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Using Corresponding State Theory to Obtain Intermolecular Potentials to Calculate Pure Liquid Shock Hugoniot

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ABSTRACT

Determination of product species, equations-of-state (EOS) and thermochemical properties of high explosives and pyrotechnics remains a major unsolved problem. Although, empirical EOS models may be calibrated to replicate detonation conditions within experimental variability (5-10%), different states, e.g. expansion, may produce significant discrepancy with data if the basic form of the EOS model is incorrect. A more physically realistic EOS model based on intermolecular potentials, such as the Jacobs Cowperthwaite Zwisler (JCZ3) EOS [1], is needed to predict detonation states as well as expanded states.

Predictive capability for any EOS requires a large species data base composed of a wide variety of elements. Unfortunately, only 20 species have known JCZ3 molecular force constants. Of these 20 species, only 10 have been adequately compared to experimental data such as molecular scattering or shock Hugoniot data. Since data in the strongly repulsive region of the molecular potential is limited, alternative methods must be found to deduce force constants for a larger number of species. The objective of the present study is to determine JCZ3 product species force constants by using a corresponding states theory.

Intermolecular potential parameters were obtained for a variety of gas species using a simple corresponding states technique with critical volume and critical temperature. A more complex, four parameter corresponding state method with shape and polarity corrections was also used to obtain intermolecular potential parameters. Both corresponding state methods were used to predict shock Hugoniot data obtained from pure liquids. The simple corresponding state method is shown to give adequate agreement with shock Hugoniot data.

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INTRODUCTION

Predictive capability for any EOS requires a large species data base composed of a wide variety of elements. Unfortunately, only 20 species have known JCZ3 molecular force constants. Of these 20 species, only 10 have been adequately compared to experimental data such as molecular scattering or shock Hugoniot data. The thermochemical properties of pyrotechnics are difficult to calculate at high pressures due to complex compositions which produce various condensed-phases. For example, 33 gas-phase species and 24 condensed-phase species composed of Al, Cl, K, O, or Ti, typical components in a report charge (Ti/Al/KClO₄), have been used with the empirical BKWS-EOS [2] to calculate detonation states. An overview of detonation physics is found in Ref. [3].

JCZ3-EOS - The JCZ3-EOS uses an equation based on P-V-T relationships similar to the Mie-Grüneisen EOS [4]

$$P = \frac{G(V, T)nRT}{V} + P_0(V) \quad (1)$$

where P , n , R , T , and V represent the pressure, number of moles, universal gas constant, and volume, respectively. The form of the Grüneisen function, G , and the volume dependent internal pressure function, P_0 , is documented (e.g., Ref. 1). The volume-dependent internal pressure function, $P_0(V)$ is composed of the exponential 6 potential function:

$$\varphi(r) = \varepsilon \left[\left(\frac{6}{\eta - 6} \right) \exp[\eta(1 - r/r^*)] - \left(\frac{\eta}{\eta - 6} \right) \left(\frac{r^*}{r} \right)^6 \right] \quad (2)$$

where ε is the well depth for the pair potential and r^* is the radius of the minimum pair potential energy. The molecular force parameters ε , η , and r^* are required for each product species. The force constant, ε , is often given as ε/k , where k is Boltzmann's constant.

Corresponding States Methods - The idea of the corresponding states method as originally proposed by van der Waals [5] is that the behavior of all substances is the same at the same reduced temperature (T/T_c), pressure (P/P_c), and volume (V/V_c). Pitzer [6] derived van der Waals' corresponding states principle by assuming 1) classical statistics, 2) spherically symmetric nonpolar molecules, 3) similar molecular vibrations for both liquid and gaseous states, and 4) conformal molecules. The conformal assumption implies that the functionality of the intermolecular potential is the same although the force constants vary from molecule-to-molecule.

The corresponding states method can be applied with confidence to molecules which comply to Pitzer's assumptions. These molecules include the heavier rare gases such as Argon, Krypton, and Xenon as well as spherically symmetric molecules such as methane. Hydrogen, Helium, and Neon do not follow corresponding states because of quantum effects [7].

Pitzer's Deviation - Deviations from corresponding states estimates were determined by Hougen and Watson [8] to range from 5 to 35%. These deviations result from molecules which are not perfectly spherical or nonpolar. To improve corresponding states estimates for molecules which are not perfectly spherical, Pitzer and coworkers [7,9], introduced the *acentric factor*, ω , to account for deviations from spherical molecules:

$$\omega = -\log P_r - 1.000 \quad (3)$$

where the reduced pressure, P_r , is evaluated at a reduced temperature, T_r , of 0.7. The form of Eq. (3) was chosen since the reduced vapor pressure is almost precisely 0.1 at the reduced temperature of 0.7 for corresponding molecules Ar, Kr, Xe, and CH_4 , giving an ω of essentially zero for these molecules.

