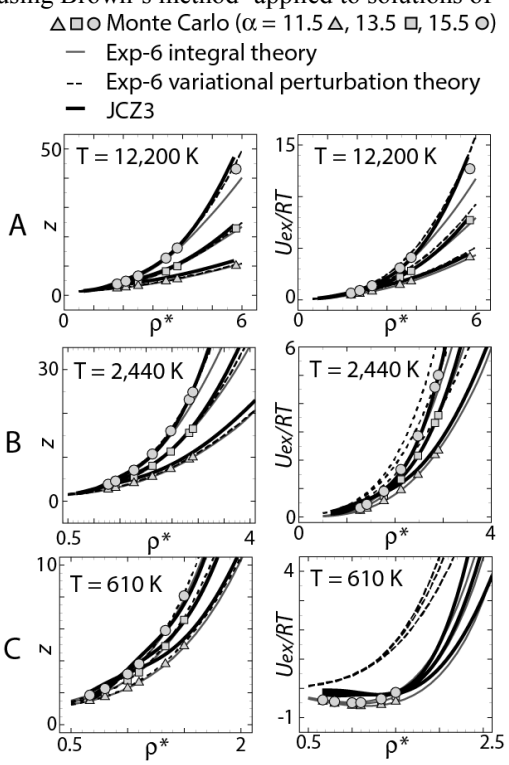

Fig. 1. Comparison of predicted compressibility (z) and excess internal energy (U_{ex}/RT) with Monte Carlo calculations with $\rho^* = Nr^{*3}/V$.

either integral theory[10] or variational perturbation theory[12] as solved in the CHEETAH thermochemical code.[11]

Fitting Hugoniots with a constant α

We fit Hugoniot data using two adjustable parameters (r^* and ε/k) and let α be constant at 13. Other investigators have used three adjustable parameters (r^*, ε/k, and α) to match Hugoniot data, with α varying substantially. For example, Stiel et al.[13] determined that a high stiffness (α = 18.2) for CF_4 was necessary to match the polytetrafluoroethylene (PTFE or Teflon™) shock Hugoniot. Similarly, others have used high stiffness parameter for CF_4 such as 15.5 by Fried and Howard.[14]

Figure 2 shows the shock Hugoniot of Teflon with symbols representing data from Marsh.[15] Predictions were made with parameters from Stiel

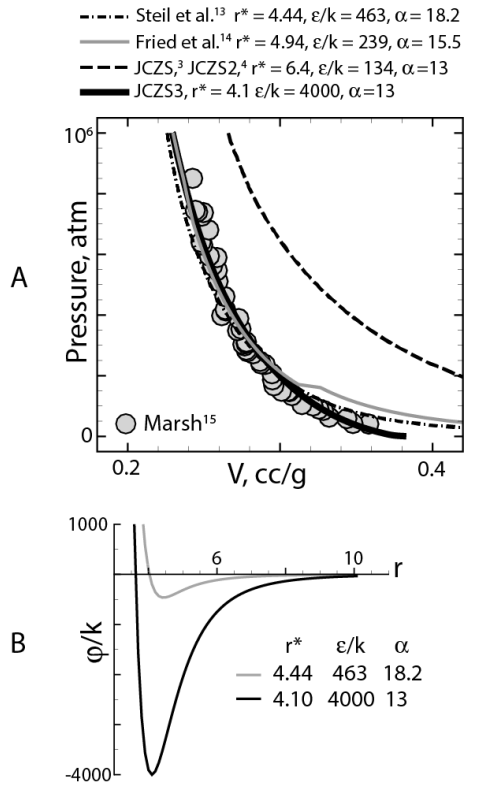

Fig. 2. A) PTFE Hugoniot and B) CF_4 potential.

et al.,[13] Fried, et al.,[14] JCZS[3] and JCZS2[4] libraries (same line), and the JCZS3 library. The parameters for the potential are given in the legend of Fig. 2. We have found that stiffness can be enhanced by keeping α constant, decreasing r* and increasing ε/k. This "potential compensation" effect is similar to the "kinetic compensation effect" described by Brill et al.[16] where a relationship exists between the pre-exponential factor and the activation energy, where one effect is compensated for by the other.

