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JCZS2i: An Improved JCZ Database for EOS Calculations at High Temperature and Pressure

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Abstract. The Jacobs-Cowperthwaite-Zwisler-Sandia (JCZS) database[1] has been used for over 15 years with the JCZ3[2] equation of state (EOS) to calculate detonation properties and product shock Hugoniots for a variety of explosives. The scope of the JCZS database has been increased by including species, and ions, that are currently used in the National Aeronautics and Space Administration (NASA) Lewis Research Center's computer program CEA[3] (Chemical Equilibrium with Applications), which uses the ideal gas EOS as opposed to an EOS good at high pressure such as the JCZ3-EOS that uses intermolecular potentials. We have also included piecewise fits for specific heat capacities (C_p) to insure reasonable extrapolations to temperatures as high as 20,000 K. The new library with the piecewise C_p fits and exponential 6 parameters have been implemented into the CTH-TIGER equilibrium code, which is a high-pressure equilibrium solver[4,5] coupled to our shock physics code, CTH. Predictions in the current work include detonation velocity for 59 explosives, water and air properties, and composition of an air shock created by detonation of Comp-B (60% RDX and 40% TNT).

Background and History

Gas phase detonation calculations can be done using the ideal gas EOS since temperatures are high, pressures are low, and the detonation products are far enough apart that intermolecular interactions are negligible. However, condensed phase explosives produce higher pressures and require use of an EOS that accounts for reaction product volume, such as the BKW-EOS[6] or better yet, accounts for intermolecular attraction and repulsion, such as the JCZ3-EOS.[2]

Figure 1 shows a brief history of some of the codes and equations of state used to calculate detonation properties for condensed explosives at our laboratory. In the 1950's, the Lawrence Radiation Laboratory (LRL) in Livermore California used the RUBY code to calculate detonation properties. The Los Alamos Scientific Laboratory (LASL) used the BKW program to do similar calculations. Both the RUBY and BKW codes were complex with the EOS mixed intimately with the thermodynamic and hydrodynamic calculations within the code.

In the 1960's, Stanford Research Institute (SRI) developed the TIGER code[4,5] with a goal to simplify the detonation calculations by using modular subroutines for the hydrodynamics, thermodynamics, and the EOS. In the 1970's, Cowperthwaite and Zwisler[5] put the JCZ EOS into TIGER giving the code options for ideal, BKW, and JCZ-EOS. Only 12 gases consisting of carbon (C), hydrogen (H), oxygen (O), nitrogen (N), and aluminum (Al) had JCZ parameters.

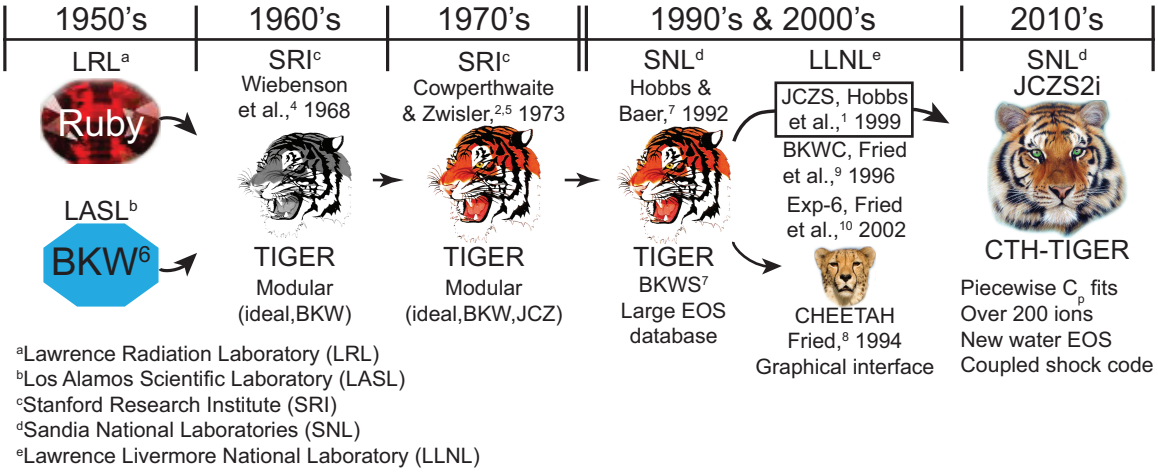

Fig. 1. Brief history of SNL's EOS work[1,7] based on SRI's original TIGER code.[4,5]

The original TIGER code[4] could consider up to 30 gas species and 10 condensed products composed of up to 10 elements, although the code was typically only used for reactants containing C, H, N, O, and Al. In the 1990's, these restrictions were eliminated when Hobbs et al. created the BKWS[7] and JCZS[1] EOS databases, which considered 56 elements, 747 gases, and 401 condensed products. BKW covolumes and parameters for an exponential-6 intermolecular potential were determined for all of these gases.

