Equilibrium Chemical Composition and Thermodynamic Properties of Air-Carbon Mixtures at High Temperatures

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THE RECENT need for laboratory simulation of high speed flight and atmospheric re-entry has created interest in the high temperature gas flow produced by a constricted electric arc (*1, 7, 9*). When the arc is operated with graphite electrodes and with air as the working fluid, the flow is contaminated with quantities of carbon. Since knowledge of the chemical and thermodynamic properties of the flow is important in simulation, the properties of air-carbon mixtures must be determined.

In the calculations reported here, the constituents of the mixtures are assumed to be N, O, A, C, N_2, O_2, C_2, NO, CO, CN, and C_3. Calculations have been made of the free energy, enthalpy, entropy, average molecular weights, and mole fractions for equilibrium mixtures containing 1 to 30% carbon by weight in the temperature range 4000° to 10,000° K. and pressures in the range 0.1 to 100 atm. Only representative portions of the data are reported in this article.

PROCEDURE

The free energy F of any n component, ideal gas system at temperature T is given by

$$F = \sum x_i F_i^0 + RT \sum x_i \ln p_i \qquad (1)$$

where x_i is the number of moles, p_i the partial pressure, and F_i^0 the standard molar free energy of the i^{th} constituent. The equilibrium composition of the mixture consists of that set of nonnegative values x_i which minimizes the free energy and satisfies the mass balance restraints:

$$\sum_{i=1}^{n} A_{ij} x_i = B_j \qquad (j = 1, \ldots, m) \qquad (2)$$

where A_{ij} is the number of atoms of elements j in a molecule of component i, and B_j is the total number of gram atomic weights of j originally present in the mixture.

A method reported by White, Johnson, and Danzig (*10*) was used to linearize the free energy equation and establish an iterative linear programming procedure to compute the x_i and minimize F. The initial basic feasible solution was taken as

$$x_i = B_i \quad (i = j = 1, \ldots, m),$$

$$x_i = 0 \quad (i > m)$$

The only modification of the method as described by White and others (*10*) was in the halving of the "alpha grid," because successive values of $(x_i/\sum x_i)$ did not always stay within the range set up by the previous cycle.

Throughout the iterations the mole fractions of species present in trace amounts assumed a zero value. The linear programming procedure was used until four decimal place accuracy in $(x_i/\sum x_i)$ was obtained. The nonzero values of $(x_i/\sum x_i)$ were then used in a set of chemical equilibrium equations involving each "zero level" component to obtain values for mole fractions of the trace components. Equilibrium constants were calculated using the free energy functions (Table III) discussed below.

The accuracy of all mole fraction values was then improved by setting

$$\left(\frac{x_i}{\sum x_i}\right)_{\text{improved}} = \left(\frac{x_i}{\sum x_i}\right) + \epsilon_i \qquad (3)$$

$$\left(\sum x_i\right)_{\text{improved}} = \left(\sum x_i\right) + \bar{\epsilon} \qquad (4)$$

and using these equations in the chemical equilibrium equations.

Since the values of ϵ_i and $\bar{\epsilon}$ are relatively small, their products may be considered negligible. Thus the $(n - m)$ chemical equilibrium equations were obtained as linear functions of the $(n + 1)$ unknowns ϵ_i and $\bar{\epsilon}$. The mass balance restraints provide m additional equations of the form;

$$\left[\left(\sum x_i\right) + \bar{\epsilon}\right] \sum_i A_{ij} \left[\left(\frac{x_i}{\sum x_i}\right) + \epsilon_i\right] = B_j \; (j = 1, \ldots, m) \qquad (5)$$

Since

$$\sum_{i=1}^{n} \left(\frac{x_i}{\sum x_i}\right) \equiv 1 \qquad (6)$$

and it is required that

$$\sum_{i=1}^{n} \left[\left(\frac{x_i}{\sum x_i}\right) + \epsilon_i\right] = 1, \qquad (7)$$

the $(n + 1)$ st equation is

$$\sum_{i=1}^{n} \epsilon_i = 0 \qquad (8)$$

These $(n + 1)$ simultaneous equations were then solved for for the unknowns $\epsilon_i (i = 1, \ldots, n)$ and $\bar{\epsilon}$, and the improved set of mole fraction values was obtained. This improvement process was then repeated to give the values reported in Table I. An IBM 704 computer was used for the computations.

