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Computational Algorithm for Thermodynamic Properties of Air to Extreme Temperatures and Pressures

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Introduction

THE current study was motivated by the need for an easily applied computational method to determine the thermodynamic properties of extremely high-temperature air. This need arose during our investigations of the atmospheric entry of large meteors. These entry bodies' trajectories are significantly effected by aerothermal ablation, and a reasonable estimate of the ablation rates requires a knowledge of the thermodynamic state of the shock layer. Previous investigators have published widely used curve fits for the thermodynamic properties of high-temperature air.[1–4] The works of Tannehill and Mugge[1] and Srinivasan et al.[2] extend to 25,000 K and 1000 atm pressure, whereas the original curve fits of Gupta et al. extended to approximately 30,000 K and 100 atm pressure.[3] Reference 4 extended Gupta's curve fits to a maximum of 1000 atm pressure and 32,600 K. Whereas these methods are sufficient to allow the calculation of equilibrium shock layer temperatures for meteors entering Earth's atmosphere at speeds up to about 20 km/s, most comets enter at velocities between 20 and 30 km/s (Ref. 5). Hence, a rapid computational method that extends to more extreme conditions is needed.

Methodology

The derivation of the desired computational algorithm was made possible by the use of thermodynamic data developed and reported by the Chance Vought Research Center in the early 1960s.[6] The thermodynamic properties in the Chance Vought Research Center report were calculated for a gas mixture model that included 30 species (up to the fifth level of ionization for nitrogen, the sixth level for oxygen, and the eighth level for argon), whereas the data used to develop previously published curve fits accounted for only 11 species.[3,4] The higher number of species considered in the Chance Vought Research Center study allows the range of applicability to extend from 3,000 to 100,000 K and from a density of $1.2(10^{-6})$ kg/m^3 to approximately 70 kg/m^3 (Fig. 1). Unfortunately, the data in the report were presented only in graphical form, and the computer models used to produce the document are no longer in existence. This is in marked contrast to the work of Refs. 1–3, which present both plotted data and computer curve fits designed for the rapid calculation of thermodynamic properties. Therefore, to use the Chance Vought Research Center data in our meteor entry studies, it was necessary to develop an algorithm to accurately calculate the desired data over a very wide range of conditions. The method devised uses well over 1500 data points read from the published plots. To fit this large quantity of data accurately, a surface fit interpolation subroutine known as ITPLBV[7] was employed. ITPLBV is well suited for the required task because it is a bivariate routine (one designed to evaluate parameters that are functions of two independent variables) and uses local procedures. (The term local procedures refers to an approach in which only known data points near the desired point are used in the interpolation, rather than all of the known data points.) This was appropriate in our case because thermodynamic data can vary by as much as 10 orders of magnitude over the range analyzed. The interpolation routine develops a set of bicubic polynomials where