In 1994, Fried[8] converted our laboratories version of TIGER with the BKWS database to the computer language C and added a graphical user interface (GUI). Fried et al.[9] also created a BKW parameterization called the BKWC database, which was limited in scope since it lacked important species such as dissociated hydrogen (H). Fried et al.[10] created a more useful EOS database referred to as the EXP6 EOS. The EXP6 database contains many of the same potential parameters as the JCZS database but is not as accurate as the JCZS database when calculating detonation properties.[10]

Problems with JCZS database occur when the temperature exceeds 6,000 K. The specific heats for the JCZS databases were fit to polynomials using data from the JANAF tables,[11] which were typically good to 6,000 K for the gases and 1,500 K for the condensed products. The condensed C_p's were extrapolated to 6,000 K with a monotonically increasing polynomial. Above 6,000 K, the C_p extrapolations are not good and sometimes decrease with temperature, even going negative as shown in Fig. 2 for C, CO and CO. The C_p fits for these gases used in the NASA-CEA[3] code are also shown in Fig. 2.

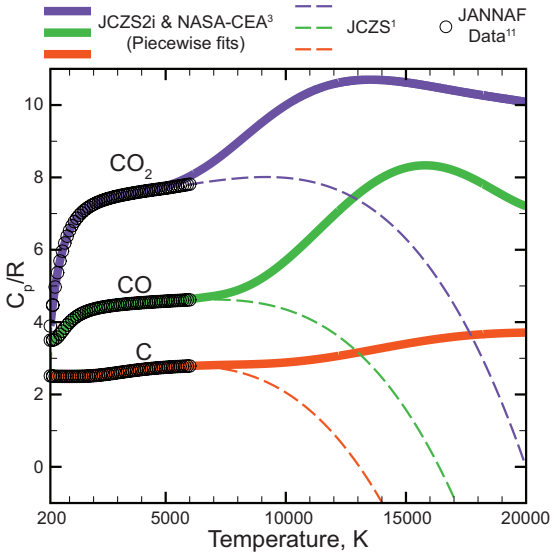

Fig. 2. C_p fits for JCZS and JCZS2i databases.

Temperatures in shocks can easily exceed 10,000 K. For example, the air shock produced

during open-air detonation of Comp-B can exceed 10,000 K. To simulate such phenomena using our shock physics code, CTH, we have coupled our version of the TIGER-EOS code to CTH. The coupled code will be referred to as CTH-TIGER.

The primary objective of the current work is to describe a new EOS library, which we have called the JCZS2i database. The database acronym retains the same JCZS as in reference 1, the "2" refers to version 2 of that database, and the "i" refers to "ions" in the database. This database retains the EOS parameters such as BKW covolumes and JCZ potential parameters.

The new database uses the same piecewise specific heat fits as the NASA-CEC code[3], with all of the monoatomic, diatomic, and some polyatomic specific heat fits good to 20,000 K. We have also included a new condensed EOS for solid and liquid water. The new database can be used to successfully reproduce the water phase diagram, and considers ice, liquid water, and water vapor. We also 1) compare the JCZS2i predictions to the JCZS[1] and EXP6[10] predictions of detonation properties for 59 explosives, 2) compare JCZS2i predictions of rarified air composition at 0.01 atm from 2,000 to 16,000 K with the NASA-CEC[3] code, and 3) predict the composition of an air shock produced by detonating a 5 inch (12.7 cm) radius cylinder of Comp-B in air.

Piecewise Thermodynamic Properties

The JCZS2i database contains coefficients that can be used to determine the dimensionless specific heat at 1 bar from about 100 K to 20,000 K. We use two temperature dependent polynomial functions to calculate the specific heat and refer to them as the "NASA" and "TIGER" polynomials. The two specific heat functions are:

NASA[3]:

$$\frac{C_p}{R} = a_1T^{-2} + a_2T^{-1} + a_3 + a_4T + a_5T^2 + a_6T^3 + a_7T^4 \qquad (1)$$

TIGER[4,5]:

$$\frac{C_p}{R} = C_1 + C_2\theta + C_3\theta^2 + C_4\theta^3 + C_5\theta^{-1} + C_6\theta^{-2} + C_7\theta^{-3} \qquad (2)$$

where $\theta = T[K]/1000$. The entropy and enthalpy at 1 bar can be obtained as a function of temperature with the following two equations:

$$h = \int C_p\,dT \text{ and } s = \int \frac{C_p}{T}dT\,. \qquad (3)$$

Equation (3) can be solved by substituting the specific heats from (1) and (2) into (3). The integration constants can be obtained by assuming that the enthalpy and entropy at the reference temperature (298.15 K) is equal to the heat of formation (ΔH^o_{f298}) and entropy of formation at 298.15 K (S^o_{298}), respectively. The dimensionless Gibb's free energy is found from the dimensionless entropy and enthalpy:

$$\mu / RT = h / RT - S / R\,. \qquad (4)$$

Piecewise fits insure extrapolations are reasonable without having the problems such as negative heat capacities as shown in Fig. 2. JCZS2i specific heats are extrapolated to high temperatures linearly using the specific heat at the highest known temperature and the following value of the dimensionless specific heat at 10^6 K, depending on the number of atoms (N) in the molecule:

Monatomic gases	2.5
Diatomic gases	4.5
Polyatomic gases	3*N-1.75

All of our C_p fits were plotted to 20,000 K by Miller et al.[12] to insure reasonable extrapolations.

