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Thermodynamic Property Characterization for Plasmas Generated by an Ablating-Capillary Arc

by Michael J. McQuaid and Michael J. Nusca

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Abstract

The thermodynamic property database developed by McBride and Gordon for use with their program for calculating the chemical compositions of complex gas mixtures has been employed in a computational fluid dynamics (CFD) model for simulating plasma jets generated by ablating-capillary arc igniters. In this report, the methods employed in the development of the McBride and Gordon data are compared to those based on the "standard" (Debye-Huckel) theory employed for gases in which Coulomb interactions need to be considered. Predictions based on these two approaches are compared over pressure and temperature ranges relevant to an ablating-capillary arc jet. The comparison indicates that McBride and Gordon data, which does not include a "first principles" correction for the influence of Coulomb interactions, still yields property determinations that are in good agreement with the standard. Moreover, it is shown that properties obtained from their database should not be corrected with terms that account for Coulomb interactions.

Acknowledgments

The authors would like to thank Dr. Bonnie McBride (NASA) for providing us with her programs (CEA and PAC99) and databases (THERMO.INP and PAC99 input files) for calculating the thermodynamic properties of gases, and the publications which describe their basis and use. We are also thankful for the assistance of Dr. Anthony Kotlar of the U.S. Army Research Laboratory (ARL), who helped clarify various points in published derivations of Coulomb interaction corrections, and who reviewed this manuscript.

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1. Introduction

Ablating-capillary arcs are a means of converting electrical energy into a form suitable for the ignition of propulsion charges in large-caliber gun systems [1–4]. In ignition systems that utilize this approach, electrical energy stored in a pulse-forming network (PFN) is initially discharged via a thin metallic wire strung through the capillary. The initial discharge explodes the wire, “instantaneously” producing an ionized (plasma) gas into which the PFN continues to dump energy. Ablation of material from the capillary wall, which is generally attributed to (and modeled as) a radiation-driven process [5], serves to sustain the arc by replenishing gas that exits the capillary. The overall process produces a “dense” (10^{23} – 10^{26} m⁻³), “low-temperature” (10,000–30,000 K) plasma whose composition is primarily derived from decomposed capillary material [5]. This plasma exits the capillary as a jet, and flows into the propellant bed, igniting it directly. Ablating capillary arcs were one of the first electrothermal-chemical (ETC) ignition concepts to be investigated, and experimentally observed attributes (including short, reproducible ignition delays [1], propellant burn-rate enhancement [2] and “temperature compensation” [3, 4]) have been bases for believing that ETC-based concepts are capable of significantly enhancing the ballistic performance of fielded and proposed weapons systems.

In order to better understand the mechanisms by which ablating-capillary-arc igniters yield desirable ballistic performance characteristics, the U.S. Army Research Laboratory (ARL) has been developing a computational fluid dynamics (CFD) model to simulate the dynamics of arc discharges and their interaction with propellant [5–7]. The primary computational engine for simulating the plasma after it exits the capillary is NSRG2, a solver for the Navier-Stokes equations characterizing mass, momentum, and energy transport in gaseous, reactive, unsteady, two-dimensional (2-D)/axisymmetric flowfields [6, 7]. In NSRG2, the partial differential equations are cast in conservation form and converted to algebraic equations using a finite-volume formulation. The primary dependent variables in the formulation are density (ρ), velocity (v), specific internal energy (E), and specie mass fractions (c_i). Other thermodynamic properties, such as the temperature (T) and pressure (P), are found via (equation-of-state) relationships that determine these properties from ρ , E , and c_i . Subroutines for the representation

of (nonequilibrium) chemical reactions, multispecies diffusion, viscosity, and thermal conductivity are also included in the model [7].

This report summarizes an investigation into means for refining the model's calculation of thermodynamic properties. In previously reported efforts, these properties were calculated from the thermodynamic property database (THERMO.INP) developed by McBride and Gordon [8-10]. Designed for use with their program for calculating the chemical compositions of complex gas mixtures (CEA) [9], THERMO.INP is extremely convenient for calculating such properties and (with CEA) is widely utilized within the combustion community. The data, which are based on "the method of partition functions," are popular and valuable for several reasons. One is, that for systems in which polyatomic species are important, the arduous and time-consuming task of compiling the data needed as input for the method of partition functions can be avoided. (This was our original reason for using it.) It was also learned (later) that, though based on simple equations, there are a number assumptions/judgments that need to be made when applying the method of partition functions. Thus, a certain level of acquired expertise is required in order to obtain good results with the method. Through THERMO.INP, McBride and Gordon provide the necessary expertise. Moreover, their data is reduced into a computationally efficient package, with heat capacity, entropy and the Gibb's free energy being obtained from the specification of temperature (alone) via simple polynomial expressions. (Other properties, such as the specific internal energy and Helmholtz free energy, can be found from the three established properties through appropriate thermodynamic relationships.) This structure is attractive because it avoids the need to carry partition function input data and recompute multiterm summations prior to actually calculating a specie's properties.

Unfortunately, THERMO.INP has a potential shortcoming with respect to determining the thermodynamic properties of plasmas, i.e., the methodologies employed to calculate the data assumes the ideal gas law applies. While it is considered that the ideal gas law reasonably describes the gases generated by an ablating-capillary arc, a more rigorous characterization would include corrections that account for the Coulomb interactions between charged particles. Though Coulomb interaction-based corrections are expected to be small, because of the

nonlinear nature of the equations describing the plasma jet, their absence from the arc plasma jet CFD model is difficult to justify.

McBride and Gordon [11] recognize that Coulomb interactions may influence the thermodynamic properties of an ionized gas, but they do not provide an option within CEA that implements a correction for such interactions, stating that “special programming” would be required. This statement is (presumably) related to the fact that in the “standard” (Debye-Huckel) theory for quantifying the effect of Coulomb interactions, partition functions depend on a mixture’s electron number density and temperature. Since these parameters are interdependent, rigorous application of the theory requires that partition functions be computed as a function of a mixture’s temperature, density, and chemical composition. To incorporate such corrections into the derivation of properties from THERMO.INP, where temperature is the only available variable, would thus, indeed, seem to require special programming. This consideration initially dissuaded us from pursuing the matter. However, it was learned that Kappen [12], following the work of Kovitya [13], computes thermodynamic property data for ETC simulations from an “extended” version of THERMO.INP (the details of which are unknown to us) and a CEA-like approach that includes Coulomb interaction-based correction terms. This knowledge prompted the authors to reconsider whether that approach should be taken here as well.