Pitzer et al. [7,9] chose to expand the compressibility factor function as a power series in the acentric factor

$$z = z_o + \omega z_1 + \dots \quad (4)$$

where z_o , z_1 , etc. are each functions of T_r and P_r giving a three parameter corresponding states equation to predict compressibility. This approach improved predictions over simple corresponding state theory for nonspherical molecules [7]. Pitzer et al. [7,9] concluded that a three parameter corresponding state theory is inadequate for highly polar molecules such as water or ammonia. A fourth parameter is necessary for accurate corresponding state correlation.

Lee and Kesler's Improvements - Lee and Kesler improved Pitzer's corresponding states model given in Eq. (4) using a Taylor's series expansion about the simple fluid with respect to the acentricity factor:

$$z = z_o + \frac{\omega}{\omega_r}(z_r - z_o) \quad (5)$$

where the subscripts o and r refer to a simple reference fluid with an acentric factor of zero and a heavy reference fluid, respectively. The data used to determine the constants for the simple fluid were principally Ar, Kr, and methane. N-octane was chosen as the heavy reference fluid. The Lee-Kesler (LK) model is useful for predicting the thermodynamic properties of nonpolar and slightly polar fluids. The success of the LK corresponding states method is due to the accurate analytic equation of state which represent the two reference fluids [10]. The LK model is a three parameter corresponding states method in ω , T_c , and P_c .

Extension to Polar Molecules - To predict thermodynamic properties for both polar and nonpolar fluids, Wilding and Rowley [10] extended the LK model to account for both geometric as well as polar contributions. The Extended Lee-Kesler (ELK) model [10] is written as a dimensionless Taylor's series expansion about a simple fluid with respect to geometry and polarity:

$$J = J_o + (\partial J / \partial \alpha)_{T_r, P_r, \beta}(\alpha - \alpha_o) + (\partial J / \partial \beta)_{T_r, P_r, \alpha}(\beta - \beta_o) + O(\alpha^2, \beta^2, \alpha\beta) \quad (6)$$

where J_o is the simple fluid dimensionless property such as compressibility at the given reduced conditions, α is a size and shape constant, and β is a polarity constant. To apply Eq. (6) to an arbitrary molecule, high order terms are assumed negligible and both partial derivatives, the geometric constant, and the polarity constant must be defined. The LK model considers only the first two terms on the right-hand-side of Eq. (6).

The partial derivatives can be determined by using corresponding molecules at the same T_r and P_r as the test molecule. The partial derivative with respect to shape, $(\partial J / \partial \alpha)_{T_r, P_r, \beta}$, is determined using argon and n-hexane. In the present study, n-hexane is used instead of n-octane, which was used by Rowley et al. as well as Lee and Kesler, because pure shock Hugoniot data

needed to deduce force constants is available for n-hexane and not for n-octane. The shape partial derivative becomes:

$$(\partial J/\partial \alpha)_{T_r, P_r, \beta} = (J_{hx} - J_{ar})/\alpha_{hx} \quad (7)$$

where the subscripts ar and hx refer to argon and n-hexane, respectively. The shape factor for argon is assumed to be zero.

The polar partial derivative can be obtained by using water and a hypothetical molecule which is the same size as water but is nonpolar (*i.e.* β is zero). Since the hypothetical molecule is nonpolar, thermodynamic properties for the hypothetical molecule can be obtained using Eq. (6) or by Eq. (7). The polar partial derivative becomes:

$$(\partial J/\partial \beta)_{T_r, P_r, \alpha} = (J_{h2o} - J_{hyp})/\beta_{h2o} \quad (8)$$

$$J_{hyp} = J_{Ar} + \alpha_{h2o}(J_{hx} - J_{ar})/\alpha_{hx} \quad (9)$$

where the subscripts *h2o* and *hyp* refer to water and the hypothetical molecule, respectively. Substitution of Equations (7)-(9) into Equation (6) gives the general four-parameter ELK equation applicable to all types of molecules:

$$J = J_{ar} + \alpha(J_{hx} - J_{ar})/\alpha_{hx} + \beta\{J_{h2o} - [J_{Ar} + \alpha_{h2o}(J_{hx} - J_{ar})/\alpha_{hx}]\}/\beta_{h2o} \quad (10)$$

In summary, the ELK method is a four parameter (T_c , P_c , α , and β) corresponding states technique that uses three well-characterized reference fluids. The first reference fluid is a pure corresponding states fluid (argon), the second fluid is used to correct for geometric effects (hexane), and the third fluid is used to correct for polar effects (water).