Condensed Water EOS

We have implemented the following equation of state for solid and liquid water.

$$V = A + BT + CP\exp\left(1 - P/D\right), \qquad (5)$$

where A, B, C, and D are 19.03, 0.002, -0.00018, 7000 for ice and 15.7, 0.008, -0.000318, and 7000 for liquid water, respectively. The molar volume for ice and liquid water at 1 atm using Eq. (5) is shown in Fig. 3.a with data.[13]

Figures 3.b-f show the calculated and measured[11] specific heat, water shock Hugoniot with data[14,15] with the universal liquid Hugoniot[16], water sound speed with data[17], pressure dependent melting point of liquid water with data[13], and the

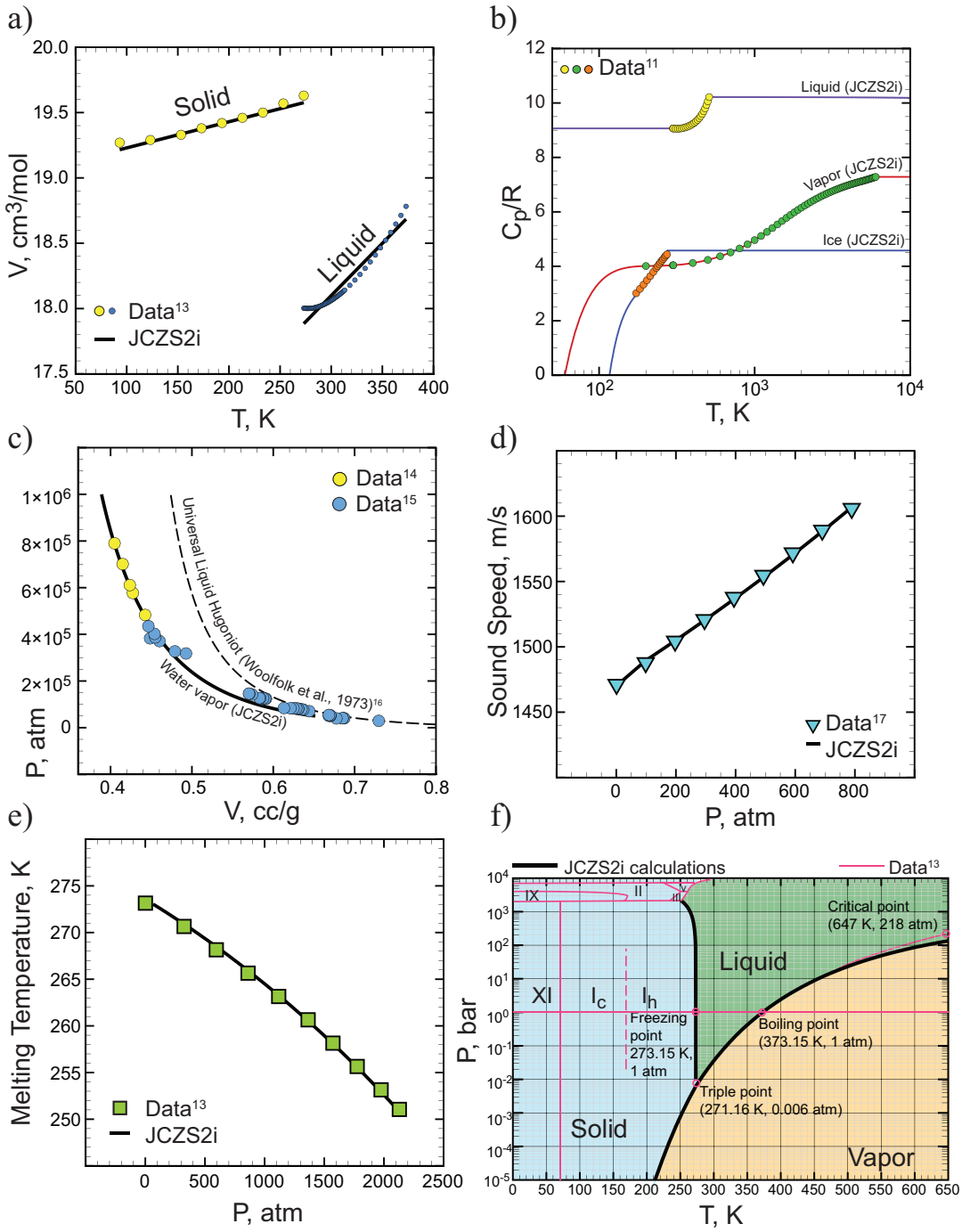

Fig. 3. Water a) EOS, b) specific heat, c) Hugoniot, d) sound speed, e) melting temperature, and f) phase diagram calculated with the JCZS2i database and compared to data from various sources.

water phase diagram calculated using CTH-TIGER with the JCZS2i database. Currently, CHEETAH's EXP6-EOS[10] does not consider liquid water and expansion states are suspect. The addition of the JCZS2i water EOS will make expansion calculations more accurate.

