jugate problem is then decoupled. Note that Eqs. (5–9) also describe an imperfect contact problem, i.e., when two rough solid boundaries are pressed together, only certain scattered regions are in perfect contact, while voids exist in other regions.[3]

Although direct numerical integration such as finite difference or finite elements can be used, the number of computations needed would be much larger than that used in the present Note. The sharp corners and the infinite boundary would also be compromised.

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Extension of Curve Fits for Enthalpy of Equilibrium Air to 1000 Atmospheres

Richard M. Fought*
University of Tennessee, Knoxville, Tennessee 37996
Roop N. Gupta†
NASA Langley Research Center, Hampton, Virginia 23681
and
James E. Lyne‡
University of Tennessee, Knoxville, Tennessee 37996

Introduction

THE present study was initiated in response to the need for high-temperature thermodynamic data for equilibrium air. In investigating the physics of meteors entering Earth's atmosphere at hypersonic velocities, the radiation heat transfer from the hot gases behind the bow shock wave is of major importance. To calculate the radiation intensity, the temperature behind the shock wave must be known. Enthalpy is conserved across the shock wave and the pressure can be approximated using Newtonian theory; these two properties can be used to fix the thermodynamic state at a given position behind the shock wave. However, thermodynamic data for such high enthalpies and pressures (up to 2.0E8 J/kg and close to 1000 atm) are not readily available. Determining the equilibrium composition of air at such states is not trivial, and requires complex computations for exact theoretical values. References 1 and 2, for example, have carried out such computations and obtained curve fits to the computed values.

The curve fits presented by Gupta et al.[1] have an effective limit of 30,000 K and 100 atm for temperature and pressure, respectively. Although the fits provided by Tannehill and Mugge[2] have a higher pressure limit of 1000 atm, the temperature limit is only 25,000 K. These fits are also older and less robust than those of Gupta et al.[1] Although recent improvements have been made to the fits of Tannehill and Mugge[2] by Srinivasan et al.,[3] the temperature limit of 25,000 K still remains. In addition, both the former and latter use a Grabau-function technique that leaves discontinuities in the curves. These discontinuities can result in numerical convergence problems as noted by Oberkampf et al.[4] The following overview demonstrates a scheme used to extrapolate data for enthalpy as a function of temperature to a pressure of 1000 atm, using the existing fits of Gupta et al.[1] In addition, this new 1000-atm curve is valid up to a temperature of approximately 32,600 K, some 7600 K higher than those given by Tannehill and Mugge[2] or Srinivasan et al.[3]

The enthalpy curves of Gupta et al.[1] are presented in terms of h (kcal/g) vs a nondimensional temperature term χ defined as

$$\chi = \ell n(T/10{,}000) \tag{1}$$

where T is in Kelvin. The equations are of the general form

$$h = \exp(A\chi^4 + B\chi^3 + C\chi^2 + D\chi + E) \tag{2}$$

where A, B, C, D, and E are constant coefficients. Curves are presented for pressures ranging from 10^{-4} to 10^2 atm, in intervals of one order of magnitude (i.e., 10^{-3}, 10^{-2} atm, etc.). For any one pressure, the complete curve is made up of several pieces; each piece covers a temperature interval and has a unique set of coefficients. These curves have characteristic inflection points where the change in slope (or $d^2h/d\chi^2$) is zero. These correspond to points where different species begin and cease to dissociate. Any one characteristic inflection point follows a reasonably smooth pattern in terms of h–χ location across the pressure spectrum. This pattern can be extrapolated to a higher pressure for which there is no curve available. From the extrapolated data, a curve consisting of equations like Eq. (2) can easily be reconstructed.

For each of the curves presented by Gupta et al.,[1] Eq. (2) is differentiated to yield

$$\frac{dh}{d\chi} = (4A\chi^3 + 3B\chi^2 + 2C\chi + D)\exp(A\chi^4 + B\chi^3 + C\chi^2 + D\chi + E) \tag{3}$$

$$\frac{d^2h}{d\chi^2} = [(4A\chi^3 + 3B\chi^2 + 2C\chi + D)^2 + 12A\chi^2 + 6B\chi + 2C]\exp(A\chi^4 + B\chi^3 + C\chi^2 + D\chi + E) \tag{4}$$

Equation (4) is used to find the inflection points for the curves by substituting the appropriate coefficients, setting it equal to zero, and solving for χ. With χ known, Eqs. (2) and (3) are used to find the enthalpy h and slope $dh/d\chi$ at the inflection points, respectively. These three equations [Eqs. (2–4)] will be used later for evaluation of curve-fit coefficients in the extended pressure range.

