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**MODIFICATION OF THE USER FRIENDLY THERMODYNAMIC
CODE TO INCLUDE THE EFFECTS OF MINOR SPECIES**

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13. ABSTRACT (Maximum 200 words) Three year ago, a user friendly thermodynamic code was developed at Picatinny Arsenal for the personal computer. This code enabled the engineer to calculate the flame temperature of a new propellant formulation on a personal computer thus eliminating the need for access to a mainframe computer. The new code uses the highly accurate equation of state for propellant gases developed by Powell, Wilmot, Haar and Klein and does not rely on the two term virial expansion employed in BLAKE and the ICT codes. This equation of state was developed to accurately calculate the pressures of mixtures of water, carbon monoxide, carbon dioxide, hydrogen, and nitrogen but was not designed to take into account the contributions of minor species. As a result, the effects of all minor species were described in a very approximate way. This defect in the code has now been removed. For many minor species which are predicted to occur in a propellant gas after combustion, the equation of state parameters are not known. Both BLAKE and the ICT codes assign generic parameters to all of these minor species. Second and third virial coefficients are then calculated and used in their virial expansion. The contribution of all minor species are assumed to be approximated by a Lennard-Jones gas with epsilon divided by Boltzmann's Constant = 100K and sigma = 3.0 Angstrom. Expressions were developed for the second virial coefficient and the molecular volume and incorporated as a (cont)			
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sixth species into the equation of state proposed by Powell, Wilmot, Haar and Klein. Generally good agreement with BLAKE and the ICT code was observed up to a loading density of 0.2 gm per cubic centimeter. As density increases, real gas effects cause the calculated flame temperature to decrease and the calculated pressure to increase. A computer program to perform the calculations has been devised for a personal computer.

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INTRODUCTION

Flame temperature calculations are very important in combustion for several reasons. They indicate the maximum temperature at which the energy released during combustion is available to do useful work and they also signify possible material and cooling requirements. The chemical equilibria involved in these calculations can be quite complex as can be ascertained by reading the review article by Zeleznik and Gordon (ref 1). Since most combustion takes place at atmospheric pressure it is perfectly valid to treat the combustion products as ideal gases. Perhaps the best known of these types of computer programs is the NASA Lewis (ref 2) code. More recently STANJAN (ref 3) has been developed which will run on a personal computer. However, there is one area of combustion research where the ideal gas approximation is not valid. This area involves the development of propellants for gun applications. Propellants are burned in high pressure vessels and the pressure achieved can exceed 700 MPa. An early attempt to model this type of experiment was developed by Hirschfelder and Sherman (ref 4). The advantage of this method was that the calculations could be done by hand. As electronic computers became more readily available, there was a great deal of interest in developing computer codes which were more accurate. BLAKE (ref 5) and ICT (ref 6) codes were designed for high pressure applications, taking real gas effects into account by using a virial equation of state terminated after the third term. Volk and Bathelt (ref 6) use the Stockmayer and the Lennard-Jones potentials to calculate virial coefficients for polar and nonpolar molecules respectively. Freedman (ref 5) computed the third virial coefficient using the assumption that the molecules are hard spheres with a radius equal to 0.81 time the Lennard-Jones radius.

An important contribution to the theory of hot, dense gases was provided by Haar and Shenker (ref 7). These workers approximated the equation of state for a real gas using the second virial coefficient and a closed form expression for all the other virial coefficients using the solution to the hard sphere Percus-Yevick equation. In their equation the hard sphere diameter or "molecular volume" was treated as a parameter and was assumed to be temperature dependent. This approach was developed for H_2O , CO , CO_2 , H_2 , and N_2 by Powell, Wilmot, Haar and Klein (ref 8). A BLAKE implementation of this work was achieved by Powell, Wilmot, and Almeyda (ref 9). More recently, a new thermodynamic code was developed by Vladimiroff, Carignan, Chiu and Macpherson (ref 10) specifically designed for the personal computer. This code also used the Haar and Shenker (refs 7 and 8) approach except that the contributions of all minor species were described in a very approximate way. The purpose of the present work is to develop a more reasonable approximation of the effects of all the minor species.