Our approach to answering this question was framed by a specific concern about the appropriateness of correcting the properties calculated from the “standard” THERMO.INP database, i.e., the one provided by McBride and Gordon. That concern was related to the fact that the data for monatomic species generated by an ablating (polyethylene) capillary arc—C and H, in particular—have been calculated with a method that biases partition function calculations so that better ionization equilibrium values are obtained [10]. Given the use of this method in the development of the database, we were concerned that an additional correction for Coulomb interactions might lead to “overcorrected” results.

To investigate this issue, approaches are reviewed for calculating the thermodynamic properties of “low-density” gases in (local) thermodynamic equilibrium and their implementation by McBride and Gordon in the development of their THERMO.INP library. The nature of errors that can occur if Coulomb interaction corrections are included (or omitted) in the computation of properties from this database is then considered from a theoretical standpoint. Finally, plasma property determinations obtained (1) directly from the McBride and Gordon library, and (2) those same results adjusted with “formal corrections” for Coulomb interactions, are compared to those generated by a “standard model” developed previously [14]. Based on the results, it was concluded that for this application (CFD simulations of the plasma discharged from an ablating-capillary arc), the THERMO.INP data provided by McBride and Gordon should not be corrected with terms that account for Coulomb interactions. Alternate THERMO.INP libraries, which, when subsequently corrected for Coulomb interactions, yield results that are in slightly better agreement with the standard model, are presented. But, it will be shown that for the range of conditions that we have studied, the need to develop and exploit such libraries does not appear to be necessary.

2. Background

This section provides a brief review of the formulae employed to characterize the thermodynamic properties of a low-density gas. Such a discussion starts (of course) with the ideal gas law, which (in conjunction with the law of partial pressures) may be written as

$$P = k_b T \left(N_e + \sum_{i,j} N_{i,j} \right), \quad (1)$$

where N_e is the number density of electrons, $N_{i,j}$ is the number density of specie $X_{i,j}$ (the i^{th} “heavy” nuclear configuration in its j^{th} ionization state), T is the temperature, and k_b is Boltzmann’s constant. It should be noted that the interpretation of notation is a consistently vexing issue when reading the literature on plasma thermodynamics. The notation employed here, with electrons labeled and carried distinct from the heavy species, follows the practice of

Griem [15]. Because electrons have “status” as particles that is equal to that of species with heavy nuclei within the ideal gas law, there is the temptation to condense the notation by lumping them in with the heavy species. However, when Coulomb interactions are introduced, electrons acquire special status, and thus labeling them separately throughout the discussion lessens the potential for confusion.

For gases that obey the ideal gas law, the method of partition functions is “the most rigorous and consistent method for finding all of [its] thermodynamic functions” [16]. Details of this method can be found in texts on statistical physics, e.g., Kittel [17]. Of particular relevance to this study are the relationships for computing the Helmholtz free energy (F), the entropy (S), and the internal energy (E). For a constant specific volume (V), these relationships are:

$$F_{i,j}^{\text{ideal}} = N_{i,j} k_b T \ln Z_{i,j}, \quad (2)$$

$$S_{i,j}^{\text{ideal}} = - \left(\frac{\partial F_{i,j}^{\text{ideal}}}{\partial T} \right)_{V,N} = N_{i,j} k_b \left(T \left(\frac{\partial \ln Z_{i,j}}{\partial T} \right) + \ln Z_{i,j} \right), \quad (3)$$

and

$$E_{i,j}^{\text{ideal}} = F_{i,j}^{\text{ideal}} + TS_{i,j}^{\text{ideal}} = N_{i,j} k_b T^2 \left(\frac{\partial \ln Z_{i,j}}{\partial T} \right)_V = \left(\frac{N_{i,j} k_b T^2}{Z_{i,j}} \right) \left(\frac{\partial Z_{i,j}}{\partial T} \right)_V. \quad (4)$$

The partition function ($Z_{i,j}$) for monatomic specie $X_{i,j}$ is calculated per

$$Z_{i,j} = \sum_k g_{i,j}^k \exp \left(\frac{\epsilon_{i,j}^k}{k_b T} \right), \quad (5)$$

where $g_{i,j}^k$ is the statistical weight associated with the k^{th} energy state ($\epsilon_{i,j}^k$). (The partition functions for polyatomic species include contributions for vibrational and rotational motions, but

such species are not specifically considered in this report and so the details of the partition functions for these species are not given.) Electrons and protons represent special cases. For electrons, because they are spin 1/2 particles with no electronic energy levels, Z_e is a constant equal to 2. Like electrons, protons are spin 1/2 particles with no electronic energy levels, but it is assumed that Z_{H^+} is a constant equal to 1. (A reference has not been found by the authors that states this assumption explicitly, but it is clear from their data for H^+ that McBride and Gordon [10] set Z_{H^+} equal to 1.) Characterization of the properties for a mixture is determined by summing mole fraction-weighted contributions of the individual constituents.

Equations (2)–(4) are derived based on the assumption that the particles in the gas do not interact, i.e., the gas is “perfect.” In an ionized (plasma) gas, however, ions tend to be surrounded by charges of opposite sign, resulting in a net attractive force between particles. One result of such forces is that the pressure of an ionized gas will be less than that calculated, assuming it is perfect. In addition, the energy required to ionize a constituent is reduced from that which would be required for the constituent in isolation. (The amount of the reduction depends on the charge of the particle, the plasma density, and the temperature.) This so-called “lowering of the ionization energy” manifests itself in two ways. First, the lowering of the ionization potential implies that bound states whose energies are between the uncorrected ionization potential and the lowered ionization potential become free states. The consequence is that the electronic energy that can be carried by a plasma constituent will be lower than that calculated assuming the ionization potential of the constituent is not affected by the interactions, and the “statistical weight” of the constituent’s population will be reduced. Second, the energy (of formation) of the cation for the next ionization state will be reduced relative to the reference state for the mixture. As will be discussed, both of these effects favor higher degrees of ionization. How these effects are quantified and subsequently manifest themselves in the estimates of the properties of the gas has to be understood in order to assess the desirability of employing the approach to property characterization utilized by Kappen [12].