Once the inflection points are found, it is observed that only three points exist for the 100-atm curve. These three and their corresponding points on the other pressure curves are well behaved at the higher pressure ranges. These three point classes (termed class 3, 4, and 5 points) are used for the extrapolation. Lagrangian polynomials are used to fit the trend of each point class across the pressure range. These are of the form (from Ref. 5)

$$f(x) = \sum_{k=0}^{n} \frac{l_k(x)}{l_k(x_k)} f_x \tag{5}$$

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*Graduate Student; currently Engineer, Lockheed Martin Corporation, Denver, CO 80201. Member AIAA.

†Senior Research Engineer, Gas Dynamics Division. Associate Fellow AIAA.

‡Assistant Professor, Mechanical and Aerospace Engineering and Engineering Science Department. Member AIAA.

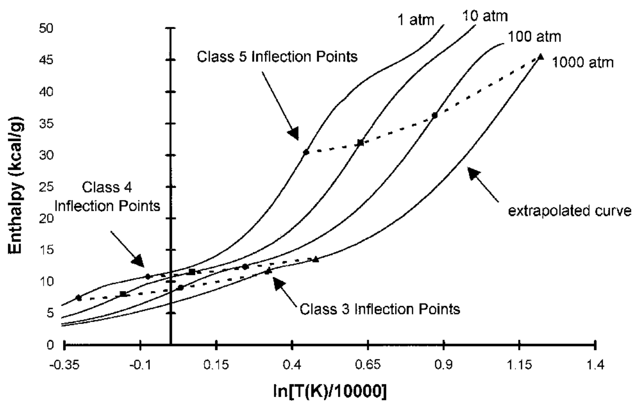

Fig. 1 Enthalpy of equilibrium air with inflection points for various pressures.

where

$$l_0(x) = (x - x_1)(x - x_2) \cdots (x - x_n) \tag{6}$$

$$l_k(x) = (x - x_0) \cdots (x - x_{k-1})(x - x_{k+1}) \cdots (x - x_n) \tag{7}$$

$$l_n(x) = (x - x_0)(x - x_1) \cdots (x - x_{n-1}) \tag{8}$$

Polynomials for the 3, 4, and 5 class inflection points are set up using $\log(P/P_0)$ as the independent variable x (not to be confused with χ, chi). Polynomials of the order $n = 2$ are used for all three classes, using data from $\log(P/P_0) = 0$, 1, and 2. The function $f(x)$ is used to represent χ, h, and $dh/d\chi$. Once the polynomials are set up, an internal point different from the known points is solved for at $\log(P/P_0) = 0.5$. Then polynomials of one order higher are set up to include the unknown curve of 1000 atm. Using the derived data at $\log(P/P_0) = 0.5$, the unknown function at 1000 atm can be calculated. This is required because if any of the original points are used, all other points go to zero, leaving only an equality. Extrapolated inflection points for 1000 atm that fall in the temperature range of Tannehill and Mugge's[2] fits are compared to data from the same 1000-atm curve. The class 3 point shows an error of 2.1%, whereas the class 4 point shows an error of less than 1%. The class 5 point is out of the temperature range of Ref. 2, and no comparison can be made. These inflection points can be seen in Fig. 1. The 1-, 10-, and 100-atm curves are those of Gupta et al.[1]; the 1000-atm curve is that constructed by the present method.

Once χ, h, and $dh/d\chi$ data are found for the class 3, 4, and 5 inflection points at 1000 atm, they are used to reconstruct the curves. This is done using Eqs. (2), (3), and (4) containing the coefficients A, B, C, D, and E at each inflection point. Since χ, h, and $dh/d\chi$ are known for each inflection point, and $d^2h/d\chi^2$ is equal to zero, there are six equations and five unknowns for each interval between two inflection points. The logarithmic nature of Eq. (2) allows for easy substitution into the derivatives, such that a linear system of equations involving the coefficients can be easily derived and solved using matrix inversion. Using this method, three equations are used:

$$\ell n(h|_{\chi_{ip}}) = A\chi_{ip}^4 + B\chi_{ip}^3 + C\chi_{ip}^2 + D\chi_{ip} + E \tag{9}$$

$$h'|_{\chi_{ip}}/h|_{\chi_{ip}} = 4A\chi_{ip}^3 + 3B\chi_{ip}^2 + 2C\chi_{ip} + D \tag{10}$$

$$-(h'|_{\chi_{ip}}/h|_{\chi_{ip}})^2 = 12A\chi_{ip}^2 + 6B\chi_{ip} + 2C \tag{11}$$