THE EQUATION OF STATE

The flame temperature calculation is straightforward in concept. First it is necessary to guess a flame temperature. Then an equilibrium composition for the elements in the propellant is computed at the assumed temperature by minimizing the free energy. The energy available is obtained by subtracting the heat of formation of the products from the heat of formation of the propellant. This energy is used to heat up the products to some new temperature. The equilibrium products are calculated at the new temperature and the procedure continues in an iterative manner until the temperature does not change in two successive steps. Mathematical complexities are introduced when many combustion products are involved since minimizing the free energy is a nonlinear process. Also, additional problems are introduced when the products are assumed to obey an equation of state more complicated than the ideal gas equation. The problem of interest is to determine the chemical composition of products in an adiabatic closed bomb at constant volume and temperature (the flame temperature). The condition for equilibrium is that A , the Helmholtz free energy is a minimum. The minimization procedure is carried on as before (refs 2 and 10).

Since guns operate at high pressure, the ideal gas equation can not be used. Both BLAKE (ref 5) and the ICT (ref 6) codes employ a truncated virial expansion, keeping the second and third virial coefficients. However, as the pressure level at which guns operate increases, there is some doubt as to the accuracy of this approximation. Also, it is of interest to establish the real gas effects dictated by a more accurate equation of state. In this work the equation of state proposed by Haar and Shenker (ref 7) is used. Molecular dynamics calculations have shown (ref 11) that this approach should be accurate for most ballistic calculations. The equation of state proposed by Haar and Shenker (ref 7) uses temperature dependent second virial coefficients and temperature dependent molecular volumes for each species. The compressibility factor, Z is then given as the sum of the second virial coefficient and a closed form formula for all the other virial coefficient given by the hard sphere solution (ref 12) to the Percus-Yevick equation (ref 13). The molecular volumes are also assumed to be temperature dependent. The resulting expression is (ref 7)

$$Z_j = (1 + y_j + y_j^2)/(1 - y_j)^3 + \rho_j(B_{jj} - b_j) \quad (1)$$

where B_{jj} is the the temperature dependent second virial coefficient of species j , b_j is the temperature dependent molecular volume of species j , ρ_j is the density and $y_j = b_j\rho_j/4$. Powell et. al. (ref 8) developed expressions for b and B for water, carbon monoxide, carbon dioxide, hydrogen and nitrogen but did not consider the minor species. Equation of state information is usually not available for most of the minor species predicted to exist as byproducts of combustion. Following Volk and Bathelt (ref 6) we

assume that all minor species can be assigned Lennard-Jones parameters of $\epsilon/k = 100\text{K}$ and $\sigma = 3.0\text{\AA}$. Thus a sixth generic species with these Lennard-Jones parameters was incorporated into our code. The second virial coefficient was found to be approximated by

$$B_{66} = 13.9025 + 483.55/\sqrt{T} - 13606/T \text{ cm}^3/\text{mole} \quad (2)$$

where T is the temperature. The Lennard-Jones compressibility factor was calculated using a five term virial expansion. The second and third virial coefficients were obtained from the work of Volk and Bathelt (ref 6). Fourth virial coefficients were taken from the tabulations of Selevanyuk and Tsykalo (ref 14). Fifth virial coefficients calculated by Barker, Leonard and Pompe (ref 15) were employed. These values were supplemented by fifth compressibility virial coefficients calculated by Kim, Henderson and Oden (ref 16) using Verlet's extension (ref 17) of Percus-Yevick theory (ref 13). For several densities and temperatures equation 2 was substituted into equation 1 and the b was adjusted so as to yield the same Z as the five term virial expansion. The core volume obtained were represented by the following equation