Correction terms that quantify the effects of Coulomb interactions have been derived by the Debye-Huckel method. The Debye-Huckel method envisions a spherically symmetric,

non-uniformly charged cloud of like charges formed about each electron or ion. From this starting point, it can be shown that the specific internal energy reduction resulting from Coulomb interactions is [15],

$$E^{\text{coul}} = -\frac{e^3}{8\pi} \left(\frac{1}{\epsilon_0^3 k_b T} \right)^{1/2} \left(N_e + \sum j^2 N_{i,j} \right)^{3/2}. \quad (6)$$

The correction to the Helmholtz free energy (F^{coul}) can be found by integrating the thermodynamic relationship [16],

$$\frac{E}{T^2} = \frac{\partial(F/T)}{\partial T}, \quad (7)$$

to give [15]

$$F^{\text{coul}} = -\frac{e^3}{12\pi} \left(\frac{1}{\epsilon_0^3 k_b T} \right)^{1/2} \left(N_e + \sum j^2 N_{i,j} \right)^{3/2} = \frac{2}{3} E^{\text{coul}}. \quad (8)$$

The reduction in the pressure can be found from the relationship [15]

$$P^{\text{coul}} = -\left(\frac{\partial(E^{\text{coul}} V)}{\partial V} \right)_{T, N_i} = \frac{E^{\text{coul}}}{3}. \quad (9)$$

Derived under the assumption that they are perturbations to the relationships obtained via the ideal gas law, these corrections terms are simply added to the associated ideal gas property to get the refined property prediction.

Assuming that the plasma ejected by an ablating-capillary arc is a weakly imperfect gas, the primary technical issue in determining its thermodynamic properties is the computation of partition functions. The difficulty in computing partition functions arises (in part) because the

summation in equation (5) is not a convergent series. For a “theoretically isolated” molecule, k can go to infinity, and because near the series limit the exponential term remains nearly constant while the statistical weight increases with k , the summation will too. Of course, in a system of particles the association of a given electron with a given nucleus will only span a finite distance, limiting the values of k that actually exist in a population. Since the values for a partition function calculation depend on the values of k employed, the selection of a technique for identifying the values to use in the summation is an integral aspect of the development of the method.

For an ionized gas, the usual basis for limiting the summation in equation (5) is to calculate the reduction in ionization potential ($\Delta\epsilon^\infty$) and employ it formally as a truncation criterion in the equation

$$\epsilon_{i,j}^{\max} \leq \epsilon_{i,j}^\infty - \Delta\epsilon_{i,j}^\infty, \quad (10)$$

where $\epsilon_{i,j}^\infty$ is the (uncorrected) ionization potential for specie $X_{i,j}$. One method of calculating $\Delta\epsilon_{i,j}^\infty$ follows from arguments related to the minimization of the Helmholtz free energy for the reactive system $X_{i,j} \rightarrow X_{i,j+1} + e^-$ [16]. For reference, these arguments yield [18],

$$\Delta\epsilon_{i,j}^\infty = \frac{je^2}{4\pi\epsilon_0(\lambda_D + \Lambda/8)}, \quad (11)$$

where ϵ_0 is the permittivity of free space and λ_D is the Debye length,

$$\lambda_D = \left(\frac{\epsilon_0 k_b T}{N_e e^2 (1 + \tilde{z})} \right)^{1/2}. \quad (12)$$

The parameter \tilde{z} in equation (12) represents the effective charge on an ion, this parameter being computed via the equation

$$\tilde{z} = \frac{\sum_i \sum_j j^2 N_{i,j}}{\sum_i \sum_j j N_{i,j}}. \quad (13)$$

The inclusion of a dependence on the DeBroglie wavelength (Λ) in equation (11),

$$\Lambda = \frac{h}{(2\pi m_e k_b T)^{\frac{1}{2}}}, \quad (14)$$

is a slight modification to the formula for $\Delta\epsilon_{i,j}^\infty$ given in standard texts [15, 16]. Powell and Zielinski [5] adopted equation (11) for their model of ablating-capillary-arc dynamics, and their lead was followed in subsequent studies [14]. The practice is retained here for consistency with these prior efforts.

If it is further assumed that Coulomb interactions have a negligible effect on the energy level structure of plasma constituents, the issue of calculating $Z_{i,j}$ reduces to one of characterizing all of the energy levels of all constituents up to the limit imposed by equation (10). For plasmas generated by ablating-polyethylene-capillary arcs, at temperatures above $\sim 12,000$ K, the plasma will consist almost exclusively of monatomic species and the reduction in ionization potentials will be relatively large [14]. Under such conditions, "complete" energy level information can be obtained for all species in the mixture, this information being available in experimentally based data tables and/or through computational techniques. Thus, the computation of partition functions is a relatively straightforward matter when temperatures are in this range.

For temperatures below 12,000 K, however, the concentration of polyatomic species becomes important and the reduction in the ionization potential becomes smaller [14]. Under such conditions, application of the methodology is less clear cut. One problem that arises is the mismatch in information available for monatomic and polyatomic species. Quoting Gurvich et al. [19]:

“It is almost impossible to take account of the Rydberg electronic states in the partition functions of diatomic and especially of polyatomic molecules, as for the majority of molecules there are no data for these states. For atoms and monatomic ions, the experimental data for a significant part of the Rydberg states are lacking, especially those originating during the excitation of one of the electrons in states with large values of the orbital quantum number ... [While] for the majority of atoms the number of these states can be established on the basis of the configuration of the electron shell of the atom and approximate values of the energies of these states can be estimated with sufficient accuracy ... for molecules, including the simplest diatomic molecules, the determination of the bonding Rydberg states is very difficult.”

As will be shown, this situation can create problems because the use of mismatched information can bias the calculation of equilibrium constants.

In addressing this issue, Gurvich et al. [19] observe (empirically) that, while the thermodynamic functions of an individual constituent depend strongly on the number of states employed in the calculation of its partition function, this type of dependence does not carry over to the property determinations for complex mixtures. Rather, as long as “comparable” information is employed to calculate the partition function of each constituent, the properties calculated for a mixture tend to be insensitive to amount of information used. Consistent with this conclusion, they calculate properties for all of the species in their database based on sums that include only the contributions of valence states.