The geometrical parameter α must be independent of polarity. Wilding and Rowley [10] based α on the radius of gyration, r , a purely geometric quantity available from molecular structure information. The functionality of α is determined by correlating the acentricity factor, ω , for nonpolar fluids with the radius of gyration:

$$\alpha = -7.706 \times 10^{-4} + 0.0330r + 0.01506r^2 - 9.997 \times 10^{-4}r^3 \quad (11)$$

This correlation is applicable to all fluids regardless of polarity and represents only geometrical effects [10]. The value of α is zero for the reference fluid argon.

The polar parameter β is obtained by application of Eq. (10) to any known value of J . Wilding and Rowley [10] use the liquid density at some T_r and P_r to determine the compressibility by setting J equal to Z and calculating β directly from Eq. (10). The value of β for the reference molecule water is set equal to one. For hydrogen bonding molecules, especially alcohols, enthalpic properties are not predicted as well as volumetric properties. For more accuracy, the heat of vaporization, ΔH_v , at the normal boiling point can be used to calculate β and may give better results. To differentiate between the two methods of calculating the polar parameter β , a subscript h is used to denote the enthalpic origins: β_h .

APPLICATION OF ELK TO JCZ3 FORCE CONSTANTS

The force constants for the JCZ3-EOS can be determined by applying Eq. (10) to the dimensionless force constants as follows:

$$\underbrace{\frac{r^*}{V_c^{1/3}} = \frac{r_{ar}^*}{V_{c,ar}^{1/3}}}_{\text{Corresponding States}} + \underbrace{\frac{\alpha}{\alpha_{hx}} \left(\frac{r_{hx}^*}{V_{c,hx}^{1/3}} - \frac{r_{ar}^*}{V_{c,ar}^{1/3}} \right)}_{\text{Shape Corrections}} + \underbrace{\frac{\beta}{\beta_{h2o}} \left\{ \frac{r_{hx}^*}{V_{c,hx}^{1/3}} - \left[\frac{r_{ar}^*}{V_{c,ar}^{1/3}} + \frac{\alpha_{h2o}}{\alpha_{hx}} \left(\frac{r_{hx}^*}{V_{c,hx}^{1/3}} - \frac{r_{ar}^*}{V_{c,ar}^{1/3}} \right) \right] \right\}}_{\text{Polar Corrections}} \quad (12)$$

$$\underbrace{\frac{\epsilon/k}{T_c} = \frac{\epsilon_{ar}/k}{T_{c,ar}}}_{\text{Corresponding States}} + \underbrace{\frac{\alpha}{\alpha_{hx}} \left(\frac{\epsilon_{hx}/k}{T_{c,hx}} - \frac{\epsilon_{ar}/k}{T_{c,ar}} \right)}_{\text{Shape Corrections}} + \underbrace{\frac{\beta}{\beta_{h2o}} \left\{ \frac{\epsilon_{hx}/k}{T_{c,hx}} - \left[\frac{\epsilon_{ar}/k}{T_{c,ar}} + \frac{\alpha_{h2o}}{\alpha_{hx}} \left(\frac{\epsilon_{hx}/k}{T_{c,hx}} - \frac{\epsilon_{ar}/k}{T_{c,ar}} \right) \right] \right\}}_{\text{Polar Corrections}} \quad (13)$$

The first terms marked "Corresponding States" of Eq. (12) and (13) represent the simple-corresponding states law used by Ross and Ree [11] to deduce force constants as proposed originally by Hirschfelder et al. [12]. The last two terms on the right hand side of Eq. (12) and (13) represent geometrical deviations and polar deviations, respectively.

Force Constants - Table 1 gives the force constants found in the literature for the JCZ-EOS. Accurate force constants for argon, n-heptane, and water are needed to apply Eq. (12) and (13). As shown in Table 1, the exponential 6 potential parameters differ significantly between investigators. Pure shock Hugoniots for Ar, CH₄, CO₂, H₂, H₂O, N₂, NH₃, O₂, and Xe predicted using the JCZ3-EOS as implemented in the CHEETAH code [19] using force constants from Table 1 are compared to measurements in Fig 1. The force constants which fit the Hugoniot data the best are shaded in Table 1. Note that η is 13 for the best fits. Within experimental uncertainty, Ross and Alder [20] indicate that the potential for argon can be fit with any η between 12 and 14 with 13 being the best value. This seems to be the case for other molecules as shown in Fig 1. For the present study, η is assumed to be 13 for all molecules.