$$b_6 = (4.10857 - 0.18413\log(T))^3 \text{ cm}^3/\text{mole} \quad (3)$$

Equation 1 along with equations 2 and 3 were used to calculate the compressibility factor as a function of temperature and density. The results are compared to the five term virial expansion in table I. Errors as large as 6.2% are encountered at high density and low temperature. However, it should be pointed out that the density of 0.030 moles/cm^3 is close to the liquid density and other considerations (ref 8) effectively limit the use of our approach to temperatures above 850K. The expressions for b_6 and B_{66} given above were assigned to all the minor species and combined with the expressions given by Powell, Wilmot, Haar and Klein (ref 8) for the main species. Mixed second virial coefficients were assumed to be given by

$$B_{jk} = \sqrt{B_{jj} B_{kk}}$$

and mixture parameters were calculated using

$$b_{\text{mix}} = \sum X_j b_j \quad (4)$$

and

$$B_{\text{mix}} = \sum \sum X_j X_k B_{jk} \quad (5)$$

In these expressions X_j is the mole fractions of species j . The pressure is then given by

$$P = \rho_{\text{mix}} RT Z_{\text{mix}}$$

$$\rho_{\text{mix}} = \sum n_j / V$$

n_j is the number of moles of species j , V is the volume, R is the universal gas constant and Z_{mix} is calculated using equation 1 in conjunction with equations 4 and 5. The Helmholtz free energy is given by

$$A = RTJ_{\text{mix}} + A_o \quad (6)$$

where J_{mix} is defined in reference 8 and A_o is the contribution to the free energy from the molecular degrees of freedom. The assumption is made (ref 8) that these molecular degrees of freedom are not effected by the presence of other species. The chemical potential is given by (ref 8)

$$\mu_j = \left(\frac{\partial A}{\partial n_j} \right)_{T, p, n_k, k \neq j} \quad (7)$$

The internal energy U is also required in order to calculate the heat absorbed by the propellant gases

$$\frac{U}{RT} = \frac{A}{RT} - \frac{\partial}{\partial T} \left(\frac{A}{R} \right)_p \quad (8)$$

The Helmholtz free energy is minimized using the Newton-Raphson method advocated by Gordon and McBride (ref 2). However, the gradients are computed as if the chemical potentials were obtained from an ideal gas equation of state. This approximation does not seem to affect the speed of calculation but it does simplify the computer program. Convergence criteria are the same as in reference (ref 2).

THE COMPUTER PROGRAM

The mathematical considerations discussed above were coded in FORTRAN and incorporated into MCVECE (micro computer very easy chemical equilibrium) on an IBM RT PC. A real gas equation of state is used as discussed above but an ideal gas equation can be used as well by setting the parameter IDEAL = true. The program uses 40 elements and 800 product species. Thermodynamic data from the latest JANNAF tables (ref 18) are employed. Input is of the interactive type with the units being quite flexible. Data on 165 propellant constituents are contained on a file called FUELS. If it

is desirable to use some other propellant ingredient, the user will be prompted for the necessary inputs. Presently, the program is restricted to 800 product species that are contained on a file called PRODUCTS. The products are those commonly expected with standard propellants which are based on carbon, oxygen, hydrogen, and nitrogen. For special cases, special product files may have to be developed. The output of the program consists of the calculated flame temperature, the pressure in atmospheres, psi, and MPa, the impetus in Joules/gram and foot-pounds/pound and the mole fractions of the more abundant product species. An option is provided to rerun the same composition at a different loading density or to input a new composition.