Major CHNO Species Parameters

Ten liquid Hugoniots with the initial temperature, density, and heat of formation are presented in Table 2. Parameters determined for the major species that were obtained from these

Hugoniots are listed in Table 3. JCZS3 parameter r^* and ε/k for species containing C, H, N, and O where obtained by matching the predicted Hugoniot with the measured Hugoniot.

The predicted and measured Hugoniots are presented in Figures 3 and 4. The Hugoniot for liquid oxygen gives a good example of how various parameters are obtained for species that are composed exclusively of oxygen. For example, the parameters for O_2 where obtained with the lower pressure data below 250 kbar. The parameters for O_3 were obtained with data from 250 to 400 kbar. Parameters for O were obtained with data from 400 to 500 kbar. And parameters for the ions O_2- and O_2+ were obtained with data between 500 and 800 kbar. Figures 3 and 4 also shows the predicted composition of the gases along the Hugoniot. Most of the ions do not form until the higher pressure and temperature region of the Hugoniot.

Table 2. Hugoniots for major CHNO species

	Ref.	**T, K**	**ρ_o, g/cc**	**h_f, kJ/mol**
CH_4	17	111.5	0.424	-14.6
CO	17	77.4	0.808	-123.58
CO_2	18-19	218	1.173	-147.1
C_6H_6	15, 20, 21, 22	298	0.875	48.95
H_2	15, 23	20	0.071	-8.8
H_2O	15, 24	298	1.000	-285.83
NH_3	15, 25	203	0.726	-72.5
N_2	15, 26, 27	75	0.820	-12.1
NO	28	122	1.263	79.5
O_2	15, 27	90	1.141	-13

Table3. JCZS3 potential parameters (α = 13)

Species	***r****	**ε/k**
C	2.50	100
CH_4	3.90	200
CHNO	4.32	180
CO	4.10	30
CO_2	4.30	240
H	2.70	3
H_2	3.75	4
H_2O	3.85	50
N	2.30	80
N_2	4.11	103
N_2H_2	4.26	150
N_2H_4	4.75	205
NH_3	4.10	70
O	3.20	50
O_2	3.83	130
O_2-	4.00	125
O_2+	3.00	125
O_3	4.30	250
OH	3.30	80

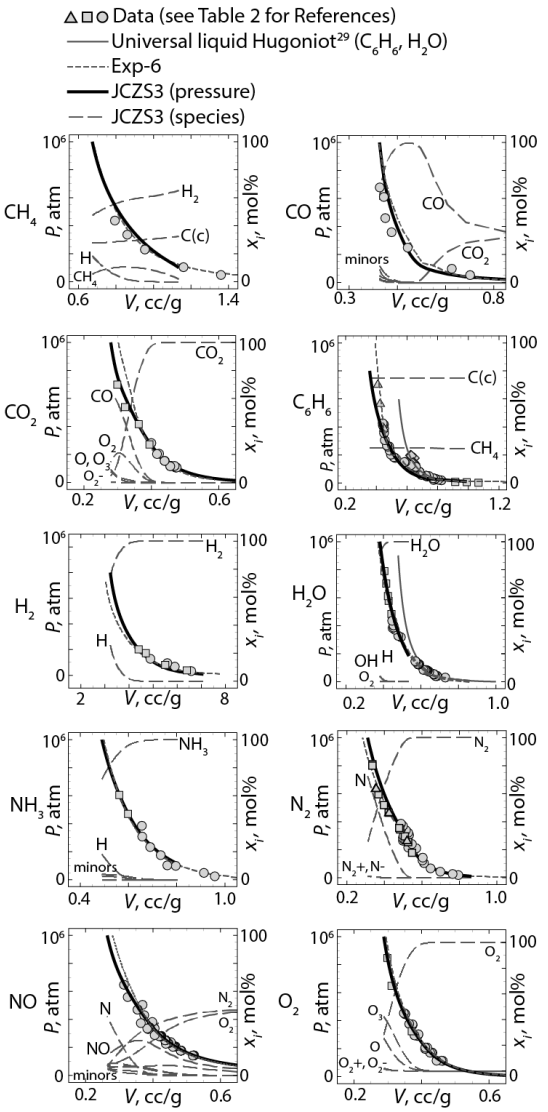

Fig. 3. Hugoniots listed in Table 2.