Detonation Velocity Calculations

The detonation performance calculations with the JCZS2i database are essentially the same as the JCZS database since intermolecular parameters are the same and the specific heats at typical detonation temperatures are the same. The addition of ions to the database does not change the calculations much since dissociation and ion formation takes place at temperatures higher than typical detonation temperatures.

Figure 4 shows a plot of measured versus calculated detonation velocities for 59 different explosives, which are listed in Table 1. These are the same explosives tested by Hobbs and Baer.[18] Common acronyms are given for the explosive with additional detail such as heat of formation available in Ref. 18. Predicted detonation velocities from three databases are given in Table 1: 1) JCZS[1] database, 2) JCZS2i database, and the 3) EXP6[10] database.

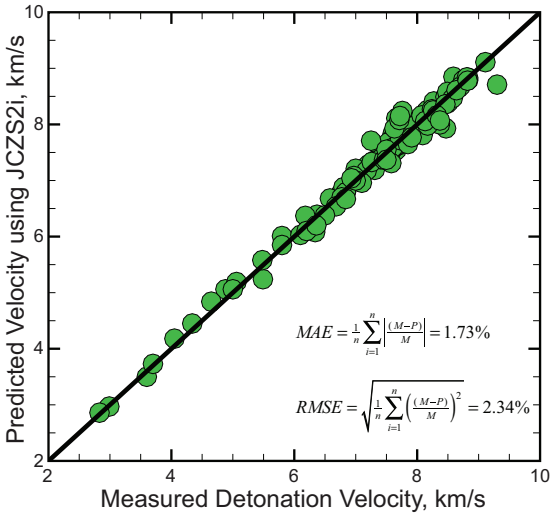

Fig. 4 Measured (M) versus predicted (P) detonation velocity for explosives in Table 1.

Some of the explosives have measured detonation velocities at several different initial densities. For example, the measured and predicted detonation velocity for HMX, RDX, PETN, and TNT are shown in Fig. 5 for several densities. These predictions are similar to JCZS predictions.

Air at High Temperatures and Pressures

Figure 6 shows the composition of rarefied air at 0.01 atm and temperatures ranging from 2,000 K to 16,000 K. In Fig. 6.a, shows a prediction from Vincenti and Kruger[19] based on work in the 1950's. Figure 6.b, shows predictions from both the CTH-TIGER using the JCZS2i database and a prediction from the NASA-CEC code using the ideal gas EOS. Both the NASA code and the CTH-TIGER code give the same results at these low pressures and high temperatures.

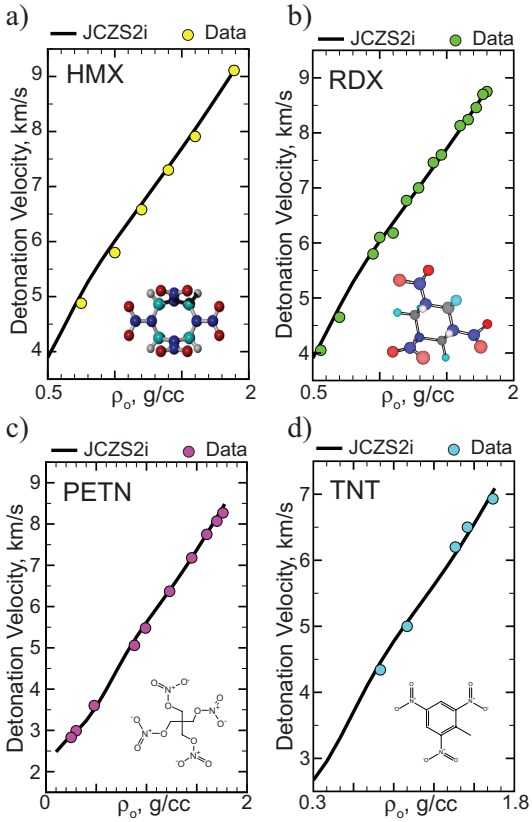

Fig. 5. Detonation velocities for a) HMX, b) RDX, c) PETN, and d) TNT. Experimental velocities are listed in Table 1.

Table 1. Measured and predicted detonation velocities with explosives from Ref. 18.