N-hexane Hugoniot - In order to apply Eq. (12) and (13) to any molecule, the force constants for n-hexane need to be determined. Fig 2 shows predicted and measured pure shock Hugoniot for n-hexane. The n-hexane force constants were obtained by using simple-corresponding states theory to obtain r_{hx}^* and best fitting ϵ/k to data. The value for r_{hx}^* and ϵ/k were determined to be 6.6 Å and 300 K, respectively.

HUGONIOT CALCULATIONS

To determine the validity of the ELK method applied to the JCZ3 force constants, Eq. (12) and (13) were applied to various test molecules. The predicted JCZ3 force constants are given in Table 2 using the simple corresponding states method, the ELK method using β , and the ELK method using β_h . The parameters required for each molecule are given in Table 3. The size and shape parameter, α , and the polar parameters β and β_h were obtained from Ref. [32].

Predictions using simple corresponding state theory (SCS) as well as the ELK method are compared to measured Hugoniots in Fig 3 and 4. In general, the predictions using the ELK

method are better than using the SCS method. The exceptions are dibromomethane, methanol and acetone, although the ELK predictions are in acceptable agreement with the limited set of Hugoniot data available. Only two Hugoniot points are available for methanol and acetone.

The comparison between the predicted and experimental shock Hugoniot data for hexane and water, as shown in Figure 4, show the influence of shape and polar contributions. Shape effects move the Hugoniot curve up, whereas polar effects move the Hugoniot curve down in relation to the experimental data. The agreement with Hugoniot data in these high pressure regimes is promising for increasing the JCZ3-EOS product species database.

CAVEATS

Unfortunately, not all chemical species have critical properties. Out of 750 gas species listed in the JANNAF tables [33], 150 species have both the critical temperature and critical volume. Thus alternative methods must be used to determine the intermolecular force constants. Hobbs et al. [34, 35] have obtained intermolecular force constants for all 750 gases using a combination of corresponding state theory, pure liquid shock Hugoniot data from the present study, and fit values using an empirical EOS. The large database can be used with the CHEETAH computer program [19] to permit intermolecular potential based calculations of exotic energetic materials of complex elemental composition.

SUMMARY AND CONCLUSION

Pure shock Hugoniot calculations have been performed with the JCZ3-EOS which is based on the exponential 6 potential function. The radius of the minimum pair potential energy and the well depth of the exponential 6 potential well has been estimated using simple corresponding states methods as well as the ELK corresponding states method. The simple corresponding state method is shown to give adequate agreement with shock Hugoniot data.

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Table 1. Repulsive force constants for an exponential 6 potential function

Species	r^* , Å	ϵ/k , K	η^*	Ref	Species	r^* , Å	ϵ/k , K	η	Ref
Ar	3.83	119	15	13	HCl	4.14	262	---	19
Ar	3.85	122	13	11	HCO ₂ H	4.15	463	---	19
Ar	3.93	120	12.9	14	He	3.14	9.16	12.4	17
C	3.15	100	---	15	HF	3.30	100	---	16
CF ₄	5.00	220	---	16	F ₂	3.50	200	---	16
CH ₄	4.29	154	14	13	N ₂	4.05	120	15	13
CH ₄	4.22	154	13	11	N ₂	4.09	102	13	11
CH ₄	4.20	156	13.5	17	N ₂	4.11	117	13.5	17
CH ₄	4.39	136	12.2	14	N ₂	4.10	101	13.5	14
Cl ₂	4.61	337	---	19	NF ₃	4.10	200	---	16
CO	4.05	120	15	13	NH ₃	3.35	138	---	16
CO	4.09	108	13	11	NH ₃	4.15	154	---	15
CO	4.12	108	13	18	NH ₃	3.44	474	13	18
CO ₂	4.20	200	15	13	NH ₃	3.50	138	17	17
CO ₂	4.17	246	13	11	NH ₃	4.00	200	11.2	14
CO ₂	4.21	249	13.8	14	NO	3.97	105	15	13
H ₂	3.34	37.0	14	13	NO	3.97	113	13	18
H ₂	3.43	36.4	11.1	18	NO	3.56	131	---	15
H ₂	3.00	30	13.5	17	NO	3.9	105	12	17
H ₂	3.60	36.4	10.8	14	O ₂	3.73	132	15	13
H ₂ O	3.35	138	14	13	O ₂	3.84	125	13	11
H ₂ O	3.06	356	13	18	O ₂	3.93	133	12.6	14
H ₂ O	3.37	135	13.5	17	Xe	4.47	235	13	11
H ₂ O	3.68	300	10.3	14	Xe	4.45	231	13	17

* Fickett [13] uses 15 for η and Ross and Ree [11] use 13 for η when it has not been determined experimentally. Blank values for η in this table have not been reported.