The Hugoniot plots for water and benzene (C_6H_6) shows predictions from the universal liquid Hugoniot.[29] Deviations from the universal liquid Hugoniot signifies the transformation from liquid to gas. The "kinks" in the water and benzene may be related to this transition.

Overdriven Shock Hugoniots

Shocks in explosives that reach pressures higher than the Chapman-Jouguet (CJ) pressure are referred to as overdriven shock Hugoniots, which are a good test of the JCZS3 database. Figure 4 presents several predictions of overdriven shock Hugoniots for PETN, PBX 9501, and a mixture of HMX, TATB, and Estane, at nominal formation enthalpies and initial densities of 1.72, 1.836, and 1.83 g/cc, respectively. The data for these Hugoniots were presented in references 14 and 30. The inability of the older JCZS databases to match these Hugoniots at extreme pressures was due to inaccurate potential values for the radicals H and N rather than the form of the JCZ3-EOS as implied by other authors.

Gas Detonation at Elevated Initial Pressures

Another test of the JCZS3 database is prediction of gas detonations. Typical gas detonations occur when the initial pressure is near ambient pressure. These ambient gas detonations do not reach CJ pressures where a non-ideal equation of state is necessary. However, when the initial pressure is elevated, a non-ideal equation of state is necessary. Compressibility in gases at elevated initial pressure reach values of 1.03 to 1.2. In contrast, the compressibility of HMX detonation products reaches 16 in the CJ plane.

Figure 5 presents a comparison of measured[31] and predicted detonation velocity of stoichiometric hydrogen with oxygen ($2H_2 + O_2$) at various initial pressures using the BKWC,[32] Exp-6, JCZS3, and ideal gas. Fried et al.[33] stated that "BKWC is not reliable when applied to explosives with very high in hydrogen content." Table 4 shows the products predicted when the initial pressure was 30 atm. The BKWC library does not consider H, O, and OH. This is the primary reason that the BKWC predictions disagree with data in Fig. 5.

The Exp-6 used in the CHEETAH database predicts higher detonation velocities for the H_2/O_2 system in Fig. 5. The database did not consider OH as a possible detonation product. Omitting OH does not matter for typical explosive calculations but is absolutely necessary for this system. In contrast, the JCZS3 database considers 23 different species, with six being significant (H_2O, H_2, OH, H, O_2, and O).

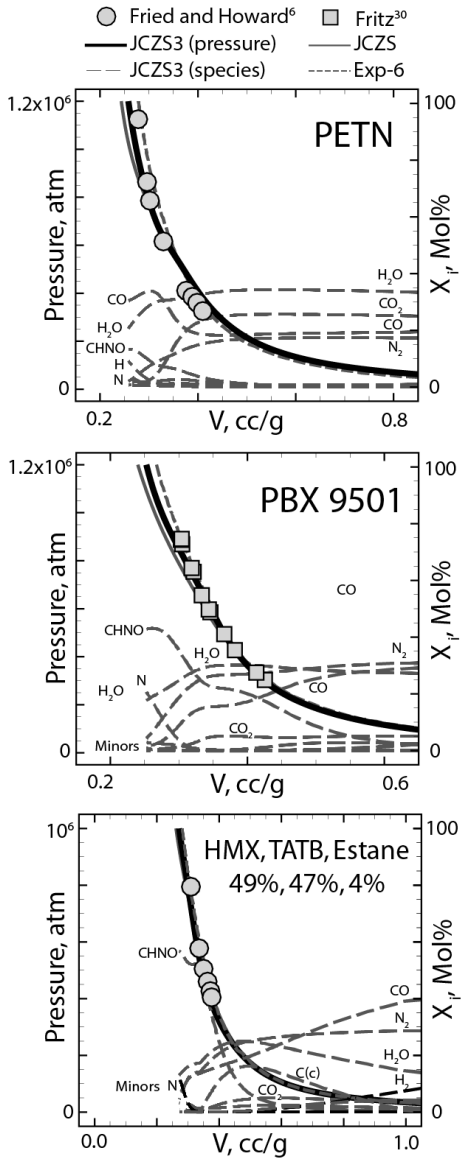

Fig. 4. Overdriven shock Hugoniots.