Explosive	ρ_o	Exp.	JCZS	JCZS2i	EXP6	% Error = (P-M)/M) JCZS	JCZS2i	EXP6
ABH	1.64	7200	7276	7281	7010	1.05%	1.13%	-2.64%
COMP A-3	1.64	8470	7908	7925	7896	-6.63%	-6.43%	-6.78%
COMP B	1.72	7920	7977	7988	7922	0.72%	0.86%	0.02%
COMP B-3	1.72	7890	7956	7967	7899	0.84%	0.98%	0.12%
COMP C4	1.66	8370	7988	8003	7981	-4.57%	-4.38%	-4.65%
78/22 RDX/TNT	1.76	8310	8295	8300	8308	-0.18%	-0.12%	-0.02%
77/23 RDX/TNT	1.74	8250	8209	8215	8215	-0.50%	-0.43%	-0.42%
75/25 RDX/TNT	1.76	8300	8256	8265	8267	-0.53%	-0.42%	-0.40%
70/30 RDX/TNT	1.73	8060	8094	8105	8079	0.42%	0.56%	0.24%
65/35 RDX/TNT	1.72	8040	8007	8018	7970	-0.41%	-0.28%	-0.87%
60/40 RDX/TNT	1.74	8090	8030	8040	7977	-0.75%	-0.62%	-1.39%
"	1.72	7900	7956	7967	7899	0.71%	0.85%	-0.01%
50/50 RDX/TNT	1.63	7660	7529	7542	7624	-1.71%	-1.54%	-0.46%
DATB	1.80	7600	7819	7827	7667	2.89%	2.99%	0.88%
"	1.78	7600	7741	7749	7578	1.85%	1.95%	-0.29%
DEGN	1.38	6760	6749	6766	6953	-0.16%	0.08%	2.85%
DIPM	1.76	7400	7566	7572	7429	2.25%	2.33%	0.39%
EXP D	1.55	6850	6835	6844	6938	-0.22%	-0.08%	1.28%
"	1.48	6700	6575	6585	6678	-1.86%	-1.71%	-0.33%
HMX	1.89	9110	9108	9106	9177	-0.02%	-0.05%	0.74%
"	1.60	7910	8035	8044	8012	1.58%	1.70%	1.29%
"	1.40	7300	7346	7355	7370	0.63%	0.75%	0.95%
"	1.20	6580	6679	6682	6710	1.51%	1.56%	1.98%
"	1.00	5800	6010	6011	5961	3.62%	3.64%	2.78%
"	0.75	4880	5055	5055	4959	3.59%	3.59%	1.62%
HNAB	1.60	7310	7187	7193	6963	-1.68%	-1.60%	-4.75%
HNS	1.60	6800	6873	6881	6895	1.07%	1.19%	1.40%
"	1.70	7000	7202	7209	7270	2.89%	2.99%	3.86%
LX-01	1.24	6840	6780	6787	6834	-0.88%	-0.77%	-0.08%
LX-14	1.84	8830	8789	8787	8816	-0.47%	-0.48%	-0.16%
MEN-II	1.02	5490	5220	5241	5766	-4.91%	-4.54%	5.02%
NG	1.60	7700	7628	7625	7767	-0.94%	-0.97%	0.87%
NM	1.13	6350	6173	6187	6396	-2.79%	-2.56%	0.73%
NONA	1.70	7400	7373	7379	7175	-0.36%	-0.29%	-3.04%
NQ	1.78	8590	8849	8846	8982	3.01%	2.99%	4.57%
"	1.62	7930	7969	7970	8143	0.49%	0.50%	2.69%
"	1.55	7650	7609	7611	7790	-0.54%	-0.51%	1.83%
76.3/23.7 HMX/TNT	1.81	8450	8448	8455	8481	-0.02%	0.06%	0.37%
75/25 HMX/TNT	1.81	8480	8435	8442	8464	-0.53%	-0.45%	-0.19%
60/40 HMX/TNT	1.80	8160	8246	8254	8214	1.06%	1.16%	0.66%
PBX-9007	1.64	8090	7793	7809	7747	-3.67%	-3.48%	-4.24%
PBX-9011	1.77	8500	8368	8378	8390	-1.56%	-1.44%	-1.30%
PBX-9205	1.67	8170	7964	7978	7951	-2.53%	-2.35%	-2.68%
PBX-9501	1.84	8830	8831	8830	8844	0.01%	0.00%	0.16%
50/50 PETN/TNT	1.71	7750	7706	7717	7597	-0.57%	-0.43%	-1.97%
"	1.70	7530	7669	7681	7562	1.85%	2.00%	0.42%
"	1.68	7650	7598	7610	7494	-0.68%	-0.53%	-2.04%
"	1.64	7530	7456	7469	7370	-0.98%	-0.81%	-2.13%
PETN	1.76	8270	8403	8409	8486	1.61%	1.68%	2.62%
"	1.70	8070	8159	8164	8248	1.10%	1.17%	2.21%
"	1.60	7750	7758	7763	7871	0.10%	0.16%	1.57%
"	1.45	7180	7179	7182	7324	-0.02%	0.03%	2.01%
"	1.23	6370	6392	6393	6463	0.34%	0.36%	1.45%
"	0.99	5480	5584	5583	5462	1.89%	1.88%	-0.33%
"	0.88	5060	5188	5187	5017	2.53%	2.51%	-0.85%
"	0.48	3600	3502	3501	3577	-2.72%	-2.75%	-0.63%
"	0.30	2990	2970	2969	3038	-0.66%	-0.70%	1.59%