McBride and Gordon employ several different approaches for developing the THERMO.INP data of interest here (see Table 1). For monatomic species, they employ the TEMPER method to specify the partition function cut-off level, viz.,

$$\epsilon_{i,j}^{\max} = \epsilon_{i,j}^{\infty} - k_b T, \quad (15)$$

Table 1. Bases for THERMO.INP Data^a

Specie	Calculation Method	Temperature Range (K)
e-	Z=2	200–20,000
C	TEMPER/FILL	200–8,000
—	READ ^b	8,000–20,000
C ⁺	TEMPER/FILL	298–20,000
C ⁺⁺	See Note ^c	298–20,000
CH	READ ^d	200–20,000
CH ⁺	READ ^d	298–20,000
CN	READ ^d	200–20,000
CN ⁺	READ ^d	298–20,000
CO	READ ^d	200–20,000
CO ⁺	READ ^d	298–20,000
C ₂	READ ^d	200–20,000
C ₂ ⁺	READ ^d	298–20,000
H	TEMPER/FILL	200–8,000
—	READ ^b	8,000–20,000
H ⁺	Z=1	200–20,000
H ₂	READ ^d	200–20,000
H ₂ ⁺	READ ^d	298–20,000
N	TEMPER/FILL	300–8,000
—	READ ^b	8,000–20,000
N ⁺	TEMPER/FILL	298–20,000
NH	READ ^d	200–20,000
NH ⁺	READ ^d	298–20,000
NO	READ ^d	200–20,000
NO ⁺	READ ^d	298–20,000
N ₂	READ ^d	200–20,000
N ₂ ⁺	READ ^d	298–20,000
O	TEMPER/FILL	200–8,000
—	READ ^b	8,000–20,000
O ⁺	TEMPER/FILL	200–20,000
OH	READ ^d	200–20,000
OH ⁺	READ ^d	298–20,000
O ₂	READ ^d	200–20,000
O ₂ ⁺	READ ^d	298–20,000

^a Unless otherwise specified, the method identified is as given in PAC 91 input files provided to the authors by McBride.

^b A “special fit” is indicated, but it is assumed (based on reference [10]) the method is similar to TEMPER/FILL.

^c See reference [14].

^d Properties derived from Gurvich et al. data [19] and thus based on valence state contributions only.

and they use a fill procedure to establish a complete set of energy levels beneath this cut-off. It will be noted that the explicit temperature dependence of the cut-off criterion of the TEMPER method ($k_b T$) is different than that of equation (11), where $\Delta\epsilon_{i,j}^\infty$ is employed. Consideration of equations (11) and (12) indicate that $\Delta\epsilon_{i,j}^\infty$ increases nearly in proportion to $N_e^{1/2}$ while decreasing in proportion to $T^{1/2}$. Despite the apparently contradictory temperature dependence of these two truncation criteria, equation (15) adjusts the ionization equilibrium in the right direction because of the temperature dependence of N_e , e.g., equation (16). For all of the diatomic molecules of interest here, McBride and Gordon have based their data on that published by Gurvich et al. [19]. As mentioned, this data is based on partition function calculations that include only valence state contributions.

3. Results and Discussion

Given that the THERMO.INP data provided by McBride and Gordon have been generated based on partition-function calculations in which the contributions of empirically-limited numbers of energy levels are summed, the question arises as to whether or not Coulomb interaction corrections should be included. To better understand the basis for this question and its resolution, it is instructive to consider the Saha equation, which relates the number densities of species $X_{i,j}$ and $X_{i,j+1}$ at a given temperature and electron number density. Based on arguments that follow from the minimization of the Helmholtz free energy for the reactive system $X_{i,j} \rightarrow X_{i,j+1} + e^-$, for an ideal gas, this equation may be written:

$$\frac{N_{i,j+1}N_e}{N_{i,j}} = \frac{2Z_{i,j+1}(T)}{Z_{i,j}(T)} \left(\frac{2\pi m_e k_b T}{h^2} \right)^{3/2} \exp\left(\frac{-\epsilon_{i,j}^\infty}{k_b T} \right), \quad (16)$$

where m_e is the mass of an electron and h is Planck's constant. Coupled with appropriate specie balances, the system of equations following from the application of equation (16) is the "microscopic equivalent" of CEA. As such, this equation reveals the influence that partition

function-calculation methods have in determining the chemical composition of a mixture—insight that is difficult to glean from the macroscopic approach.

Following from the fact that $\epsilon_{i,j}^k$ is less than $\epsilon_{i,j}^\infty$ for all k , it can be shown that the ratio of $Z_{i,j+1}(T)$ to $Z_{i,j}(T)$ is bound when the same $k = \max$ level is employed in both summations, and the ratio converges to a limiting value as \max goes to infinity. This behavior, i.e., the mediation of the vagaries inherent in calculating partition functions when calculating the properties of complex mixtures, is consistent with the empirical observations of Gurvich et al. [19]. Moreover, this equation exemplifies the concern expressed by Gurvich et al. as to the bias that can be introduced if there is a mismatch in the information employed for different species.

When Coulomb interactions are included, the Saha equation becomes

$$\frac{N_{i,j+1} N_e}{N_{i,j}} = \frac{2Z_{i,j+1}(T)}{Z_{i,j}(T)} \left(\frac{2\pi m_e k_b T}{h^2} \right)^{3/2} \exp\left(\frac{-(\epsilon_{i,j}^\infty - \Delta\epsilon_{i,j}^\infty)}{k_b T} \right), \quad (17)$$

The inclusion of $\Delta\epsilon_{i,j}^\infty$ in the exponential term is derived from “first principles” based solely on replacing F^{ideal} with $(F^{\text{ideal}} + F^{\text{coul}})$ in the derivation of equation (16). Moreover, though derived from free energy considerations, in following the derivation, it is observed that there is a one-to-one correspondence between its expression in equation (17) and the reduction in the specific internal energy of $X_{i,j+1}$ with respect to the reference state. As will be appreciated by the comparison of equations (16) and (17), the inclusion of the effect leads to estimates having higher degrees of ionization.