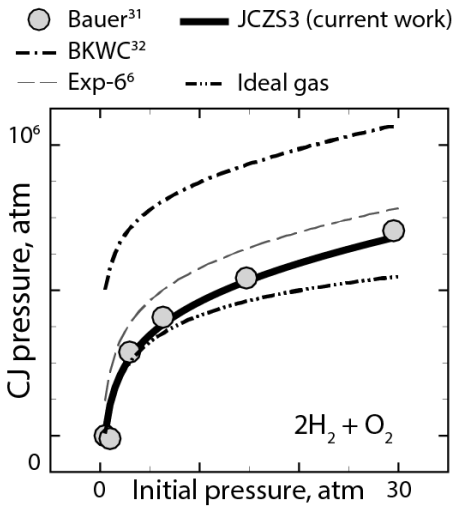

Fig. 5. Hydrogen/oxygen detonation at elevated initial pressure.

Table 4. Major detonation products in detonation at 30 atm in Fig. 5. Final two columns give mol%.[a]

BKWC	JCZS	Exp-6	JCZS	Exp-6
H_2O	H_2O	H_2O	62.7%	68.8%
H_2	H_2	H_2	13.7%	14.7%
missing	OH	missing	13.3%	missing
missing	H	H	4.5%	5.7%
O_2	O_2	O_2	3.5%	6.7%
missing	O	O	2.2%	4.1%
		Total =	99.9%	100%

[a] These minor species were also considered in the calculation:
BKWC: no other minor species
Exp-6: O_3
JCZS3: O_3, $H_2O(L)$, H_2O_2, HO_2, H_2-, H_2+, H_2O+, HO_2-, e-, O-, O+, H-, O_2-, O_2+, H+, OH-, OH+.

Detonation Predictions

We have tested the BKWS,[34] JCZS,[3] and JCZS2[4] databases using a set of 59 explosives at 108 different densities. Detail of the explosives, including initial density, heat of formation, and measured detonation velocity, pressure, and temperature can be found in reference 4. Figure 6 presents plots of measured detonation properties vs predicted detonation properties with the JCZS3 database. None of the intermolecular parameters were adjusted to match these properties. Rather, parameters were adjusted to match pure liquid Hugoniot data as discussed previously.

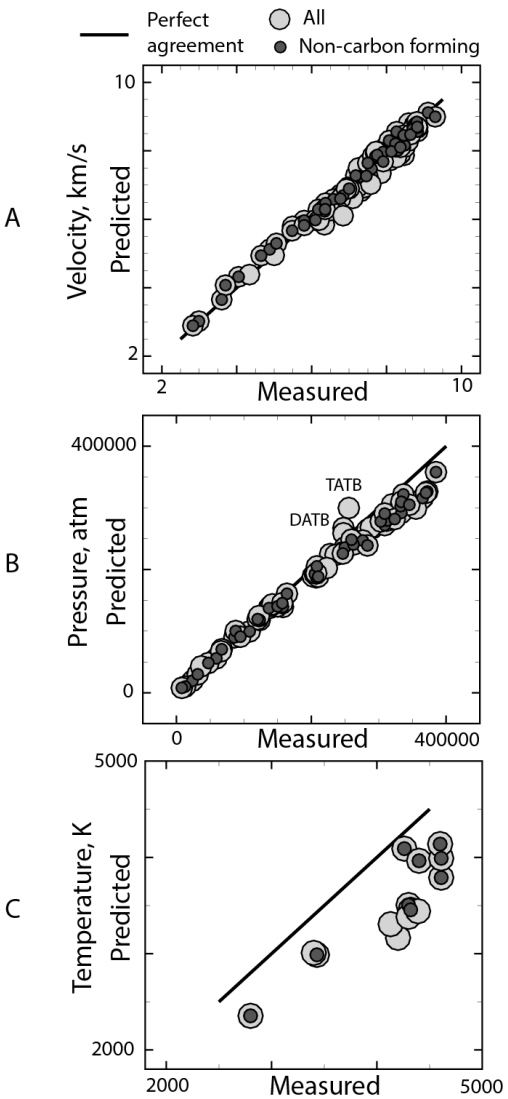

Fig. 6. Measure vs predicted detonation A) velocity, B) pressure, and C) temperature.