CALCULATION

To perform the calculations, the standard molar free energy F_i^0 of each of the i constituents must be known. The values of the standard free energy function $(F^0/RT)_i$ and enthalpy function $(H^0/RT)_i$ of N, O, A, C, N_2, O_2, NO, and CO at temperatures of 4000° to 8000° K. given by Gilmore (*2*) have been used without modification. The 9000° and 10,000° K. values for these species and the 6000° to 10,000° K. values for CN and C_2 were calculated from the spectroscopic data given by Herzberg (*5*) using the general method described by Gilmore. The thermodynamic functions from 4000° to 6000° K. for CN were taken from Johnson (*6*) and for C_2 from Gordon (*4*). The spectroscopic data used in the calculations are reproduced in Table II. The thermodynamic functions of C_3 were calculated as discussed below for the entire temperature range.

At the suggestion of Mulliken (*8*) the C_3 molecule was treated as follows: The ground state was taken as $^1\Sigma$ by analogy with CO_2. The available excited states on promotion of an electron from the $1\pi_u$ orbital to π_g orbital were chosen as $^1\Sigma_u^+$, $^1\Delta_u$, $^1\Sigma_u^-$, $^3\Sigma_u^-$, $^3\Delta_u$, $^3\Sigma_u^+$. Similarly, on promotion of an electron from the $3\sigma_u$ orbital to the π_g orbital the excited states chosen were $^1\Pi_u$, $^3\Pi_u$, $^1\Sigma_g^+$. Since little experimental data are available concerning the energies of these states, a very rough estimate based on scaling from N_2 and CO_2 was made. The energies of the nine statistical states corresponding to the $(3\sigma_u \rightarrow \pi_g)$ transition were assumed to be evenly distributed in the range 1.5 to 3.5 ev. Similarly the 16 states corresponding to the $(1\pi_u \rightarrow \pi_g)$ transition were assumed to be distributed in the range 1.5 to 4.5 ev.

The values used for the moments of inertia and fundamental vibration of the C_3 molecule were taken from Glockler (3).

The thermodynamic data which were used to calculate the composition and thermodynamic properties of the mixtures are reproduced in Table III. The composition of dry room temperature air was obtained from Gilmore (2). The compositions of four air-carbon mixtures at temperatures 5000°, 6000°, 8000°, and 10,000° K. and pressures of 0.1, 1.0, 10, and 100 atm. are reported in Table I. The last value in each column of Table I is the average molecular weight, $\bar{M}$, of the mixture. For convenience, the thermodynamic function is presented graphically as plots of temperature vs. (S/R) in Figure 1. Lines of constant density ratio (ρ/ρ_0) and constant enthalpy function (H/RT_0) are also included in the figure.

The enthalpy function (H/RT) was obtained for each mixture from the (H^0/RT) values given in Table III using the expression

$$\sum_{i=1}^{n} x_i (H^0/RT)_i = (H/RT)_{mix} \qquad (9)$$

The free energy functions $-(F/RT)_{mix}$ were obtained from the minimization of Equation 1 and the entropy functions $(S/R)_{mix}$ from the relation $(S/R = -F/RT + H/RT)_{mix}$.

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(Literature Cited follows on page 460.)