The other effect of $\Delta\epsilon_{i,j}^\infty$, which is the reduction in the capability of $X_{i,j}$'s population to carry energy via its electronic structure (as calculated via equation [4]), is expressed through its use as a truncation criterion in the computation of the partition function (equation [10]). It should be noted that because the reduction in ionization potential is employed as a basis for truncating partition function summations, it might be assumed that this criterion is somehow related to the

derivation of equation (17). It is not. Rather, equation (10) simply provides an approach that is consistent with the derivation of this relationship. Though not implicitly derivable from equation (17), this effect also favors higher degrees of ionization because, at least for the species and conditions that we have considered, $Z_{i,j}$ is reduced more by $\Delta\varepsilon_{i,j}^{\infty}$ than $Z_{i,j+1}$ is reduced by $\Delta\varepsilon_{i,j+1}^{\infty}$. This result is related to the difference in the magnitudes of the ionization potentials of $X_{i,j}$ and $X_{i,j+1}$, the spacing of the attendant Rydberg states, and the magnitudes of $\Delta\varepsilon_{i,j}^{\infty}$ and $\Delta\varepsilon_{i,j+1}^{\infty}$ relative to these first two considerations.

Because the reduction of the internal energy carried by a specie's electronic structure is the only effect of the lowering of the ionization potential that is incorporated into the property data of THERMO.INP—a reduction in the relative energy of the next ionization state being neglected—one would expect that CEA-THERMO.INP calculations would underpredict the degree of ionization. That is, for the same temperature and pressure, the ratios of $N_{i,j+1}$ to $N_{i,j}$ obtained for compositions computed via CEA-THERMO.INP would be consistently lower than the same ratios calculated via the standard model. Thus, the incorporation of Coulomb interaction-based corrections into CEA as done by Kappen [12] would appear to be warranted.

However, from the standpoint of developing a subroutine for the arc plasma jet CFD model the concern is not the determination of chemical compositions, but, rather, the determination of the temperature and pressure for a specified (possibly nonequilibrium) chemical composition, density, and internal energy. To examine the appropriateness of correcting properties obtained from the standard THERMO.INP library with terms that account for Coulomb interactions, a case study was conducted comparing “uncorrected” and “corrected” property determinations vs. those generated by the standard model. The protocol for the comparison involved employing the standard model to establish (equilibrium) chemical compositions, densities, internal energies, temperatures and pressures for plasmas derived from the decomposition of polyethylene. The temperatures and pressures for the simulated plasmas were then found from the standard library based on the chemical composition, density, and internal energy values. (This protocol reflects the way the database is employed in the CFD simulation.) One change to the standard model that was necessary for this study was the assignment of its reference state. Previously assigned

as $1/2 \text{ C(gas)} + \text{H(gas)}$ at 0 K, it was converted to $\text{C(graphite)} + \text{H}_2(\text{gas})$ at 298.15 K for compatibility with the reference state upon which the THERMO.INP data are based.

Since the internal energy, density, and chemical composition both determine and depend on the temperature, a technique for finding a self-consistent solution for these variables had to be implemented. To accomplish the task, a bisection root-finding technique was developed [20]. For the initial bounding temperature guesses (and the iterative bisections of the range that follow), the specific internal energy of the mixture was calculated directly from the THERMO.INP library. It should be noted that the data in THERMO.INP yields enthalpy ($H_{i,j}^{\text{ideal}}$ in kJ/mole). To obtain the internal energy (in kJ/m³), the relationship

$$E_{\text{mix}}^{\text{ideal}} = \rho_{\text{mix}} \left[\left(\frac{x_e H_e^{\text{ideal}}}{m_e} + \sum_{i,j} \frac{x_{i,j} H_{i,j}^{\text{ideal}}}{m_{i,j}} \right) - \frac{R_u T}{\left(x_e m_e + \sum_{i,j} x_{i,j} m_{i,j} \right)} \right] \quad (18)$$

is employed. In this equation, $x_{i,j}$ is the mass fraction of specie $X_{i,j}$, and R_u is the universal gas constant. The "correct" internal energy is then found from

$$E_{\text{mix}} = E_{\text{mix}}^{\text{ideal}} + E^{\text{coul}}. \quad (19)$$

The internal energies at the specified temperatures are then compared to the target internal energy value, and new temperature bounds selected accordingly. This procedure is continued until the bounding temperatures differ by less than 1 K. Once T is found, the pressure of the mixture follows from equations (1) and (9).

Comparisons of the temperatures and pressures for 1-bar, 10-bar, and 100-bar plasmas as computed via uncorrected and corrected approaches are shown in Figures 1-3, respectively. Below ~10,000 K, the use of the standard model as a standard is questionable, but the results are

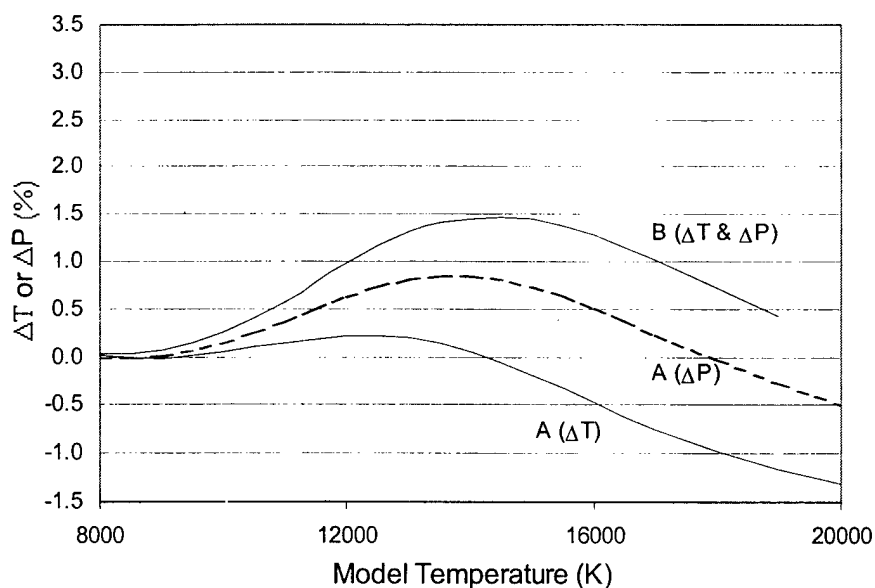


Figure 1. Percent Difference Between Temperatures and Pressures Established by the Standard Model for a 1-bar Plasma Derived From Decomposed Polyethylene and Those Determined From the THERMO.INP Library Provided by McBride and Gordon (A) Without and (B) With Corrections for Coulomb Interactions.