RESULTS AND DISCUSSION

In order to assess the validity of the present work it is useful to compare calculated results from MCVECE with outputs from other codes (refs 5, 6, and 9). A reasonable basis of comparison is afforded by the five propellant formulations suggested by Freedman (ref 5). The formulations are reproduced in table 2. Calculations for the real gas case are presented in table 3 and compared to the values computed using BLAKE and the ICT codes. The flame temperature calculated using MCVECE is lower than for the other two codes. For a loading density of 0.2 gm/cm^3 the effect is noticeable but small. Variations of the order of 1% should be considered acceptable for thermodynamic codes so that the effect could not be considered to be physically significant. At the higher loading the MCVECE flame temperature is always lower than the flame temperature computed using BLAKE and the ICT codes. The decrease in flame temperature is due to an increase in the heat capacity of the propellant gas molecules which is a consequence of the equation of state used in this work and has already been observed (ref 9). Despite the lowering of the temperature, the pressure is either higher or the same as computed with the other two codes. This is due to the effectively infinite number of virial coefficients employed in this work. The pressure calculated for propellant four seems to contradict this observation. We do not have an explanation for this discrepancy. The impetus for the five propellants seem to be independent of the code by which it is calculated although the BLAKE (ref 5) values are systematically high at 0.6 gm/cm^3 loading density.

Because of the approximate way in which all the minor species were handled, it made no sense to make comparisons between the BLAKE implementation of the NBS equation of state (ref 9) and our previous work (ref 10). Since, the contributions of all minor species are now taken into account in a reasonable way it is possible to make the comparisons. Thermodynamic calculations for the five propellants listed in table 2 were kindly provided by Dr. Wilmot. The comparison is made in table 4. With the exception of propellant 5 the flame temperatures calculated with the NAVY code is systematically higher than our results. The largest difference is 1.9% at a loading density of 0.6 gm/cm^3 for propellant 2. The calculated pressures are also systematically higher than our

calculations with the largest difference being 5% also for propellant 2 at the highest loading density considered. The discrepancies in the impetus are about the same as in the flame temperature. Since both approaches are trying to do the same thing (although not exactly in the same way) the differences seem too large. Some additional effort will be required to reconcile the two methods.

CONCLUSIONS

The thermochemical computer code developed earlier has been modified to explicitly calculate the effects of minor species. All minor products were assumed to be described by a Lennard-Jones gas with $\epsilon/k = 100\text{K}$ and $\sigma = 3.0\text{\AA}$. Computed thermodynamic properties for five propellants are compared to values calculated with computer codes which employ truncated virial equations of state (ref 5 and 6) and the NBS equation of state used in conjunction with BLAKE (ref 9). At a loading density of 0.2gm/cm^3 there is good agreement between all codes. As the loading density increases the flame temperatures calculated in this work are usually lower than calculated using the other codes. This indicates that the heat capacity of the gas is increasing (becoming more liquid like). As the loading density increases, the pressure is usually lower when calculated with BLAKE and the ICT codes and higher when the NAVY code (ref 9) is used. At a loading density of 0.4gm/cm^3 there is a certain fortuitous cancellation of errors. In fact, with the exception of propellant four there is quite good agreement between the pressure calculated using the ICT (ref 6) code and MCVECE. A lower flame temperature is computed with MCVECE but since we employ more effective virial coefficients the pressure is increased and becomes comparable to the pressure calculated using the ICT (ref 6) code which determines a higher flame temperature but uses less virial coefficients. The pressure computed by using BLAKE (ref 5) is lower, possibly because of approximate nature of the third virial coefficient employed by Freedman.

It would be interesting to determine which code is correct using experimental techniques. Flame temperatures can be measured directly using modern spectroscopic techniques (ref 19). However, differences between codes are largest at the high loading densities. This creates higher pressures which may make optical access to the gas inside a closed bomb more difficult. It may also turn out that the hot gas will be too optically dense to get a laser beam through. So it is doubtful that the discrepancies can be resolved experimentally. Instead it will be necessary to make sure that all the codes use the most accurate thermodynamic data available and employ the best model. Finally, we must conclude that at 0.2gm/cm^3 loading density the truncated virial equation of state is acceptable but for tank guns where peak pressures can be 620 MPa, the equation of state proposed by Powell, Wilmot, Haar, and Klein (ref 11) does seem to offer a significant advance in accuracy.