Table I. Mole Fractions of the Constituents of Air-Carbon Mixtures

Species	Pressure Atm. 0.1	1	10	100
	Temperature: 5000° K.; Carbon Content: 5% by Wt.			
N	7.928×10^{-2}	2.599×10^{-2}	8.317×10^{-3}	2.657×10^{-3}
O	2.289×10^{-1}	2.255×10^{-1}	1.955×10^{-1}	1.232×10^{-1}
A	7.444×10^{-3}	7.694×10^{-3}	7.904×10^{-3}	8.247×10^{-3}
C	4.402×10^{-4}	4.645×10^{-5}	5.508×10^{-6}	9.122×10^{-7}
N_2	5.792×10^{-1}	6.224×10^{-1}	6.374×10^{-1}	6.508×10^{-1}
O_2	1.083×10^{-4}	1.051×10^{-3}	7.900×10^{-3}	3.137×10^{-2}
NO	3.971×10^{-3}	1.282×10^{-2}	3.557×10^{-2}	7.163×10^{-2}
CO	1.005×10^{-1}	1.045×10^{-1}	1.074×10^{-1}	1.121×10^{-1}
CN	2.309×10^{-4}	7.986×10^{-5}	3.031×10^{-5}	1.604×10^{-5}
C_2	2.012×10^{-9}	2.240×10^{-10}	3.150×10^{-11}	8.640×10^{-12}
C_3	7.869×10^{-14}	9.246×10^{-15}	1.542×10^{-15}	7.004×10^{-16}
$\bar{M}$	24.25	25.06	25.75	26.86
	Temperature: 5000° K.; Carbon Content: 10% by Wt.			
N	7.920×10^{-2}	2.600×10^{-2}	8.312×10^{-3}	2.643×10^{-3}
O	1.205×10^{-1}	1.171×10^{-1}	1.030×10^{-1}	6.903×10^{-2}
A	7.427×10^{-3}	7.667×10^{-3}	7.799×10^{-3}	7.962×10^{-3}
C	1.748×10^{-3}	1.875×10^{-4}	2.173×10^{-5}	3.311×10^{-6}
N_2	5.781×10^{-1}	6.227×10^{-1}	6.366×10^{-1}	6.425×10^{-1}
O_2	3.000×10^{-5}	2.835×10^{-4}	2.192×10^{-3}	9.848×10^{-3}
NO	2.088×10^{-3}	6.661×10^{-3}	1.873×10^{-2}	3.994×10^{-2}
CO	2.100×10^{-1}	2.191×10^{-1}	2.233×10^{-1}	2.280×10^{-1}
CN	9.159×10^{-4}	3.225×10^{-4}	1.195×10^{-4}	5.786×10^{-5}
C_2	3.172×10^{-8}	3.652×10^{-9}	4.903×10^{-10}	1.138×10^{-10}
C_3	4.928×10^{-12}	6.086×10^{-13}	9.467×10^{-14}	3.347×10^{-14}
$\bar{M}$	25.52	26.35	26.80	27.36
	Temperature: 5000° K.; Carbon Content: 20% by Wt.			
N	7.307×10^{-2}	2.383×10^{-2}	7.582×10^{-3}	2.402×10^{-3}
O	3.279×10^{-3}	5.889×10^{-4}	1.389×10^{-4}	3.947×10^{-5}
A	6.608×10^{-3}	6.927×10^{-3}	7.097×10^{-3}	7.177×10^{-3}
C	8.937×10^{-2}	5.265×10^{-2}	2.289×10^{-2}	8.151×10^{-3}
N_2	4.920×10^{-1}	5.234×10^{-1}	5.297×10^{-1}	5.315×10^{-1}
O_2	2.222×10^{-8}	7.168×10^{-9}	3.991×10^{-9}	3.220×10^{-9}
NO	5.242×10^{-5}	3.071×10^{-5}	2.305×10^{-5}	2.074×10^{-5}
CO	2.923×10^{-1}	3.093×10^{-1}	3.174×10^{-1}	3.210×10^{-1}
CN	4.320×10^{-2}	8.301×10^{-2}	1.148×10^{-1}	1.296×10^{-1}
C_2	8.292×10^{-5}	2.878×10^{-4}	5.442×10^{-4}	6.897×10^{-4}
C_3	6.586×10^{-7}	1.347×10^{-5}	1.107×10^{-4}	4.994×10^{-4}
$\bar{M}$	25.51	26.75	27.40	27.71
	Temperature: 5000° K.; Carbon Content: 30% by Wt.			
N	6.206×10^{-2}	1.967×10^{-2}	6.114×10^{-3}	1.950×10^{-3}
O	9.589×10^{-4}	1.595×10^{-4}	3.644×10^{-5}	1.101×10^{-5}
A	5.214×10^{-3}	5.611×10^{-3}	5.925×10^{-3}	6.130×10^{-3}
C	2.434×10^{-1}	1.581×10^{-1}	7.307×10^{-2}	2.502×10^{-2}
N_2	3.549×10^{-1}	3.564×10^{-1}	3.444×10^{-1}	3.502×10^{-1}
O_2	1.901×10^{-9}	5.257×10^{-10}	2.745×10^{-10}	2.507×10^{-10}
NO	1.302×10^{-5}	6.862×10^{-6}	4.874×10^{-6}	4.698×10^{-6}
CO	2.329×10^{-1}	2.515×10^{-1}	2.657×10^{-1}	2.749×10^{-1}
CN	9.994×10^{-2}	2.056×10^{-1}	2.956×10^{-1}	3.227×10^{-1}
C_2	6.153×10^{-4}	2.594×10^{-3}	5.542×10^{-3}	6.501×10^{-3}
C_3	1.331×10^{-5}	3.644×10^{-4}	3.597×10^{-3}	1.446×10^{-2}
$\bar{M}$	23.10	24.86	26.25	27.16