Table 2. Predicted force constants using simple corresponding states and ELK*

Name	Symbol	$r^*, \text{\AA}$ scs	$\epsilon/k, \text{K}$ scs	$r^*, \text{\AA}$ β	$\epsilon/k, \text{K}$ β	$r^*, \text{\AA}$ β_h	$\epsilon/k, \text{K}$ β_h
argon	Ar	3.85	122	3.85	122	3.85	122
carbon tetrachloride	CCl_4	5.95	450	5.98	631	5.98	631
chloroform	CHCl_3	5.67	434	5.75	600	5.72	593
dibromomethane	CH_2Br_2	5.54	494	5.64	631	6.66	884
dichloromethane	CH_2Cl_2	5.20	413	5.00	459	5.11	484
diiodomethane	CH_2I_2	5.92	604	5.25	559	5.96	759
methanol	CH_3OH	4.48	415	3.96	333	3.59	240
methane	CH_4	4.23	154	4.23	154	4.23	154
carbon dioxide	CO_2	4.15	246	4.16	264	4.16	264
acetone	$\text{C}_3\text{H}_6\text{O}$	5.42	411	5.02	441	5.16	472
hexane	C_6H_{14}	6.56	411	6.60	600	6.60	600
water	H_2O	3.52	523	3.06	356	3.06	356
nitrogen	N_2	4.09	102	4.10	106	4.06	104
ammonia	NH_3	3.81	328	3.42	254	3.47	268
oxygen	O_2	3.82	125	3.83	131	3.83	131
xenon	Xe	4.48	234	4.48	234	4.48	234

* scs stands for simple-corresponding states theory. β and β_h indicate that the polar interactions were estimated using compressibilities and enthalpies, respectively.

Table 3. Parameters required by ELK method for selected polar and nonpolar molecules

Name	Symbol	T _c K	P _c atm	V _c cc/mol	r Å	ρ g/cc	T _r K	P _r atm	T _{bp} K	α	β	β _h
argon	Ar	151	48	75	0	1.41	86	1.97	87	-0.0008	0*	0
carbon tetrachloride	CCl ₄	556	45	276	3.46	1.58	298	1	350	0.2522	0	0
chloroform	CHCl ₃	536	54	239	3.18	1.49	293	1	334	0.2242	-0.0665	-0.0264
dibromomethane	CH ₂ Br ₂	611	71	223	2.36	2.48	298	1	270	0.1479	-0.1143	-1.5322
dichloromethane	CH ₂ Cl ₂	510	60	185	2.34	1.32	298	1	313	0.1463	0.3333	0.1667
diiodomethane	CH ₂ I ₂	747	54	272	2.44	3.31	298	1	455	0.1548	0.895	-0.0266
methanol	CH ₃ OH	513	80	118	1.54	0.79	293	1	338	0.0819	0.9086	1.5357
methane	CH ₄	191	46	99	0.023	0.43	112	1	112	0	0	0
carbon dioxide	CO ₂	304	73	94	0.99	0.78	293	10	195	0.0458	0	0
acetone	C ₃ H ₆ O	508	46	209	2.74	0.79	293	1	329	0.1822	0.603	0.3961
hexane	C ₆ H ₁₄	508	30	370	3.81	0.66	293	1	342	0.2885	0.	0.
water	H ₂ O	647	218	57	0.62	1.00	298	1	373	0.025	0.9997	0.9992
nitrogen	N ₂	126	34	90	0.55	0.81	77	1	78	0.0216	-0.022	0.0518
ammonia	NH ₃	406	111	73	0.85	0.68	240	2	240	0.0378	0.7914	0.6787
oxygen	O ₂	155	50	73	0.68	1.14	90	1	90	0.0283	0	0
xenon	Xe	290	58	118	0	2.95	165	1	165	-0.0008	0	0

* βs are zero for nonpolar molecules.

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- Fig 1. Measured (symbols) and predicted (lines) pure shock Hugoniot: A) argon, B) methane, C) carbon dioxide, D) hydrogen, E) water, F) nitrogen. References shown in legend.
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- Fig 2. Measured and JCZ3 predicted shock Hugoniot for n-hexane.
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Pressure, thousand of atmospheres

Volume, cc/g

Pressure, thousand of atmospheres

Volume, cc/g

Pressure, thousand of atmospheres

Volume, cc/g

Pressure, thousand of atmospheres

Volume, cc/g

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