The line in Fig. 6 represents perfect agreement between the predicted and measured detonation property. The large circle represents the 108 velocities, 63 detonation pressures, and 14 detonation temperatures. The smaller circles represent the results that do not have substantial amounts of carbon in the equilibrium products. Detonation experiments that do not form carbon approximate complete reaction to equilibrium, since carbon may react slower and not be in chemical equilibrium.

TATB (triamino-trinitro-benzene) and DATB (diamino-trinitro-benzene) both have oxygen balances of -56% and each form significant amounts of carbon in the detonation products. TATB and DATB are labeled as outliers in Fig. 6.B. The predicted concentration of carbon in the TATB detonation front is about 25 mol%.

Detonation velocities are the most accurate detonation measurement and error is expected to be within 2-5%, at least for ideal detonations. For example, the JCZS2i database,[4] which used detonation velocities for calibration, gives an RMS (root mean squared) error of 2.3%. The Exp-6 database,[6] which has a more sophisticated 3 phase carbon model, gives an RMS of 2.5%. The RMS error for the JCZS3 database was 2.9%. A better condensed carbon model may increase the accuracy of the JCZS3 database.

Figure 7 presents a comparison of the measured and predicted detonation velocity of HMX, RDX, PETN, and TNT as a function of density with the source of the data given in reference 4. The predictions using the JCZS2 and the JCZS3 database give an overall RMS error of 1.8% and 2.6%, respectively. The potential parameters for the JCZS2 database were optimized with the detonation velocities. In contrast the parameters for the JCZS3 model were obtained from pure liquid Hugoniot data.

Engelke et al.[35] measured a detonation velocity if 6.14 km/s in 90.5 wt% H_2O_2 and 9.5 wt% H_2O at an initial density of 1.39 g/cc. The predicted detonation velocity with the JCZS2 database was 5.54 km/s (9.8% lower than the measured values) with a composition of 70.6 mol% H_2O vapor and 29.4 mol% O_2 in the CJ plane. The new JCZS3 database described in the current work gave the same composition in the CJ plane (70.6 mol% H_2O and 29.4% O_2); however, the detonation velocity was predicted to be 6.11 km/s, which is only 0.5% lower than the measured velocity of 6.14. The better predictions with the JCZS3 database is attributed to a better fit of the water Hugoniot for the water vapor potential parameters.

Summary and Conclusions

We have presented a third parameterization of the JCZ3-EOS, which is referred to as the JCZS3 database. The original JCZS database was the first

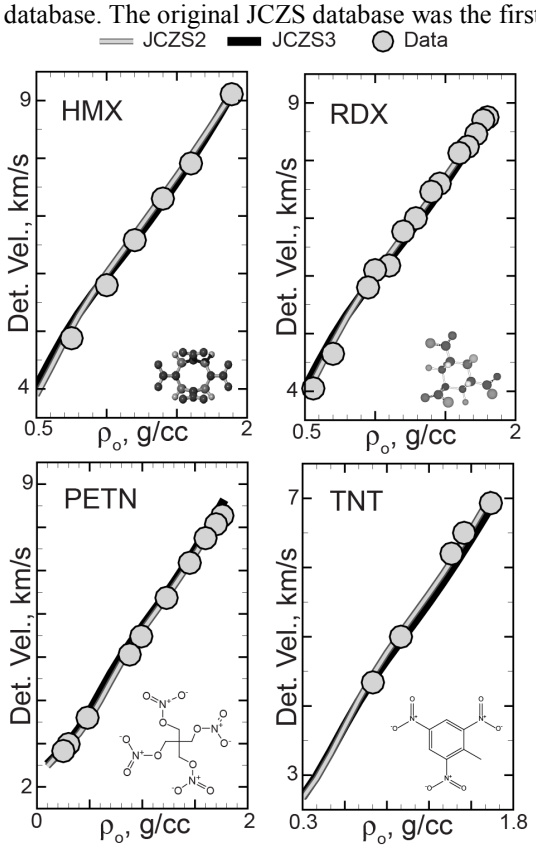

Fig. 7. Detonation velocities as a function of initial density. Experimental velocity found in 4.