Table I. Continued

Species	Pressure, Atm. 0.1	1	10	100
	Temperature: 6000° K.; Carbon Content: 5% by Wt.			
N	4.055×10^{-1}	1.676×10^{-1}	5.760×10^{-2}	1.869×10^{-2}
O	2.110×10^{-1}	2.203×10^{-1}	2.166×10^{-1}	1.797×10^{-1}
A	5.987×10^{-3}	7.079×10^{-3}	7.593×10^{-3}	7.928×10^{-3}
C	2.301×10^{-2}	3.589×10^{-3}	4.095×10^{-4}	5.191×10^{-5}
N_2	2.947×10^{-1}	5.032×10^{-1}	5.947×10^{-1}	6.262×10^{-1}
O_2	1.158×10^{-5}	1.262×10^{-4}	1.220×10^{-3}	8.397×10^{-3}
NO	1.310×10^{-3}	5.650×10^{-3}	1.909×10^{-2}	5.140×10^{-2}
CO	5.597×10^{-2}	9.111×10^{-2}	1.022×10^{-1}	1.075×10^{-1}
CN	2.408×10^{-3}	1.552×10^{-3}	6.087×10^{-4}	2.504×10^{-4}
C_2	2.027×10^{-6}	4.929×10^{-7}	6.419×10^{-8}	1.031×10^{-8}
C_3	7.608×10^{-11}	2.885×10^{-11}	4.287×10^{-12}	8.732×10^{-13}
$\bar{M}$	19.50	23.06	24.73	25.82
	Temperature: 6000° K.; Carbon Content: 10% by Wt.			
N	3.946×10^{-1}	1.663×10^{-1}	5.756×10^{-2}	1.869×10^{-2}
O	1.549×10^{-1}	1.274×10^{-1}	1.150×10^{-1}	9.507×10^{-2}
A	5.754×10^{-3}	6.994×10^{-3}	7.542×10^{-3}	7.788×10^{-3}
C	5.708×10^{-2}	1.243×10^{-2}	1.601×10^{-3}	2.026×10^{-4}
N_2	2.790×10^{-1}	4.957×10^{-1}	5.937×10^{-1}	6.258×10^{-1}
O_2	6.240×10^{-6}	4.223×10^{-5}	3.438×10^{-4}	2.351×10^{-3}
NO	9.355×10^{-4}	3.243×10^{-3}	1.013×10^{-2}	2.719×10^{-2}
CO	1.019×10^{-1}	1.826×10^{-1}	2.121×10^{-1}	2.219×10^{-1}
CN	5.813×10^{-3}	5.336×10^{-3}	2.377×10^{-3}	9.768×10^{-4}
C_2	1.247×10^{-5}	5.917×10^{-6}	9.805×10^{-7}	1.570×10^{-7}
C_3	1.161×10^{-9}	1.200×10^{-9}	2.560×10^{-10}	5.187×10^{-11}
$\bar{M}$	19.77	24.04	25.92	26.76
	Temperature: 6000° K.; Carbon Content: 20% by Wt.			
N	3.599×10^{-1}	1.530×10^{-1}	5.281×10^{-2}	1.709×10^{-2}
O	7.843×10^{-2}	2.165×10^{-2}	4.529×10^{-3}	1.097×10^{-3}
A	5.041×10^{-3}	6.207×10^{-3}	6.792×10^{-3}	7.051×10^{-3}
C	1.623×10^{-1}	1.024×10^{-1}	5.728×10^{-2}	2.485×10^{-2}
N_2	2.321×10^{-1}	4.198×10^{-1}	4.999×10^{-1}	5.236×10^{-1}