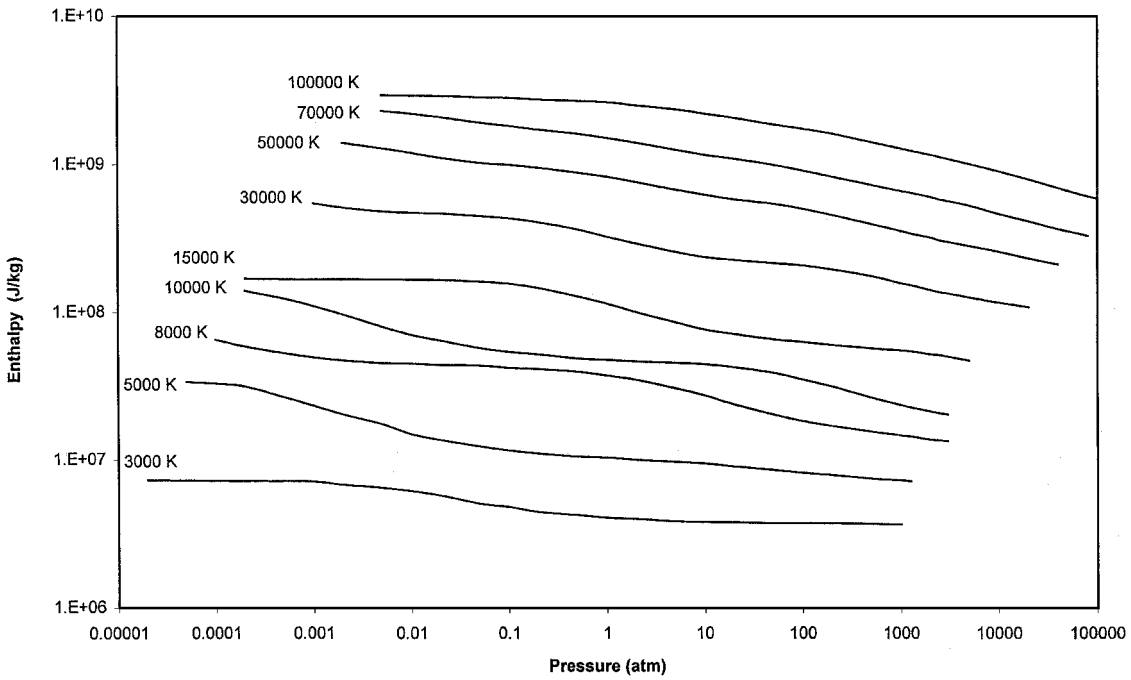

Fig. 1 Range of Chance Vought Research Center data.

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each polynomial is applicable over a given region of the input data set. The region of applicability of a given polynomial is established by the two data points to either side of the point of interest in both the x and y directions, and by one data point in each diagonal direction (for a total of 12 data points used for each interpolation). The algorithms containing the ITPLBV calls acted as an administrator for the interpolation routine by organizing the necessary input data and performing iterations when needed to achieve the proper inputs and output. A major benefit of ITPLBV was that it did not perform an iterative solution; this meant a faster solution and eliminated convergence and computational stability problems.[7]

Results and Conclusion

The method described in this study was incorporated into a FORTRAN algorithm. To evaluate the accuracy of this new algorithm, 10,000 randomly chosen values of density and pressure were used as input to calculate temperature and enthalpy using both the Tannehill and Mugge[1] and Srinivasan et al.[2] curves, as well as our new code. To remain well within the range of applicability of both methods, it was necessary to limit temperature to values between 3,000 and 23,000 K and density to values between approximately $1.23(10^{-6})$ and 68 kg/m^3 for this comparison. For the temperature calculation, our model showed an average difference of 1.05% with respect to the Refs. 1 and 2 results, whereas for enthalpy, the average difference was 0.84%. The distribution of the percent difference is given in Table 1 for temperature and in Table 2 for enthalpy.

A comparison was also made with the Fought et al. curve fits[4]; for this case, the input state variables were enthalpy and pressure, and the output was temperature. Pressure was restricted to a maximum of 100 MPa and temperature to a maximum of 29,000 K. The average difference in calculated temperature was 0.73% with a maximum difference of 6.52%. Table 3 shows the distribution of the percent difference for this case.

Table 1 Distribution of percent difference between temperatures calculated from pressure and density by the current method and by that of Ref. 2

Range, %	Percent of 10,000 points
0–1	55.72
1–2	33.72
2–3	8.36
3–4	0.67
4–5	0.70
5+	0.83

Table 2 Distribution of percent difference between enthalpy values calculated from pressure and density by the current method and by that of Ref. 2

Range, %	Percent of 10,000 points
0–1	69.88
1–2	22.76
2–3	5.59
3–4	1.50
4–5	0.19
5+	0.08

Table 3 Distribution of percent difference between temperatures calculated from pressure and enthalpy by the current method and by that of Ref. 4

Range, %	Percent of 10,000 points
0–1	76.14
1–2	19.19
2–3	3.10
3–4	1.00
4–5	0.39
5+	0.18

More details comparing results obtained using the newly developed method with results found by the methods of Srinivasan et al.[2] and Fought et al.[4] are given in Ref. 8.

The FORTRAN algorithm developed using the new method is capable of using several combinations of independent state variables to determine other thermodynamic properties. Specifically, 1) enthalpy and pressure can be used to determine temperature and density, 2) pressure and temperature can be used to find density and enthalpy, 3) enthalpy and temperature can be used to find density and pressure, 4) enthalpy and density can be used to find pressure and temperature, and 5) pressure and density can be used to determine enthalpy and temperature. Note, however, that the only routines that have been fully evaluated for accuracy are the three cases described (temperature and enthalpy as functions of density and pressure and temperature as a function of pressure and enthalpy). The algorithm is available on the Internet and can be downloaded free of charge and with no restrictions at http://web.utk.edu/~comet/mollier.html [cited 9 December 2000]. Alternatively, the web site offers the user the option of performing individual calculations of thermodynamic properties. Efforts are currently well underway to include entropy among the input and output state variables.

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