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Technical Notes

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Errors in JANAF Thermodynamic Formation Functions for Acetylene

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Introduction

THE JANAF Thermochemical Tables[1] present temperature-dependent thermal and formation functions for elements and compounds and represents a widely used source of thermodynamic information for scientists and engineers. The nomenclature of this Note is consistent with that of Ref. 1. The third and latest edition of these tables contains errors in the thermodynamic formation functions for acetylene (C_2H_2, or, using the systematic name, ethyne). Specifically, the enthalpy of formation ($\Delta_f H^0$), Gibbs energy of formation ($\Delta_f G^0$), and the logarithm of the equilibrium constant ($\log K_f$) tabulated for acetylene are inconsistent with the tabulated values of Gibbs energy function and enthalpy for acetylene and its formation from carbon graphite (C_{gr}) and diatomic hydrogen (H_2).

Analysis

The temperature-dependent formation functions for a compound formed from the reference elements are written in Ref. 1 as

$$\begin{aligned}\Delta_f H^0(T) &= \Delta_f H^0(298.15\ \mathrm{K}) \\ &+ [H^0(T) - H^0(298.15\ \mathrm{K})]_{\mathrm{compound}} \\ &- \Sigma\, [H^0(T) - H^0(298.15\ \mathrm{K})]_{\mathrm{elements}} \qquad (1)\end{aligned}$$

$$\Delta_f G^0(T) = \Delta_f H^0(T) - T[S^0(T)_{\mathrm{compound}} - \Sigma\, S^0(T)_{\mathrm{elements}}] \qquad (2)$$

$$K_f = -\Delta_f G^0(T)/(RT) \qquad (3)$$

where T is the temperature, S^0 is the entropy, H^0 is the enthalpy, and R is the universal gas constant. Equivalently, the formation functions are simply

$$\Delta_f H^0(T) = H^0(T)_{\mathrm{compound}} - \Sigma\, [H^0(T)]_{\mathrm{elements}} \qquad (4)$$

$$\Delta_f G^0(T) = G^0(T)_{\mathrm{compound}} - \Sigma\, [G^0(T)]_{\mathrm{elements}} \qquad (5)$$

where G^0 is the Gibbs free energy. The reaction forming acetylene from the reference elements is

$$C_2H_2 = 2C_{gr} + H_2 \qquad (6)$$

The tabulated values of the formation functions can therefore be compared with formation functions calculated using Eqs. (3–5) and the tabulated thermal functions of acetylene and the reference elements found in Ref. 1. The results of such comparisons are shown in Figs. 1–3. Figure 1 shows the comparison of the tabulated enthalpy of formation with the cal-

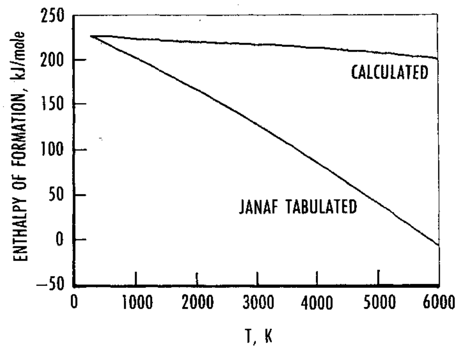

Fig. 1 Comparison of calculated and JANAF tabulated enthalpy of formation for acetylene.

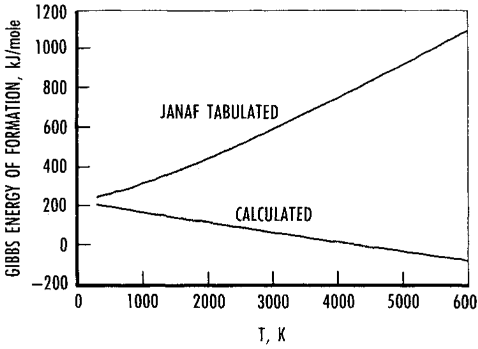

Fig. 2 Comparison of calculated and JANAF tabulated Gibbs energy of formation for acetylene.

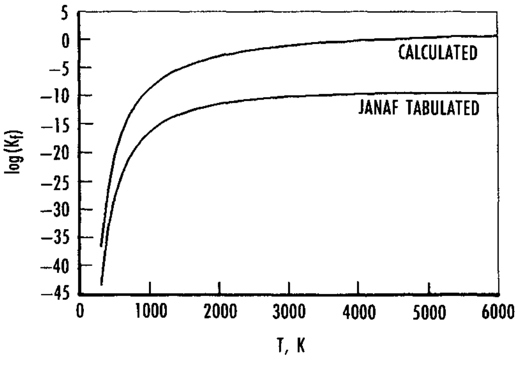

Fig. 3 Comparison of calculated and JANAF tabulated equilibrium constant of formation for acetylene.