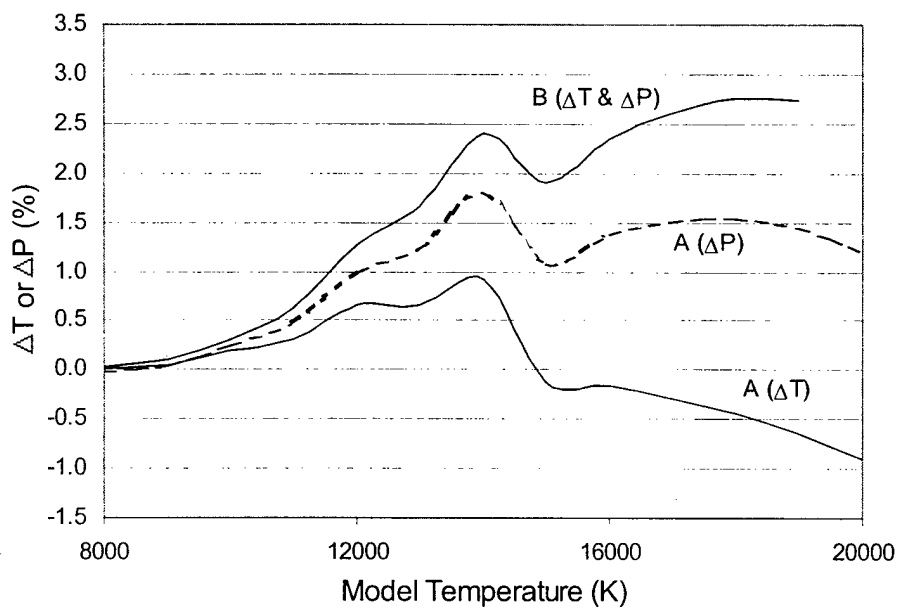


Figure 2. Percent Difference Between Temperatures and Pressures Established by the Standard Model for a 10-bar Plasma Derived From Decomposed Polyethylene and Those Determined From the THERMO.INP Library Provided by McBride and Gordon (A) Without and (B) With Corrections for Coulomb Interactions.

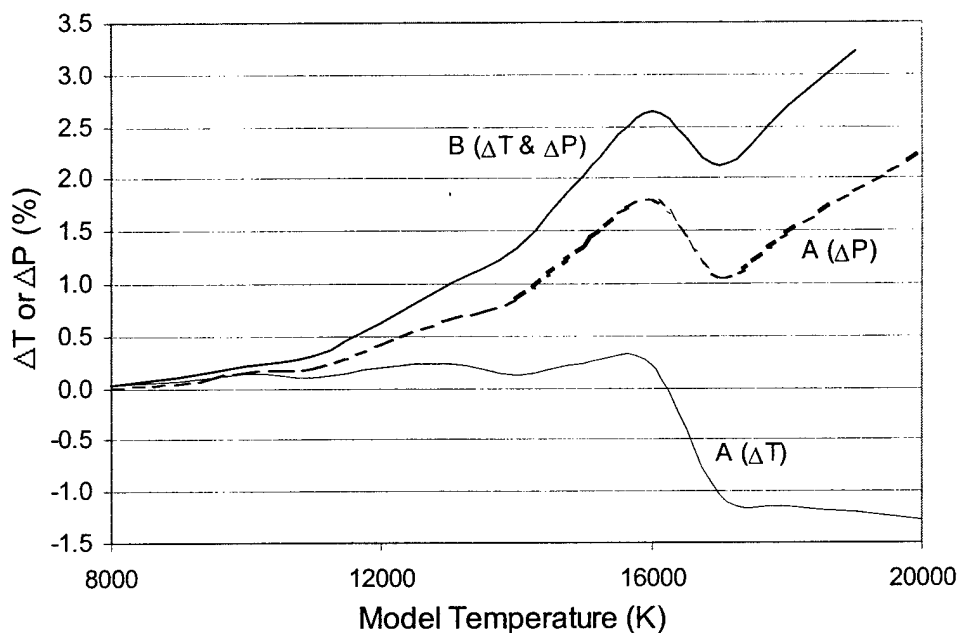


Figure 3. Percent Difference Between Temperatures and Pressures Established by the Standard Model for a 100-bar Plasma Derived From Decomposed Polyethylene and Those Determined From the THERMO.INP Library Provided by McBride and Gordon (A) Without and (B) With Corrections for Coulomb Interactions.

provided to show that the estimates obtained with the three approaches converge to the same values as the temperature is reduced and the influence of Coulomb interactions becomes (truly) negligible. Over the given temperature range, it is observed that the temperatures derived from the corrected approach are higher than those derived from the uncorrected approach; a result consistent with the fact that the reduction in internal energy incorporated into the corrected approach has to be compensated for by an increase in the temperature. Moreover, this shift leads to results that are not in as good agreement with the standard as the uncorrected results except at low pressure (1 bar) and high temperature (>18,000 K).

Several other observations are worth noting. First, based on the same argument used to explain the difference in temperatures obtained via the corrected and uncorrected approaches, it was expected that the temperatures determined via the uncorrected approach would be less than those determined via the standard model. However, for temperatures up to ~15,000 K, it is observed that the uncorrected approach yields higher values. These results can be understood by

consideration of the magnitude of the truncation criterion employed to establish the THERMO.INP data and the $\Delta\varepsilon_{j,k}^\infty$ values calculated by the standard model (see Figure 4). It is observed that the TEMPER method significantly overestimates the magnitude of the lowering of the ionization potential, and, as a result, the internal energy carried by the electronic structure of the neutrals (C and H) is significantly underpredicted. Coupled with the fact that the neutrals predominate in this temperature range, the underprediction of the specific internal energies of C and H more than offsets the fact that cation (C^+ and H^+) energies are not lowered corresponding to the reduction in the ionization potential of their respective neutrals. At high temperatures, where the concentrations of C^+ and H^+ become more significant, the lack of an accounting for the latter effect is observed.