PETN	0.25	2830	2859	2858	2900	1.04%	1.00%	2.46%
52/48 EXPD/TNT	1.63	6970	7071	7081	7174	1.45%	1.59%	2.92%
PICRID ACID	1.76	7570	7500	7505	7611	-0.93%	-0.86%	0.55%
"	1.71	7260	7324	7330	7427	0.89%	0.96%	2.30%
"	1.60	7100	6950	6956	7000	-2.11%	-2.02%	-1.41%
RDX	1.80	8750	8783	8785	8793	0.37%	0.40%	0.49%
"	1.77	8700	8671	8675	8667	-0.34%	-0.29%	-0.38%
"	1.72	8460	8485	8491	8467	0.30%	0.37%	0.08%
"	1.66	8240	8266	8274	8240	0.31%	0.41%	0.00%
"	1.60	8130	8050	8060	8028	-0.98%	-0.86%	-1.26%
"	1.46	7600	7565	7575	7573	-0.46%	-0.32%	-0.35%
"	1.40	7460	7363	7373	7386	-1.30%	-1.17%	-1.00%
"	1.29	7000	6997	7003	7033	-0.04%	0.04%	0.47%
"	1.20	6770	6697	6700	6726	-1.08%	-1.03%	-0.66%
"	1.10	6180	6364	6366	6361	2.97%	3.00%	2.92%
"	1.00	6100	6027	6028	5976	-1.19%	-1.17%	-2.04%
"	0.95	5800	5854	5855	5778	0.94%	0.95%	-0.38%
"	0.70	4650	4842	4842	4774	4.14%	4.13%	2.66%
"	0.56	4050	4177	4176	4232	3.13%	3.11%	4.50%
TACOT	1.85	7250	7707	7711	7461	6.31%	6.36%	2.92%
TATB	1.88	7760	8229	8236	8168	6.05%	6.13%	5.25%
"	1.85	7660	8104	8112	8020	5.80%	5.90%	4.70%
TETRYL	1.73	7720	7706	7715	7587	-0.18%	-0.06%	-1.72%
"	1.71	7850	7638	7647	7516	-2.70%	-2.58%	-4.25%
"	1.68	7500	7536	7546	7418	0.49%	0.62%	-1.09%
"	1.61	7580	7304	7314	7235	-3.65%	-3.50%	-4.56%
"	1.36	6680	6528	6539	6433	-2.27%	-2.11%	-3.69%
"	1.20	6340	6076	6084	6053	-4.17%	-4.04%	-4.53%
TNT	1.64	6930	7028	7039	7124	1.42%	1.57%	2.80%
"	1.45	6500	6372	6383	6438	-1.98%	-1.80%	-0.95%
"	1.36	6200	6085	6096	6153	-1.85%	-1.67%	-0.76%
"	1.00	5000	5056	5063	5119	1.13%	1.25%	2.38%
"	0.80	4340	4449	4453	4513	2.52%	2.60%	3.98%
BTF	1.86	8490	8585	8585	8710	1.12%	1.12%	2.59%
"	1.76	8260	8248	8248	8324	-0.14%	-0.14%	0.78%
HNB	1.97	9300	8716	8711	9340	-6.28%	-6.34%	0.43%
TNM	1.64	6360	6203	6200	6364	-2.47%	-2.52%	0.07%
TNTAB	1.74	8580	8467	8467	8739	-1.32%	-1.32%	1.85%
FEFO	1.59	7500	7317	7373	7345	-2.44%	-1.69%	-2.07%
LX-04	1.86	8460	8353	8356	8268	-1.27%	-1.23%	-2.27%
LX-07	1.87	8640	8605	8606	8543	-0.41%	-0.40%	-1.13%
LX-09	1.84	8810	8835	8836	8834	0.29%	0.29%	0.27%
LX-10	1.86	8820	8778	8778	8748	-0.47%	-0.48%	-0.81%
LX-11	1.86	8320	8146	8159	8040	-2.09%	-1.93%	-3.36%
AP	1.00	3700	3729	3729	3936	0.78%	0.78%	6.37%
LX-15	1.58	6840	6639	6669	6765	-2.94%	-2.51%	-1.10%
LX-17	1.91	7630	7924	7933	8008	3.86%	3.97%	4.96%
PBX-9010	1.78	8370	8062	8069	8247	-3.67%	-3.59%	-1.47%
PBX-9407	1.60	7910	7761	7769	7804	-1.88%	-1.78%	-1.34%
PBX-9502	1.91	7710	8070	8078	8112	4.67%	4.78%	5.21%
PBX-9503	1.90	7720	8138	8146	8218	5.42%	5.51%	6.45%
					MAE[a] =	1.76%	1.73%	1.90%
					RMS =	2.37%	2.34%	2.51%

[a]Mean absolute error (MAE) is defined in the inset equation in Fig. 4.
[b]Root mean squared (RMS) error is defined in the inset equation in Fig. 4.