In each equation, χ_{ip} denotes the location of the inflection point. Equations (9) and (10) are used twice, at the inital and final inflection points of the interval being solved for. Equation (11) is used once, taken at the final inflection point of the interval. For the initial point at $T = 500$ K ($\chi = -2.99573$) on the first interval up to the class 3 inflection point, h and h' data are assumed from the approximation given by Gupta et al.[1] as h (kcal/g) = 0.00024 T (K). Thus, $h = 0.12$ kcal/g and $h' = 0.12$ kcal/g at $\chi = -2.99573$.

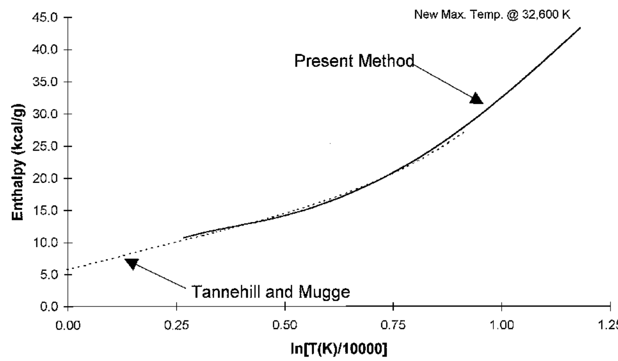

Fig. 2 Enthalpy of equilibrium air at 1000 atm.

The results from this method are best at the higher temperatures (above around 13,000 K), as there are nuances at the lower temperatures that could not be picked up with the inflection point technique. These nuances are present at the lower pressures, but quickly die out as pressure increases. Errors in the low-temperature region as high as 40% are present when comparing the extrapolated data to that presented by Tannehill and Mugge[2] for 1000 atm. Another contributor to this error at low temperatures is the use of the approximate relationship mentioned previously for the initial point. However, once the first inflection point is reached, agreement with the data of Tannehill and Mugge[2] is remarkable, and shows an average error of only 2.25%. The comparison may be seen in Fig. 2. Since sufficient curve fits already exist for enthalpy at lower temperatures and pressures, this method gives a good approximation for high-temperature data at high pressures. To present curve-fit coefficients for the entire temperature range, data derived from Tannehill and Mugge[2] are used to generate the enthalpy curve from 500 to 13,050 K. These data are converted to a curve in the form of Eq. (2) with an average absolute error of 1.5%. The curve from 13,050 to 32,600 K is from the extrapolation method. The coefficients for the curves, in the form of Eq. (2), are provided in Table 1.

One flaw of Lagrangian polynomials is instability between nodes. This arose when extrapolation of a pressure not a multiple of 10 in atmospheres was attempted. The method can theoretically be used to go to unlimited values of pressure (as long as they are multiples of 10 in atmospheres) by repeating the second Lagrangian polynomial procedure, but including the most recent extrapolation point in the equations. Thus, each new extrapolation provides another node to base further extrapolations on. There will be propagation of error involved with this method, so that validity of such a computation may be questionable, especially since there is virtually no experimental data available for comparison. The method used here for enthalpy can easily be extended to any of the other five properties presented by Gupta et al.[1] Properties such as specific heat C_p have characteristic peaks and valleys in the pressure map that would facilitate much easier recognition of patterns across the pressure spectrum. Application of this method does require some use of common sense; visual inspection of present data can determine whether or not a Lagrangian approximation would accurately predict unknown data. Certainly data with wild fluctuations would not be well predicted with this method, as it relies on smoothness of transition. There also must be sufficient data points on which to base the Lagrangian fit. At the lowest resolution, two points are needed; of course, the more points known, the better the fit.

Table 1 Curve-fit coefficients for enthalpy of equilibrium air at 1000 atm

Coefficients					Temperature range, K	χ range
A	*B*	*C*	*D*	*E*		
0.036917	0.277409	0.79532	2.171407	1.741407	500–13,050	−2.99573–0.267452
−59.90844	99.522322	−62.13573	18.320807	0.3166938	13,050–15,650	0.267452–0.448138
0.4887346	−3.011417	5.5598576	−2.320909	2.7638445	15,650–32,600	0.448138–1.18187

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