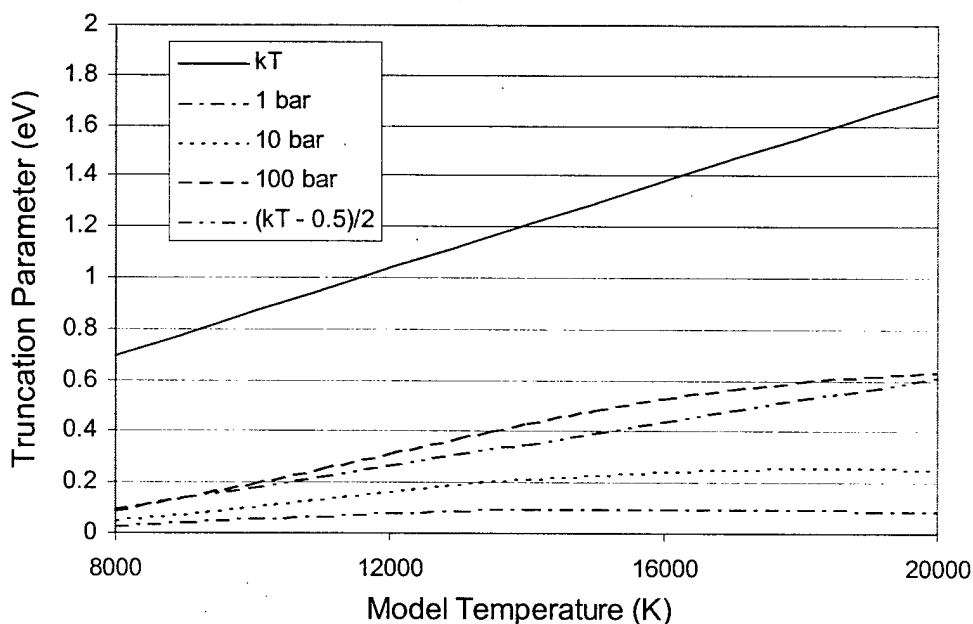


Figure 4. Comparison of Various Truncation Criteria Employed in This Study. Pressure Designations Identify Criteria Obtained From the Properties of a Plasma Derived From Decomposed Polyethylene at That Pressure.

Differences in pressure derived from the different methodologies are also shown in Figures 1–3. Since the equations employed to calculate this parameter are the same in both the standard model and the corrected approach, the differences in pressure follow the differences in

temperature. In the uncorrected case, there is an offset between ΔT and ΔP because the Coulomb interaction-induced pressure reduction is not included in the pressure calculation. However, the offset is small, corresponding to the fact that the pressure-reduction correction is small.

To determine if better agreement with the standard model could be obtained, two alternatives to the data for C, H, and C+ in THERMO.INP were constructed using PAC99.* The first alternative was built under PAC99 alone using the FIXEDN and FILL options to establish properties based on inclusion of all levels up to and including the $k = 5$ principle quantum level. This approach corresponds to the specification of a temperature independent truncation parameter of about 0.5 eV ($4,000 \text{ cm}^{-1}$). The results following from this method are shown in Figures 5–7. It is observed they are generally better than the results that follow from correcting values obtained with the standard library, but below 15,000 K the uncorrected standard library still yields results in better agreement with the standard model.

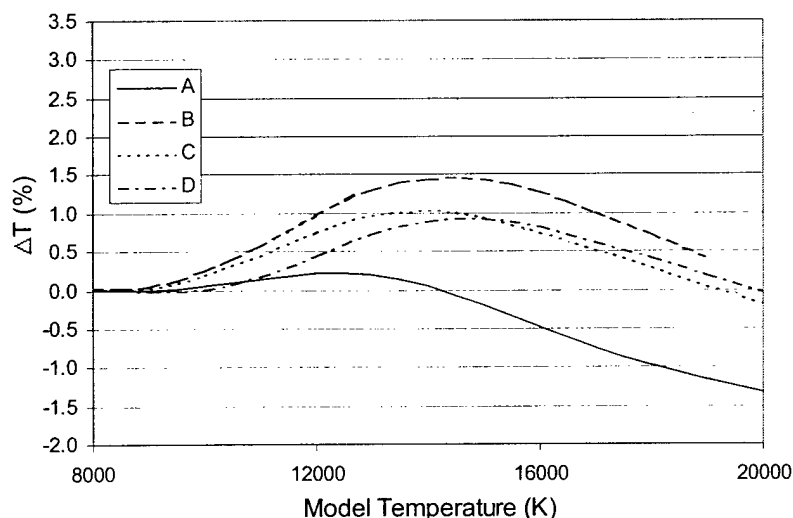


Figure 5. Percent Difference Between Temperatures Established by Standard Model for a 1-bar Plasma Derived From Decomposed Polyethylene and Those Determined From a THERMO.INP Library Developed Based on the Partition Function Truncation Criteria (C) $\Delta \varepsilon_{i,j}^{\infty} = 0.5 \text{ eV}$ and (D) $\Delta \varepsilon_{i,j}^{\infty} = (kT - 0.5)/2$. Results (A) and (B), Which Are Presented and Described in Figure 1, Are Shown for Comparison.

* B. J. McBride provided the authors a "Beta" version of PAC99 (an update of PAC91) prior to its official release.

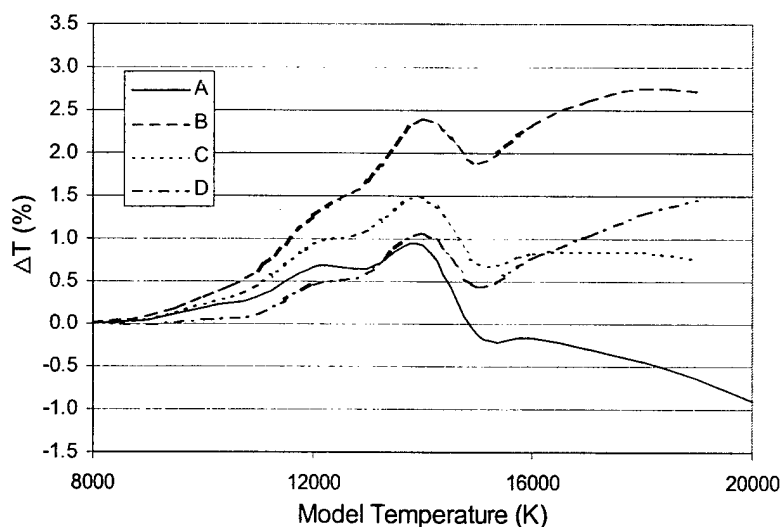


Figure 6. Percent Difference Between Temperatures Established by Standard Model for a 10-bar Plasma Derived From Decomposed Polyethylene and Those Determined From a THERMO.INP Library Developed Based on the Partition Function Truncation Criteria (C) $\Delta\varepsilon_{i,j}^{\infty} = 0.5$ eV and (D) $\Delta\varepsilon_{i,j}^{\infty} = (kT - 0.5)/2$. Results (A) and (B), Which Are Presented and Described in Figure 2, Are Shown for Comparison.