O_2	1.600×10^{-6}	1.219×10^{-6}	5.334×10^{-7}	3.123×10^{-7}
NO	4.319×10^{-4}	5.070×10^{-4}	3.661×10^{-4}	2.870×10^{-4}
CO	1.467×10^{-1}	2.555×10^{-1}	2.990×10^{-1}	3.141×10^{-1}
CN	1.507×10^{-2}	4.046×10^{-2}	7.807×10^{-2}	1.096×10^{-1}
C_2	1.008×10^{-4}	4.016×10^{-4}	1.256×10^{-3}	2.363×10^{-3}
C_3	2.670×10^{-8}	6.710×10^{-7}	1.173×10^{-5}	9.576×10^{-5}
$\bar{M}$	19.46	23.96	26.22	27.22
	Temperature: 6000° K.; Carbon Content: 30% by Wt.			
N	3.151×10^{-1}	1.311×10^{-1}	4.406×10^{-2}	1.403×10^{-2}
O	4.262×10^{-2}	7.560×10^{-3}	1.325×10^{-3}	3.113×10^{-4}
A	4.156×10^{-3}	4.970×10^{-3}	5.522×10^{-3}	5.896×10^{-3}
C	2.923×10^{-1}	2.470×10^{-1}	1.613×10^{-1}	7.361×10^{-2}
N_2	1.779×10^{-1}	3.081×10^{-1}	3.479×10^{-1}	3.527×10^{-1}
O_2	4.724×10^{-7}	1.486×10^{-7}	4.564×10^{-8}	2.520×10^{-8}
NO	2.055×10^{-4}	1.517×10^{-4}	8.933×10^{-5}	6.683×10^{-5}
CO	1.436×10^{-1}	2.152×10^{-1}	2.462×10^{-1}	2.641×10^{-1}
CN	2.377×10^{-2}	8.358×10^{-2}	1.834×10^{-1}	2.665×10^{-1}
C_2	3.271×10^{-4}	2.335×10^{-3}	9.957×10^{-3}	2.074×10^{-2}
C_3	1.560×10^{-7}	9.409×10^{-6}	2.619×10^{-4}	2.490×10^{-3}
$\bar{M}$	18.41	22.02	24.46	26.12
	Temperature: 8000° K.; Carbon Content: 5% by Wt.			
N	7.297×10^{-1}	6.729×10^{-1}	4.531×10^{-1}	1.989×10^{-1}
O	1.989×10^{-1}	2.046×10^{-1}	2.167×10^{-1}	2.105×10^{-1}
A	4.451×10^{-3}	4.688×10^{-3}	5.692×10^{-3}	6.960×10^{-3}
C	5.983×10^{-2}	5.720×10^{-2}	3.692×10^{-2}	8.936×10^{-3}
N_2	6.278×10^{-3}	5.339×10^{-2}	2.421×10^{-1}	4.664×10^{-1}
O_2	7.523×10^{-7}	7.954×10^{-6}	8.927×10^{-5}	8.426×10^{-4}
NO	7.557×10^{-5}	7.166×10^{-4}	5.112×10^{-3}	2.180×10^{-2}
CO	4.932×10^{-4}	4.849×10^{-3}	3.315×10^{-2}	7.796×10^{-2}
CN	1.888×10^{-4}	1.664×10^{-3}	7.233×10^{-3}	7.685×10^{-3}
C_2	1.180×10^{-6}	1.079×10^{-5}	4.492×10^{-5}	2.632×10^{-5}
C_3	2.779×10^{-12}	2.429×10^{-10}	6.529×10^{-9}	9.258×10^{-9}
$\bar{M}$	14.50	15.27	18.54	22.67