The equilibrium compositions in Figs. 6.a and 6.b are similar up to about 6,000 K and depart significantly at higher temperatures. The JCZS2i and NASA predictions use newer specific heat fits that are good to 20,000 K. The specific heats were calculated from molecular constant data using ideal gas partition functions.[20] The ideal gas EOS is appropriate for rarefied air at high temperatures.

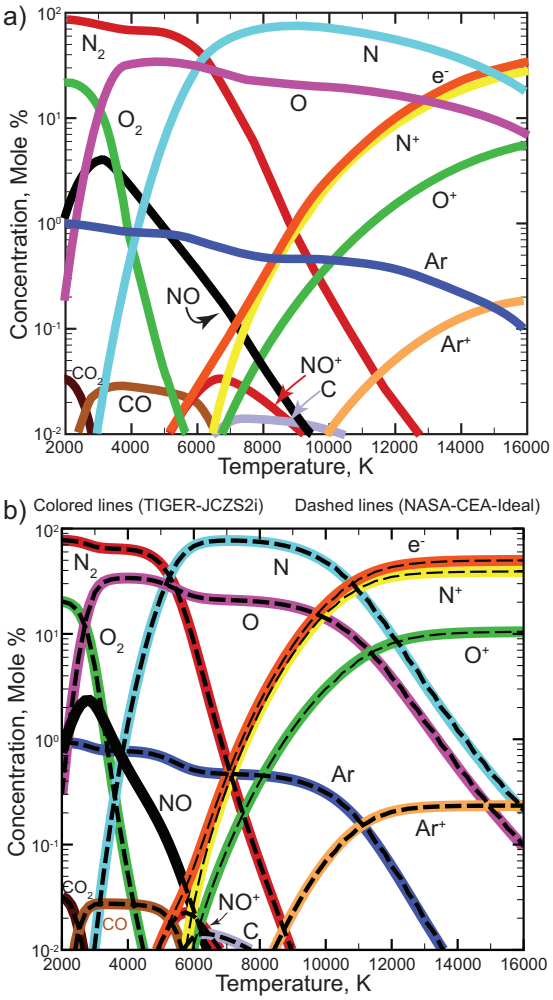

Fig. 6 Rarefied air at 0.01 atm from a) Vincenti and Kruger[19] and b) calculated with improved C_p fits[20] using both the JCZS2i database and the NASA-CEA code[3].

Figure 7 shows the effect of high pressure on the gas compressibility and the equilibrium air composition at 100,000 atm. We have assumed the Debye-Hückel effect to be negligible for the JCZS2i calculations. The Debye-Hückel effect accounts for interaction energy of the ions. This assumption is justified as shown in the inset plot in Fig. 7.A. The inset plot shows Hilsenrath and Klein's[21] calculation of the Debye-Hückel effect. Even at 15,000 K, the change in compressibility is only 0.1. However, real gas effects are significant especially at low temperatures and high pressures.

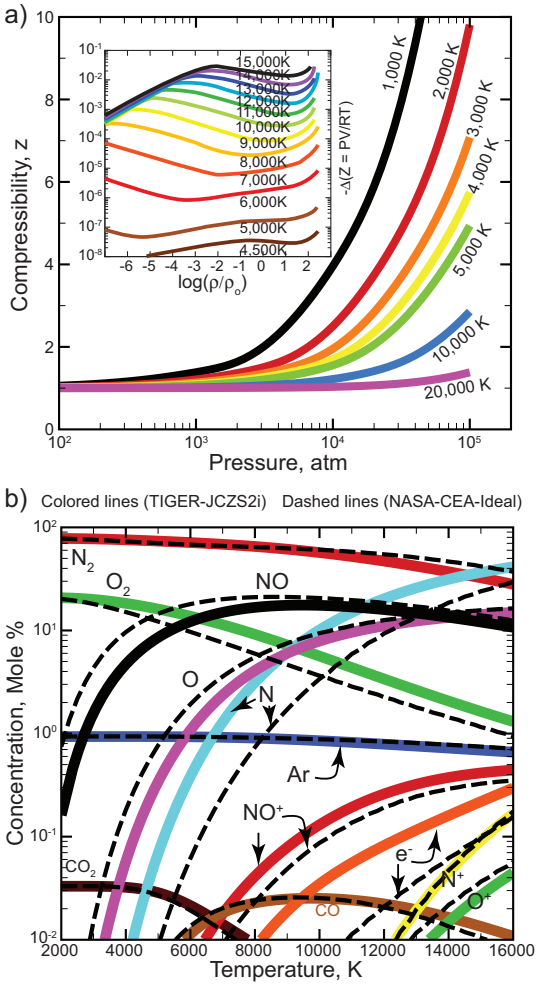

Fig. 7. The a) compressibility and b) equilibrium gas composition of air at 100,000 atm. The inset[21] shows the Debye-Hückel effect to be negligible.