large database of Exp-6,13 parameters consisting of r* and ε/k for 747 gases composed of 56 elements. The specific heat fits for these gases were only good to about 6,000 K. The JCZS parameters were determined using Lennard-Jones potential parameters, a corresponding states theory, fits to pure liquid shock Hugoniot data, fits to the BKWS-EOS at high pressures, and a final adjustment made to match detonation velocities.

The second parameterization of the JCZ3-EOS was referred to the JCZS2 database. The primary differences between this database and the JCZS database were the extension of the specific heat fits to 20,000 K and the addition of ions. The additional ions brought the number of gases in the database to 940. The potential parameters in the JCZS2 database were essentially left unchanged from the original JCZS database.

With the extension of the JCZS2 database to include ions and with the improved specific heat fits, another parameterization of the database was needed. Fitting potential parameters primarily with Hugoniots should give more accurate parameters needed for other calculations such as detonation performance. These Hugoniot can sometimes reach temperatures as high as 20,000 K where ionization becomes important.

We have also addressed several criticisms of the JCZ3-EOS. Specifically, we have shown that Brown and Amaee's[8] comments regarding poor agreement of the JCZ3-EOS with Monte Carlo data, which they refer to as the "*Sin Que Non"* test, is not true. In fact, the JCZ3-EOS matches historic[9] and recent[11] Monte Carlo data as well as other Exp-6 EOS models based on integral theory and variational perturbation theory.

Brown's criteria[5] for a good EOS is that it matches Monte Carlo data as well as that the EOS predictions agree with data. We have shown that the JCZ3-EOS combined with the large database of Exp-6,13 parameters can match pure liquid Hugoniots for CH_4, CO, CO_2, C_6H_6, H_2, H_2O, NH_3, N_3, NO, and O_2; overdriven detonation data for PETN, PBX 9501, and HMX/TATB/Estane 49%/47%/4%; gaseous detonations at elevated initial pressures; and detonation performance including detonation velocity, pressure, and temperature.

In order to match shock Hugoniots with a constant value of the repulsion constant α, we have found that a "potential compensation effect" exists wherein the steepness of the potential can be increased by lowering the potential well-depth. This compensation effect allows us to fit complex stiffness by using only two parameters, r* and ε/k, rather than the three parameters; r*, ε/k, and α; that is typically used in most Exp-6 models.

Acknowledgements

We would like to thank William Belfield for fruitful discussions of the JCZ3-EOS and the Exp-6 models as implemented using Brown's analytical representation of the Helmholtz's free energy. We discussed Hugoniot fits with Ernie Baker at the

Munitions Safety Information Analysis Center (MSIAC) located at NATO headquarters in Brussels. Ernie supplied several of his papers on fitting Hugoniots with the JCZ3-EOS. He mentioned that it is difficult if not impossible to fit Hugoniots with a constant α. We would like to acknowledge the support of Bill Erikson, who encouraged us to pursue the Hugoniot fits despite using a constant α of 13 for the JCZ3-EOS. We would also like to thank management support from Clint Hall, W. Russ Maines, and Sophia Lefantzi.

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Question from Leonard Stiel, Chemical Engineer

Concerning generating thermodynamic equations of state for overdriven Hugoniot calculations, I recommend a more advanced model than the JWL relationship, such as the JWLB EOS.

Answer from Michael L. Hobbs

We did not use JWL or JWLB EOS in our work. Our overdriven Hugoniot predictions were made with the JCZ3-EOS with the Exp-6,13 parameters listed in Table 3 using CTH-TIGER. JWL-type EOS's are typically fit to thermochemical equilibrium results calculated using equations of state such as the JCZ3-EOS at various expansions along the CJ isentrope.