FLAME TEMPERATURE CALCULATIONS AT HIGH TEMPERATURE AND PRESSURE

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D. S. Chiu, and A. K. MacPherson

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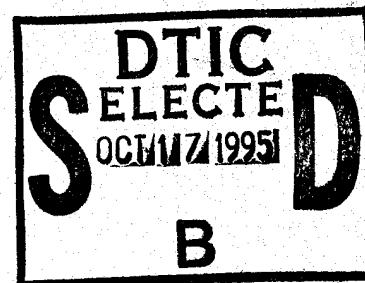
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In the past, real gas effects on the flame temperature were evaluated using the virial equation of state. Usually, the virial expansion was truncated after the third term. In this work, the equation of state for dense gases proposed by Haar and Shenker is considered. The implementation developed for H_2O, CO, CO_2, H_2, and N_2 by Powell, Wilmot, Haar, and Klein is used. The contribution of all minor species are assumed to be approximated by a Lennard-Jones gas with $\varepsilon/k = 100$ K and $\sigma = 3.0$Å. It is found that the more conventional approach is valid up to a loading density of 0.2 gm/cm³. As density increases, real gas effects cause the calculated flame temperature to decrease and the calculed 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 indicate 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 Zeleznic 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 electric 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 times the Lennard-Jones radius. Since these codes were developed, there has been little done to determine the validity of these types of approximations either by employing more virial coefficients or by using a more accurate equation of state. The purpose of this work is to indicate the limits of applicability of the truncated virial equation of state and to establish the effects of using a more accurate equation of state on the calculated flame temperature and pressure.

MATHEMATICAL CONSIDERATIONS

The flame temperature calculation is straight forward 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 Helmholt free energy is a minimum or $dA = 0$, where

$$dA = SdT - PdV + \sum \mu_j dn_j$$

In this equation S is the total entropy; P is the pressure; V is the volume; T is the temperature; n_j is the number of moles of species j; and μ_j is the chemical potential given by

$$\mu_j = \frac{\partial A}{\partial n_j}\Big)_{T,V,n_k \ k \neq j} = \frac{\partial G}{\partial n_j}\Big)_{T,P,n_k \ k \neq j}$$

and G is Gibbs free energy. Since the elements are conserved in a chemical reaction, it is necessary to introduce mass balance constraints. To formulate these constraints mathematically (ref 1), let W_i (i = 1,2,....,ℓ) be the symbol for the elements that are distributed among various species Y_j (j - 1,2,....,m). The chemical formula for species j can be written in the form

$$\prod_{i=1}^{\ell} (W_i) a_{ij}$$

where a_{ij} represents the number of atoms of the ith element in the jth species. If the system contains g_i (i = 1,2,....,ℓ) gram-atoms of element w_i, then conservation of the elements requires that

$$\sum_{j=1}^{m} a_{ij}n_j - g_i = 0 \text{ for i = 1,2,... } \ell$$

To perform the unconstrained minimization (ref 2), the method of Lagrangian multipliers is used. Each of the previous equations is multiplied by λ_i and added to the Helmholtz free energy to be minimized. At constant volume and temperature, the condition for a minimum is that

$$dA = \sum_{j=1}^{m} \left(\mu_j + \sum_{i=1}^{\ell} \lambda_i a_{ij}\right) dn_j + \sum_{i=1}^{\ell} \sum_{j=1}^{m} \left(a_{ij}n_j - g_i\right) d\lambda_i = 0$$

(1)

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Where the exact form of μ_j depends on the equation of state to be used.

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 8) 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_j 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 9) to the Percus-Yevick equation (ref 10). The molecular volumes are also assumed to be temperature dependent. The resulting expression is (ref 7)

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

where B_{jj} is 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 11), developed expressions for b_j and B_{jj} 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 by-products of combustion. Following Volk and Bathelt (ref 6), we assume that all minor species can be assigned Lennard-Jones parameters of $\varepsilon/k = 100$ K and $\sigma = 3.0\text{Å}$. 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

$$B_{66} = 13.9025 + 483.55/\sqrt{T} - 13606/T \tag{3}$$

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 12). Fifth virial coefficients calculated by Barker, Leonard, and Pompe (ref 13) were employed. These values were supplemented by fifth compressibility virial coefficients calculated by Kim, Henderson, and Oden (ref 14) using Verlet's extension (ref 15) of Percus-Yevick theory (ref 11). For several