The use of good equations of state for propellant gases should not be restricted to thermodynamic calculations. They should also be used in the interpretation of closed comb data and in interior ballistic calculations. It would be very useful to perform an equilibrium gas calculation for each step of the ballistic cycle and establish the gas composition and pressure. It was shown many years ago (ref 20) that the Abel-Noble equations which is usually used in these applications is not very accurate. The covolume would no longer be required for each individual propellant and could be replaced by the equation of state parameters developed by Powell, Wilmot, Haar and Klein (ref 8) and in this work. This approach would be valid for all propellants which are based on carbon, hydrogen, nitrogen and oxygen. As interior ballistic codes become more sophisticated propellant gas transport properties will have to be taken into account. Both viscosities and thermal conductivities should be important. Since different propellant gases have different transport properties, the composition of the propellant gas will have to be known as a function of temperature and volume. Both the pressure and the composition can be easily computed using the methods outlined in this work. It is our plan to investigate these possibilities and to report the work in the near future.

Table 1. Comparison of compressibility factor calculate with five term virial expansion and the proposed approximation for the Lennard-Jones gas.

Temp	Density = 0.014 moles/cm ³			Density = 0.020 moles/cm ³			Density = 0.030 moles/cm ³		
	H-S	L-J	% error	H-S	L-J	% error	H-S	L-J	% error
400	1.166	1.146	-1.7	1.326	1.285	-3.2	1.772	1.669	-6.2
500	1.216	1.205	-1.0	1.389	1.367	-1.6	1.836	1.786	-2.8
600	1.246	1.241	-0.5	1.425	1.416	-0.6	1.868	1.853	-0.8
700	1.265	1.264	-0.1	1.447	1.447	-0.0	1.883	1.891	0.4
800	1.278	1.280	0.1	1.462	1.467	0.4	1.890	1.913	1.2
900	1.287	1.291	0.3	1.471	1.481	0.7	1.892	1.926	1.8
1000	1.293	1.299	0.4	1.476	1.490	0.9	1.891	1.933	2.1
2000	1.306	1.316	0.7	1.479	1.502	1.5	1.842	1.903	3.2
3000	1.301	1.308	0.5	1.464	1.484	1.3	1.796	1.851	2.9
4000	1.295	1.299	0.3	1.451	1.465	0.9	1.762	1.807	2.5
5000	1.289	1.290	0.0	1.440	1.448	0.6	1.736	1.771	2.0
6000	1.284	1.281	-0.2	1.430	1.434	0.2	1.714	1.742	1.6
7000	1.280	1.274	-0.4	1.422	1.421	-0.0	1.697	1.716	1.1
8000	1.276	1.268	-0.6	1.415	1.410	-0.4	1.682	1.694	0.7
9000	1.273	1.262	-0.9	1.409	1.401	-0.6	1.670	1.675	0.3
10000	1.270	1.257	-1.1	1.404	1.392	-0.9	1.659	1.658	-0.0
20000	1.252	1.222	-2.4	1.373	1.335	-2.8	1.595	1.553	-2.7

Table 2. Propellant formulations for code comparison

<u>Ingredient abbreviation</u>	<u>One</u>	<u>Two</u>	<u>Three</u>	<u>Four</u>	<u>Five</u>
NC	83.173	19.940	45.954	58.330	79.600
(% N in NC)	(12.60)	(13.15)	(13.15)	(13.25)	(13.15)
NG	----	18.943	21.478	40.400	9.950
NQ	----	54.536	30.669	----	----
DNT	9.843	----	----	----	----
DBP	4.429	----	----	----	8.955
KCRY	----	0.299	----	----	----
DPA	0.984	----	----	----	0.995
EC	----	5.982	1.50	0.760	----
ETOH	0.98	0.300	0.30	0.510	0.500
H2O	0.59	----	----	----	----
C	----	----	0.10	----	----

Table 3. Comparison of results from the ICT code, BLAKE and MCVECE for the real gas case.