Table I. Continued

Species	Pressure, Atm. 0.1	1	10	100
	Temperature: 8000° K.; Carbon Content: 10% by Wt.			
N	6.846×10^{-1}	6.343×10^{-1}	4.349×10^{-1}	1.951×10^{-1}
O	1.860×10^{-1}	1.874×10^{-1}	1.785×10^{-1}	1.410×10^{-1}
A	4.175×10^{-3}	4.395×10^{-3}	5.397×10^{-3}	6.766×10^{-3}
C	1.183×10^{-1}	1.139×10^{-1}	7.999×10^{-2}	2.516×10^{-2}
N_2	5.526×10^{-3}	4.743×10^{-2}	2.230×10^{-1}	4.488×10^{-1}
O_2	6.579×10^{-7}	6.678×10^{-6}	6.055×10^{-5}	3.780×10^{-4}
NO	6.630×10^{-5}	6.189×10^{-4}	4.041×10^{-3}	1.432×10^{-2}
CO	9.121×10^{-4}	8.843×10^{-3}	5.916×10^{-2}	1.470×10^{-1}
CN	3.503×10^{-4}	3.123×10^{-3}	1.504×10^{-2}	2.122×10^{-2}
C_2	4.614×10^{-6}	4.273×10^{-5}	2.109×10^{-4}	2.087×10^{-4}
C_3	2.149×10^{-11}	1.915×10^{-9}	6.642×10^{-8}	2.067×10^{-7}
M	14.35	15.10	18.55	23.25
	Temperature: 8000° K.; Carbon Content: 20% by Wt.			
N	5.969×10^{-1}	5.575×10^{-1}	3.912×10^{-1}	1.780×10^{-1}
O	1.612×10^{-1}	1.560×10^{-1}	1.191×10^{-1}	5.312×10^{-2}
A	3.639×10^{-3}	3.823×10^{-3}	4.714×10^{-3}	6.027×10^{-3}
C	2.319×10^{-1}	2.256×10^{-1}	1.811×10^{-1}	9.610×10^{-2}
N_2	4.200×10^{-3}	3.664×10^{-2}	1.804×10^{-1}	3.734×10^{-1}
O_2	4.940×10^{-7}	4.627×10^{-6}	2.696×10^{-5}	5.363×10^{-5}
NO	5.009×10^{-5}	4.528×10^{-4}	2.425×10^{-3}	4.921×10^{-3}
CO	1.549×10^{-3}	1.458×10^{-2}	8.936×10^{-2}	2.115×10^{-1}
CN	5.985×10^{-4}	5.437×10^{-3}	3.063×10^{-2}	7.395×10^{-2}
C_2	1.772×10^{-5}	1.677×10^{-4}	1.081×10^{-3}	3.044×10^{-3}
C_3	1.618×10^{-10}	1.489×10^{-8}	7.706×10^{-7}	1.151×10^{-5}
M	14.05	14.76	18.20	23.27
	Temperature: 8000° K.; Carbon Content: 30% by Wt.			
N	5.124×10^{-1}	4.816×10^{-1}	3.418×10^{-1}	1.528×10^{-1}
O	1.373×10^{-1}	1.278×10^{-1}	7.954×10^{-2}	2.412×10^{-2}
A	3.106×10^{-3}	3.251×10^{-3}	3.958×10^{-3}	5.003×10^{-3}
C	3.413×10^{-1}	3.347×10^{-1}	2.929×10^{-1}	1.984×10^{-1}
N_2	3.096×10^{-3}	2.734×10^{-2}	1.377×10^{-1}	2.753×10^{-1}
O_2	3.586×10^{-7}	3.103×10^{-6}	1.203×10^{-5}	1.106×10^{-5}
NO	3.664×10^{-5}	3.203×10^{-4}	1.415×10^{-3}	1.919×10^{-3}
CO	1.942×10^{-3}	1.772×10^{-2}	9.656×10^{-2}	1.983×10^{-1}
CN	7.562×10^{-4}	6.969×10^{-3}	4.329×10^{-2}	1.311×10^{-1}
C_2	3.840×10^{-5}	3.692×10^{-4}	2.829×10^{-3}	1.298×10^{-2}
C_3	5.159×10^{-10}	4.864×10^{-8}	3.262×10^{-6}	1.014×10^{-4}
M	13.76	14.40	17.54	22.16
	Temperature: 10,000° K.; Carbon Content: 5% by Wt.			
N	7.370×10^{-1}	7.338×10^{-1}	7.043×10^{-1}	5.433×10^{-1}
O	1.982×10^{-1}	1.985×10^{-1}	2.016×10^{-1}	2.134×10^{-1}
A	4.421×10^{-3}	4.435×10^{-3}	4.557×10^{-3}	5.264×10^{-3}
C	6.008×10^{-2}	5.996×10^{-2}	5.869×10^{-2}	4.728×10^{-2}
N_2	2.928×10^{-4}	2.903×10^{-3}	2.674×10^{-2}	1.591×10^{-1}
O_2	1.564×10^{-7}	1.569×10^{-6}	1.618×10^{-5}	1.814×10^{-4}
NO	9.319×10^{-6}	9.295×10^{-5}	9.059×10^{-4}	7.399×10^{-3}
CO	1.739×10^{-5}	1.739×10^{-4}	1.729×10^{-3}	1.474×10^{-2}
CN	1.608×10^{-5}	1.598×10^{-4}	1.501×10^{-3}	9.328×10^{-3}
C_2	1.772×10^{-7}	1.765×10^{-6}	1.691×10^{-5}	1.098×10^{-4}
C_3	7.440×10^{-14}	7.394×10^{-12}	6.934×10^{-10}	3.625×10^{-8}
M	14.40	14.45	14.84	17.15
	Temperature: 10,000° K.; Carbon Content: 10% by Wt.			
N	6.910×10^{-1}	6.881×10^{-1}	6.617×10^{-1}	5.153×10^{-1}
O	1.858×10^{-1}	1.859×10^{-1}	1.874×10^{-1}	1.888×10^{-1}
A	4.148×10^{-3}	4.160×10^{-3}	4.273×10^{-3}	4.953×10^{-3}
C	1.187×10^{-1}	1.185×10^{-1}	1.163×10^{-1}	9.636×10^{-2}
N_2	2.574×10^{-4}	2.553×10^{-3}	2.360×10^{-2}	1.432×10^{-1}
O_2	1.374×10^{-7}	1.377×10^{-6}	1.399×10^{-5}	1.420×10^{-4}
NO	8.191×10^{-6}	8.165×10^{-5}	7.913×10^{-4}	6.208×10^{-3}
CO	3.223×10^{-5}	3.220×10^{-4}	3.184×10^{-3}	2.658×10^{-2}
CN	2.980×10^{-5}	2.962×10^{-4}	2.795×10^{-3}	1.803×10^{-2}
C_2	6.924×10^{-7}	6.899×10^{-6}	6.640×10^{-5}	4.559×10^{-4}
C_3	5.744×10^{-13}	5.712×10^{-11}	5.395×10^{-9}	3.069×10^{-7}
M	14.25	14.29	14.68	17.02