densities and temperatures equation 3 was substituted into equation 2 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

$$b_6 = (4.10857 - 0.18413 \log(T))^3 \tag{4}$$

Equation 2, along with equations 3 and 4, 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 1. 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 11) effectively limit the use of our approach to temperatures above 850 K. The expressions for b_6 and B_{66} given previously were assigned to all the minor species and combined with the expressions given by Powell, Wilmot, Haar, and Klein (ref 11) 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

$$b_{mix} = \sum X_j b_j \tag{5}$$

and

$$B_{mix} = \sum \sum X_j X_k B_{jk} \tag{6}$$

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

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

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

R is the universal gas constant and Z_{mix} is calculated using equation 2 in conjunction with equations 5 and 6. The Helmholtz free energy is given by

$$A = RT J_{mix} + A_o \tag{7}$$

where J_{mix} is defined in reference 11 and A_o is the contribution to the free energy from the molecular degrees of freedom. The assumption is made (ref 11) that these molecular degrees of freedom are not effected by the presence of other species. The chemical potential is given by (ref 11)

$$\mu_j = \frac{\partial A}{\partial n_j}\bigg)_{T,\rho,n_k \; k \neq j} \tag{8}$$

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

$$\frac{U}{RT} = \frac{A}{RT} - \frac{\partial}{\partial T}\left(\frac{A}{R}\right)_\rho \tag{9}$$

Equation 1 is solved for the n_j using a descent Newton-Raphson method advocated by Gordon and McBride (ref 2), but equations 7 and 8 are used for the chemical potentials. 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.

In order to speed up the convergence, it is important to start the calculation with a good initial estimate of the flame temperature. In the work, the Hirschfelder (ref 4) method is used to supply the initial guess. The equilibrium composition is then computed a the Hirschfelder temperature. The energy available from the decomposed propellant is used to heat the product gases so that the net internal energy change, ΔU, must be zero at the flame temperature. A $\Delta U(T)$ is computed by

$$\Delta U(T) = U(T_o)_{propellant} - U(T)_{products}$$

where T_o is the initial temperature and equation 9 is used to calculate the internal energy of the products. If $\Delta U(T)$ is positive (negative), then the temperature is increased (decreased) in a stepwise manner and a new equilibrium composition is computed at each step. When $\Delta U(T)$ changes sign the next smallest temperature increment is used to change the temperature in the opposite direction. Temperature is incremented first by 80 K then 16 K, then 3.2 K, and finally by 0.6 K. Convergence criteria are the same as in reference 2. Using this procedure, it is not necessary to store the heat capacity data for all the product molecules and integration of the heat capacity data is avoided.

THE COMPUTER PROGRAM

The mathematical considerations discussed were coded in FORTRAN and implemented on an IBM compatible PC. The name MCVECE (microcomputer very easy chemical equilibrium) was adopted. The coding is extensively commented and the programming is simple and straight forward. A real gas equation of state is used as discussed, 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 JANAF tables (ref 16) 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[1] 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

The writing of any new computer code presents many opportunities for errors. Therefore, in order to generate credibility, it is necessary to compare results with established codes whose error content has diminished with time. For this reason, calculated results from MCVECE were compared with outputs from NASA-Lewis (ref 2), BLAKE (ref 5), and ICT (ref 6) codes. A reasonable basis of comparison is afforded by the five propellant formulations suggested by Freedman (ref 5). The formulations are reproduced in table 2. For the ideal gas, comparison with NASA-Lewis (ref 2) and BLAKE (ref 5) are made in table 3. No significant discrepancies are noted. Exact agreement cannot be expected because different thermodynamic data and convergence criteria are used.

For the real gas case, comparisons are made with BLAKE (ref 5) and the ICT (ref 6) codes. These results are presented in table 4. The flame temperature calculated using MCVECE is lower than for the other two codes. For a loading density of 0.2 gm/cm3, 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. The calculated pressure is also lower then computed with the other two codes. This indicates that at a loading density of 0.2 gm/cm3, the contribution of higher virial coefficient to the equation of state is negligible. At the higher loading, the MCVECE flame temperature is always lower than the flame temperature computed with the other two codes. The decrease in flame temperature is due to an increase in the heat capacity of the propellant gas molecules which is a

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[1] The impetus is defined for a propellant as the product of the number of moles of gas produced upon combustion times the flame temperature times the universal gas constant. It is used as a measure of propellant performance.

consequence of the equation of state used in this work and has already been observed (ref 17). 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 seems 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.