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Table 1 Comparison of calculated and JANAF tabulated formation functions for acetylene

	$\Delta_f H^0$, kJ/mole		$\Delta_f G^0$, kJ/mole		$\log K_f$	
T, K	Tabulated	Corrected	Tabulated	Corrected	Tabulated	Corrected
298.15	226.73	226.73	248.16	209.20	−43.48	−36.65
500	220.35	226.23	264.44	197.45	−27.62	−20.63
1000	202.99	223.67	315.14	169.61	−16.46	−8.86
2000	166.98	219.93	441.08	117.19	−11.52	−3.06
3000	128.29	217.02	586.35	66.42	−10.21	−1.16

culated values. Figures 2 and 3 show similar comparisons for the Gibbs energy of formation and the equilibrium constant of formation, respectively. The tabulated values of the formation functions are in obvious disagreement with values calculated using the tabulated thermal functions, indicating a lack of internal consistency in the JANAF tables. The calculated values presented here are in agreement with others in the literature.[2,3] Reference 3 is a previous version of the JANAF tables. As an additional check of the method of calculation, formation functions for methane (CH_4) and ethylene (C_2H_4) were calculated and found to agree precisely with the tabulated values.

Moreover, the tabulated and calculated values of the enthalpy of formation for acetylene are seen in Fig. 1 to agree precisely at 298.15 K. This seemed to indicate a systematic error in the tabulated values for acetylene rather than a random error or an error in method. By definition, the enthalpies of the reference elements are zero at 298.15 K. Therefore, regardless of the stoichiometric coefficients on the right side of Eq. (6), the correct value of the enthalpy of formation is calculated at 298.15 K. Intuitively, one might then suspect an error was made when writing Eq. (6) for the JANAF tables. Indeed, if Eq. (6) is written with the incorrect coefficient for H_2 as

$$C_2H_2 = 2C_{gr} + 2H_2 \tag{7}$$

and the formation functions are calculated on this basis, then the tabulated values are obtained precisely. Therefore, it is concluded that the JANAF tabulated values were incorrectly obtained using Eq. (7) as the formation reaction. The incorrect and corrected values for the thermodynamic formation functions are listed in Table 1 for a limited number of temperatures. The authors of Ref. 1 are aware of the error and plan to publish an addendum. The intent of this Note is to communicate the corrected values to the technical community as quickly as possible.

Summary

An error is found in the thermodynamic formation functions for acetylene presented in the third edition of the JANAF tables. The error is due to the use of an incorrect formation reaction for acetylene. Corrected values are given in both graphical and tabular form. The corrected functions are also available in digital form from the author.

References

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Numerical Study of Turbulent Offset Jets with Entrainment Boundary

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I. Introduction

THE turbulent offset jets find many important industrial applications, such as heat exchangers, environment discharges, fluid injection systems, combustion chambers, air conditions for large buildings, etc. The flow pattern of turbulent offset jets can be divided into three characteristic regions: 1) the recirculation region, 2) the impingement region, and 3) the wall jet region, as shown in Fig. 1. The flow characteristics of turbulent offset jets were studied most recently by Pelfrey and Liburdy,[1-3] Bourque and Newman,[4] and Sawyer.[5,6]

Although many investigators have studied backward-facing step flow, only a few of the offset jets are considered, especially with entrainment boundary. In this Note, the high Reynolds form of the k-ε turbulence model and wall function for the near-wall turbulence behavior are incorporated to predict the mean flow characteristics of the flowfield at the single exit Reynolds number $Re = 15{,}000$ and different offset ratio $OR = 3, 7, 11$. The computed results are compared with the experimental data reported in the literature.

II. Mathematical Formulation

The steady conservation equations for incompressible two-dimensional Cartesian coordinates mean flow characteristics of turbulent flow can be written as

$$\frac{\partial}{\partial x}(\rho u\phi) + \frac{\partial}{\partial y}(\rho v\phi) = \frac{\partial}{\partial x}\left[\Gamma_\phi \frac{\partial\phi}{\partial x}\right] + \frac{\partial}{\partial y}\left[\Gamma_\phi \frac{\partial\phi}{\partial y}\right] + S_\phi \tag{1}$$

where ϕ stands for the dependent variables u, v, k, and ε; u and v are the local time-averaged velocity in x and y directions, respectively; and Γ_ϕ and S_ϕ are the corresponding turbulent diffusion coefficient and source term, respectively, for general variable ϕ. These equations are summarized in Table 1. The turbulent viscosity μ_t can be written as

$$\mu_t = \rho C\mu(k^2/\varepsilon) \tag{2}$$

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