Table I. Continued

Species	0.1	1	10	100
	Pressure, Atm.			
	Temperature: 10,000° K.; Carbon Content: 20% by Wt.			
N	6.018×10^{-1}	5.995×10^{-1}	5.781×10^{-1}	4.568×10^{-1}
O	1.617×10^{-1}	1.617×10^{-1}	1.605×10^{-1}	1.463×10^{-1}
A	3.617×10^{-3}	3.627×10^{-3}	3.720×10^{-3}	4.318×10^{-3}
C	2.325×10^{-1}	2.322×10^{-1}	2.286×10^{-1}	1.985×10^{-1}
N_2	1.953×10^{-4}	1.938×10^{-3}	1.802×10^{-2}	1.125×10^{-1}
O_2	1.042×10^{-7}	1.041×10^{-6}	1.026×10^{-5}	8.526×10^{-5}
NO	6.211×10^{-6}	6.184×10^{-5}	5.920×10^{-4}	4.265×10^{-3}
CO	5.495×10^{-5}	5.484×10^{-4}	5.361×10^{-3}	4.243×10^{-2}
CN	5.082×10^{-5}	5.055×10^{-4}	4.801×10^{-3}	3.293×10^{-2}
C_2	2.655×10^{-6}	2.647×10^{-5}	2.567×10^{-4}	1.935×10^{-3}
C_3	4.313×10^{-12}	4.293×10^{-10}	4.100×10^{-8}	2.683×10^{-6}
$\bar{M}$	13.96	14.00	14.36	16.67
	Temperature: 10,000° K.; Carbon Content: 30% by Wt.			
N	5.161×10^{-1}	5.143×10^{-1}	4.972×10^{-1}	3.963×10^{-1}
O	1.385×10^{-1}	1.382×10^{-1}	1.352×10^{-1}	1.117×10^{-1}
A	3.089×10^{-3}	3.097×10^{-3}	3.172×10^{-3}	3.660×10^{-3}
C	3.420×10^{-1}	3.416×10^{-1}	3.374×10^{-1}	3.032×10^{-1}
N_2	1.436×10^{-4}	1.426×10^{-3}	1.333×10^{-2}	8.465×10^{-2}
O_2	7.636×10^{-8}	7.603×10^{-7}	7.274×10^{-6}	4.972×10^{-5}
NO	4.561×10^{-6}	4.535×10^{-5}	4.288×10^{-4}	2.825×10^{-3}
CO	6.919×10^{-5}	6.896×10^{-4}	6.663×10^{-3}	4.950×10^{-2}
CN	6.411×10^{-5}	6.381×10^{-4}	6.093×10^{-3}	4.364×10^{-2}
C_2	5.744×10^{-6}	5.730×10^{-5}	5.591×10^{-4}	4.515×10^{-3}
C_3	1.372×10^{-11}	1.368×10^{-9}	1.318×10^{-7}	9.564×10^{-6}
$\bar{M}$	13.69	13.72	14.05	16.22