CONCLUSIONS

A thermochemical computer code had been developed for use at high pressures and temperatures. The equation of state proposed by Powell, Wilmot, Haar, and Klein (ref 11) was used. All minor products were assumed to be described by a Lennard-Jones gas with $\varepsilon/k = 100$ K and $\sigma = 3$Å. Computed thermodynamic properties for five propellants are compared to values calculated with computer codes which employ truncated virial equations of state (refs 5 and 6). At a loading density of 0.2 gm/cm^3, there is good agreement between all three methods. However, even at a loading density of 0.2 gm/cm^3 the flame temperature calculated in this work is slightly lower. This indicates that the heat capacity of the gas is increasing (becoming more liquid like). The calculated pressure is also lower which indicates that two virial coefficients are enough to describe the pressure accurately. At a loading density of 0.4 gm/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 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 the approximate nature of the third virial coefficient employed in that work. At a loading density of 0.6 gm/cm^3, the computed flame temperature using MCVECE is always lower due to the increase of the heat capacity of the gas due to real gas effects. With the exception of propellant four the pressure calculated using MCVECE is always higher due to the large number of virial coefficients employed.

Our predication is that as loading density increases the flame temperature will decrease due to real gas effects. It would be interesting to verify this observation experimentally using modern spectroscopic techniques (ref 18). However, because of the high pressures involved, optical access to the the gas inside a closed bomb may become difficult. It may also turnout that the hot gas will be too optically dense to get a laser beam through. So it is doubtful that the lowering of flame temperature with

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loading density will ever be observed experimentally. Finally, we must conclude that at 0.2 gm/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.

Table 1
Comparison of compressibility factors calculated with the five-term virial expansion and the proposed approximation for the Lennard-Jones gas

Temp (K)	density = 0.014 (moles/cm³)			density = 0.020 (moles/cm³)			density = 0.030 (moles/cm³)		
	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	-0.9	1.389	1.367	-1.6	1.836	1.786	-2.8
600	1.246	1.241	-0.4	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	0.2	1.462	1.467	0.3	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	0.5	1.476	1.490	0.9	1.891	1.933	2.2
2000	1.306	1.316	0.8	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	3.0
4000	1.295	1.299	0.3	1.451	1.465	1.0	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	0.3	1.714	1.742	1.6
7000	1.280	1.274	-0.5	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	-1.0	1.404	1.392	-0.9	1.659	1.658	-0.1
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 intercomparison

Ingredient Abbreviation	One	Two	Three	Four	Five
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
H20	0.59	---	---	---	---
C	---	---	0.10	---	---

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Table 3
Comparison of BLAKE, NASA-Lewis and MCVECE for the ideal gas case

Loading Density*	T(K)			P(MPa)		
(g/cm^3)	BLAKE	NASA-Lewis	MCVECE	BLAKE	NASA-Lewis	MCVECE
One						
0.2	2266	2268	2270	173.7	173.8	174.0
0.4	2285	2287	2292	347.9	348.0	348.9
0.6	2306	2308	2307	522.8	522.8	522.6
Two						
0.2	2559	2553	2540	197.5	197.0	197.5
0.4	2563	2557	2549	394.8	393.7	395.4
0.6	2567	2562	2556	591.9	590.1	593.2
Three						
0.2	3221	3219	3203	221.8	221.6	221.7
0.4	3230	3227	3218	444.5	444.0	445.0
0.6	3234	3231	3221	667.2	666.3	667.7
Four						
0.2	3815	3812	3815	235.6	235.4	235.6
0.4	3865	3862	3857	475.7	475.2	474.6
0.6	3891	3887	3889	716.8	715.9	716.2
Five						
0.2	2602	2606	2593	192.6	192.8	193.4
0.4	2604	2610	2596	386.0	385.5	386.7
0.6	2610	2614	2600	578.7	578.0	579.5

* Load density is defined as the number of grams of propellant divided by the volume of the high pressure vessel.

Table 4
Comparison of results from the ICT code, BLAKE and MCVECE for the real gas case

Loading Density*	T(K)			P (MPa)			Impetus (J/g)		
(g/cm^3)	ICT	BLAKE	MCVECE	ICT	BLAKE	MCVECE	ICT	BLAKE	MCVECE
One									
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
Two									
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
Three									
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
Four									
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
Five									
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

* Load density is defined as the number of grams of propellant
divided by the volume of the high pressure vessel.

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