Loading Density (g/cm ³)	T(K)			P(MPa)			Impetus (J/g)		
	ICT	BLAKE	MCVECE	ICT	BLAKE	MCVECE	ICT	BLAKE	MCVECE
<u>One</u>									
0.2	2288	2284	2276	227.5	225.0	225.5	873.0	872.1	872.0
0.4	2348	2347	2290	600.9	585.6	600.2	874.7	877.3	871.1
0.6	2402	2427	2289	1154.0	1133.0	1220.0	868.3	881.3	863.3
<u>Two</u>									
0.2	2573	2565	2556	254.9	254.9	252.2	991.6	988.5	983.7
0.4	2590	2583	2555	664.4	659.2	663.9	988.5	987.4	981.2
0.6	2613	2617	2534	1267.0	1264.0	1335.2	978.0	984.7	970.5
<u>Three</u>									
0.2	3238	3233	3230	279.1	280.0	278.6	1114.0	1112.0	1111.4
0.4	3251	3248	3234	713.7	710.6	712.5	1116.0	1116.0	1111.6
0.6	3247	3257	3217	1355.0	1341.0	1384.7	1112.0	1116.0	1104.6
<u>Four</u>									
0.2	3852	3850	3826	294.1	293.3	290.3	1188.0	1186.0	1180.2
0.4	3920	3922	3871	750.9	737.6	729.5	1203.0	1202.0	1189.5
0.6	3948	3963	3883	1424.0	1377.0	1384.0	1208.0	1211.0	1190.4
<u>Five</u>									
0.2	2612	2615	2614	248.4	247.1	247.3	965.4	966.9	966.8
0.4	2624	2634	2612	648.1	634.3	648.3	962.4	967.4	964.1
0.6	2641	2671	2590	1240.0	1210.0	1297.3	952.5	967.1	953.8

Table 4. Comparison of predictions of gun performance using the NBS equation of state in conjunction with BLAKE and MCVECE.

Loading Density (g/cm ³)	T(K)			P(MPa)			Impetus (J/g)		
	NAVY*	MCVECE	% DIF	NAVY*	MCVECE	% DIF	NAVY*	MCVECE	% DIF
<u>One</u>									
0.2	2283	2276	0.3	229	225.5	1.5	873.1	872.0	0.1
0.4	2300	2290	0.4	616	600.2	2.6	874.6	871.1	0.4
0.6	2302	2289	0.6	1266	1220.0	3.6	870.1	863.3	0.8
<u>Two</u>									
0.2	2568	2556	0.5	258	252.2	2.2	989.1	983.7	0.5
0.4	2579	2555	0.9	688	663.9	3.5	991.8	981.2	1.1
0.6	2583	2534	1.9	1406	1335.2	5.0	991.5	970.5	2.1
<u>Three</u>									
0.2	3233	3230	0.1	282	278.6	1.2	1111.1	1111.4	0.0
0.4	3252	3234	0.6	730	712.5	2.4	1116.5	1111.6	0.4
0.6	3261	3217	1.3	1433	1384.7	3.4	1118.9	1104.6	1.3
<u>Four</u>									
0.2	3824	3826	0.0	294	290.3	1.2	1178.8	1180.2	0.1
0.4	3888	3871	0.4	748	729.5	2.5	1193.4	1189.5	0.3
0.6	3928	3883	1.1	1434	1384.0	3.5	1202.7	1190.4	1.0
<u>Five</u>									
0.2	2597	2614	-0.6	250	247.3	1.1	962.6	966.8	-0.4
0.4	2601	2612	-0.4	662	648.3	2.1	962.9	964.1	-0.1
0.6	2591	2590	0.0	1338	1297.3	3.0	957.5	953.8	0.4

*These values were kindly provided by Dr. Wilmot.

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