Air Shock from Comp-B Detonation

CTH-TIGER has the unique capability to go from the detonation state to hot ionized air. An example calculation is shown in Fig. 8, which shows various profiles 8-μs after initiating a 5-cm radius cylinder of Comp-B in the center. We used a program burn with the EOS of the reaction products calculated with the JCZS database and fit to a JWL-EOS for use in the hydrocode. The air composition was chosen to be the same as the air composition in Figs. 6 and 7: 78.08% N2, 20.95% O2, 0.93% Ar, 0.033% CO2, and 0.003% Ne.

Figure 8 shows that the air shock exceeds 10,000 K. In the 1.4 mm wide air shock, nitrogen dissociates to form significant amounts of the nitrogen radical. The temperature is hot enough to strip electrons from the nitrogen radical to form positive nitrogen ions. Significant amounts of NO and NO^+ are also formed in the air shock.

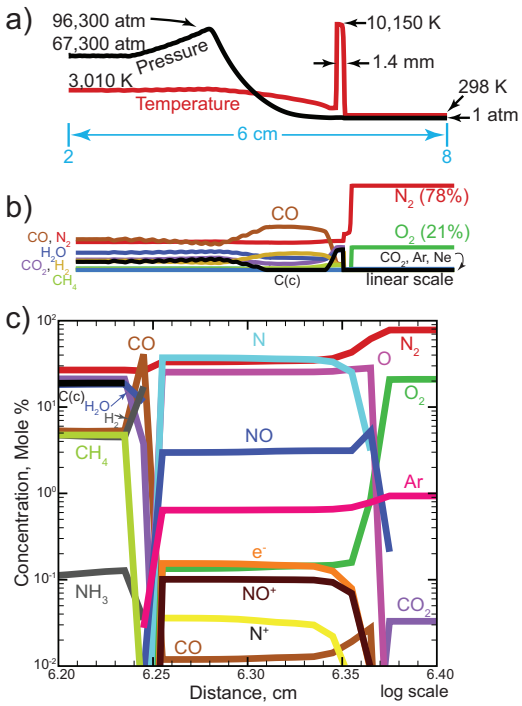

Fig. 8. Comp-B detonation in air with profiles of a) temperature and pressure, b) species composition, and c) the air shock composition.

Summary and Conclusions

The JCZS-EOS database was improved by incorporating piecewise specific heat fits of NASA's latest specific heat parameters. The new EOS database, referred to as the JCZS2i database, also considers over 200 ionic species, as well as a new condensed water equation of state.

The JCZS2i database was used to calculate various properties of water: 1) temperature dependent molar volume of condensed water, 2) shock Hugoniot, 3) sound speed, 4) pressure dependent melting point, and 5) a simple phase diagram that includes the melt line, the sublimation line, and the vapor dome. The predictions of these water properties were within experimental error.

The JCZS2i database is expected to give accurate results during expansions to low pressure when liquid water is formed. Although the JCZS database includes liquid water, the specific heat for the older database does not match measured specific heat. The EXP6 database does not include liquid water as a product.

The JCZS2i EOS database was used to calculate detonation velocity for 59 explosives at various densities. The predicted velocities were similar to the JCZS[1] database predictions, which have the same intermolecular potential parameters and the same specific heat at detonation temperatures. Detonation velocity calculations were also compared to the EXP6 EOS database. The absolute mean absolute error for the JCZS, JCZS2i, and EXP6 databases were 1.76%, 1.73%, and 1.90%, respectively. We consider these errors to be the same order as the experimental error.

The JCZS2i EOS database was used to calculate the equilibrium composition of rarified air as well as air at 100,000 atm. These results were compared to calculations performed by the National Bureau of Standards[19] in the 1950's as well as more recent predictions by the NASA – CEA[3] code using improve specific heat fits.[20] The JCZS2i predictions were identical to the newer NASA-CEA predictions, since this database uses the same specific heats. Calculations of high-pressure air show the importance of including compressibility at high pressures.

The equilibrium composition of an air shock produced by detonating Comp-B in air was calculated with CTH-TIGER. The air shock was 1.4 mm thick and was over 10,000 K. The shock was composed of primarily, N_2, N, O, NO, Ar, O_2, e^-, NO^+, N^+ and CO. The JCZS2i EOS database gives us capability to do accurate calculations of ion concentrations at high temperatures and pressures.

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