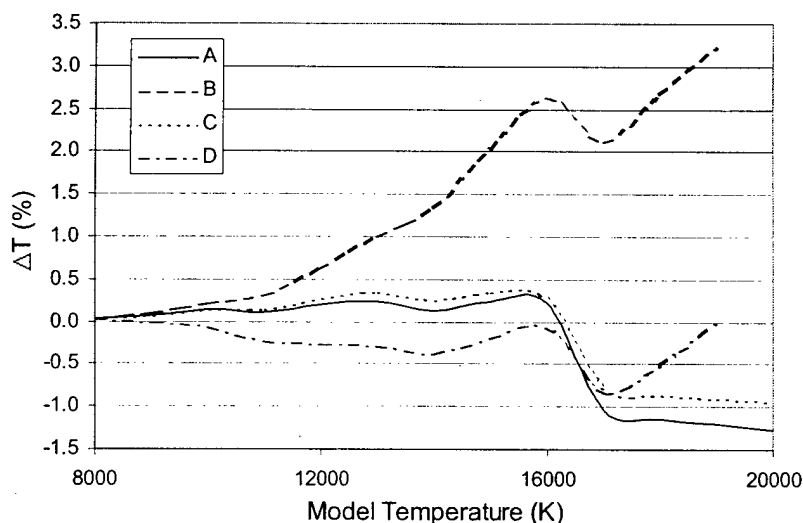


Figure 7. Percent Difference Between Temperatures Established by Standard Model for a 100-bar Plasma Derived From Decomposed Polyethylene and Those Determined From a THERMO.INP Library Developed Based on the Partition Function Truncation Criteria (C) $\Delta\varepsilon_{i,j}^{\infty} = 0.5$ eV and (D) $\Delta\varepsilon_{i,j}^{\infty} = (kT - 0.5)/2$. Results (A) and (B), Which Are Presented and Described in Figure 3, Are Shown for Comparison.

The second data-generation technique employed was to obtain c_p , ΔH , and S for C and H directly from energy level data developed previously [14] and a temperature dependent truncation parameter based on a rough empirical fit to the 100-bar data in Figure 4. The truncation criterion,

$$\begin{aligned} \Delta\varepsilon_{i,j}^{\infty} &= (kT - 0.5\text{eV})/2 \\ \text{for } 6,000 \leq T \leq 20,000, \end{aligned} \quad (20)$$

and its comparison to the other criteria employed in this study is shown in Figure 4. The READ option of PAC99 was then employed to generate the coefficients for the polynomial expressions to represent the data. The results obtained when this data is employed are also shown in Figures 5–7. The excellent agreement between the standard model and this approach for the 100-bar plasma reflects the fact that nearly identical partition-function calculations have been performed in each case. Otherwise, the agreement with the standard is comparable to that obtained with the uncorrected standard library.

The results indicate that the standard THERMO.INP data, where the TEMPER and FILL methods have been employed for generating the data for C, C^+ , and H, will give very good results for conditions relevant to an ablating-polyethylene-capillary arc when temperatures are below $\sim 16,000$ K. In the CFD studies to date, temperatures in the arc-discharge flowfield have not exceeded this value, so concerns regarding the potential inadequacy of the thermodynamic property characterizations appear to be unwarranted. Even for temperatures above 16,000 K, uncorrected results obtained with the data deviate from our standard by no more than 1.5%. When the standard THERMO.INP data is “corrected” with terms that account for Coulomb interactions, the results do not compare as well for any but very low-pressure (1 bar) and high-temperature ($\sim 20,000$ K) conditions. Thus, the incorporation of such corrections into the calculation of the property data when the standard database is employed should be avoided. Minor improvements in the agreement with the standard database can be achieved when data generated via alternatives to the TEMPER/FILL method are employed with terms that correct for Coulomb interactions. But, given the already good agreement obtained with the standard

database and the uncertainty as to how well the standard model actually represents the conditions in the arc-discharge flowfield, the effort to develop and use alternative techniques appears to be unwarranted.

Thermodynamic property data are employed by the CFD model to calculate the temperature and pressure for a fluid element based on its density, chemical composition, and specific internal energy. When this study was started, it was thought that the neglect of corrections for Coulomb interactions could lead to underpredictions of the temperature. That is, with all other parameters the same, the temperature of a fluid element calculated via equations that do not account for Coulomb interactions will be lower than that calculated via equations that do account for the interactions. One potentially important consequence of underpredicting the temperature is that the viscosity of the mixture will also be underpredicted. If the viscosity is underpredicted, the model would (presumably) overpredict the speed and pressure of the arc-discharge jet. Such overpredictions are suggested in the simulations of the experiments by White and coworkers [7]. However, the results presented here indicate that the discrepancy is probably not attributable to the use of the data provided by McBride and Gordon for characterizing the thermodynamic properties of the plasma.

4. Summary

Characterizing the thermodynamic properties of gases generated by an ablating-capillary arc is challenging because conditions in the jet are such that both Coulomb interactions and polyatomic species should be considered. Up to the present, we have employed the THERMO.INP database developed by McBride and Gordon to accomplish this task, but the fact that its data are generated based on methodologies that are not rigorously consistent with the standard theory employed for characterizing weakly-imperfect gases has been a concern. The results presented in this report indicate that despite this shortcoming, the database will provide reasonably accurate property determinations. Minor improvements in property determinations (relative to the results of a model considered to be a standard) were obtained using alternate

techniques, but for the conditions considered in this study—temperatures to 20,000 K and pressures to 100 bar—the development of such alternatives appears to be unnecessary.

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