Table II. Spectroscopic Data

N: $^4S_{3/2}$; $^2D_{5/2}$; $^2D_{3/2}$; $^2P_{3/2,1/2}$; $^4P_{1/2,3/2,5/2}$
O: $^3P_2$; $^3P_1$; $^3P_0$; $^1D_2$; $^1S_0$
A: $^1S_0$
C: $^3P_0$; $^3P_1$; $^3P_2$; $^1D_2$; $^1S_0$; $^5S_2$; $^3P_{0,1,2}$
N_2: $X^1\Sigma_g^+$; $A\Sigma_u^+$
O_2: $X^3\Sigma_g^-$; $a^1\Delta_g$; $^1\Sigma_g^+$; $^3\Sigma_u^+$
NO: X $\left\{ {}^2\Pi_{3/2} \atop {}^2\Pi_{1/2} \right.$; $A^2\Sigma^+$
CO: $X^1\Sigma^+$; $a^3\Pi_r$
CN: $X^2\Sigma^+$; $A^2\Pi_i$; $B^2\Sigma^+$
C_2: $X^3\Pi_u$; $A^3\Pi_g$; $a^1\Sigma_g^{+a}$; $b^1\Pi_u$; $c^1\Pi_g$; $B^3\Pi_g$
C_3: See text.

[a] Excitation energy assumed 5300 cm.$^{-1}$.

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Table III. Ideal Gas Dimensionless Thermodynamic Functions

T, ° K.	N	O	A	C	N_2	O_2	NO	CO	CN	C_2	C_3
					$-F^0/RT$						
4,000	8.259	15.979	22.601	1.573	29.202	31.183	28.984	33.414	18.890	6.042	9.957
5,000	11.657	18.031	23.159	6.433	30.140	32.183	30.471	33.672	22.282	10.601	16.916
6,000	14.016	19.486	23.615	9.766	30.918	33.020	31.625	33.999	24.730	16.269	21.919
7,000	15.775	20.590	24.000	12.214	31.580	33.731	32.605	34.339	26.609	20.066	24.715
8,000	17.153	21.467	24.334	14.099	32.168	34.366	33.362	34.685	28.111	22.483	28.742
9,000	18.273	22.187	24.629	15.605	32.691	34.947	34.037	35.019	29.360	24.433	31.237
10,000	19.192	22.794	24.892	16.841	33.161	35.457	34.629	35.409	30.415	26.063	33.335
					H^0/RT						
4,000	16.677	9.959	2.500	23.990	4.172	4.439	6.975	0.778	16.327	29.497	33.861
5,000	13.885	8.486	2.500	19.737	4.244	4.558	6.495	1.531	14.160	24.595	28.939
6,000	12.061	7.513	2.500	16.909	4.299	4.652	6.186	2.041	12.740	21.326	25.770
7,000	10,794	6.826	2.500	14.893	4.338	4.725	5.958	2.414	11.679	19.004	23.557
8,000	9.870	6.315	2.500	13.384	4.380	4.796	5.787	2.690	10.896	17.281	21.856
9,000	9.168	5.921	2.500	12.211	4.420	4.866	5.667	2.925	10.280	15.957	20.514
10,000	8.615	5.607	2.500	11.273	4.464	4.928	5.575	3.130	9.782	14.914	19.403
					E_0^0(Cal./Mole)						
	112,535.0	58,985	0	170,300	0	0	21,479	−27,199.2	94,000	200,200	212,300

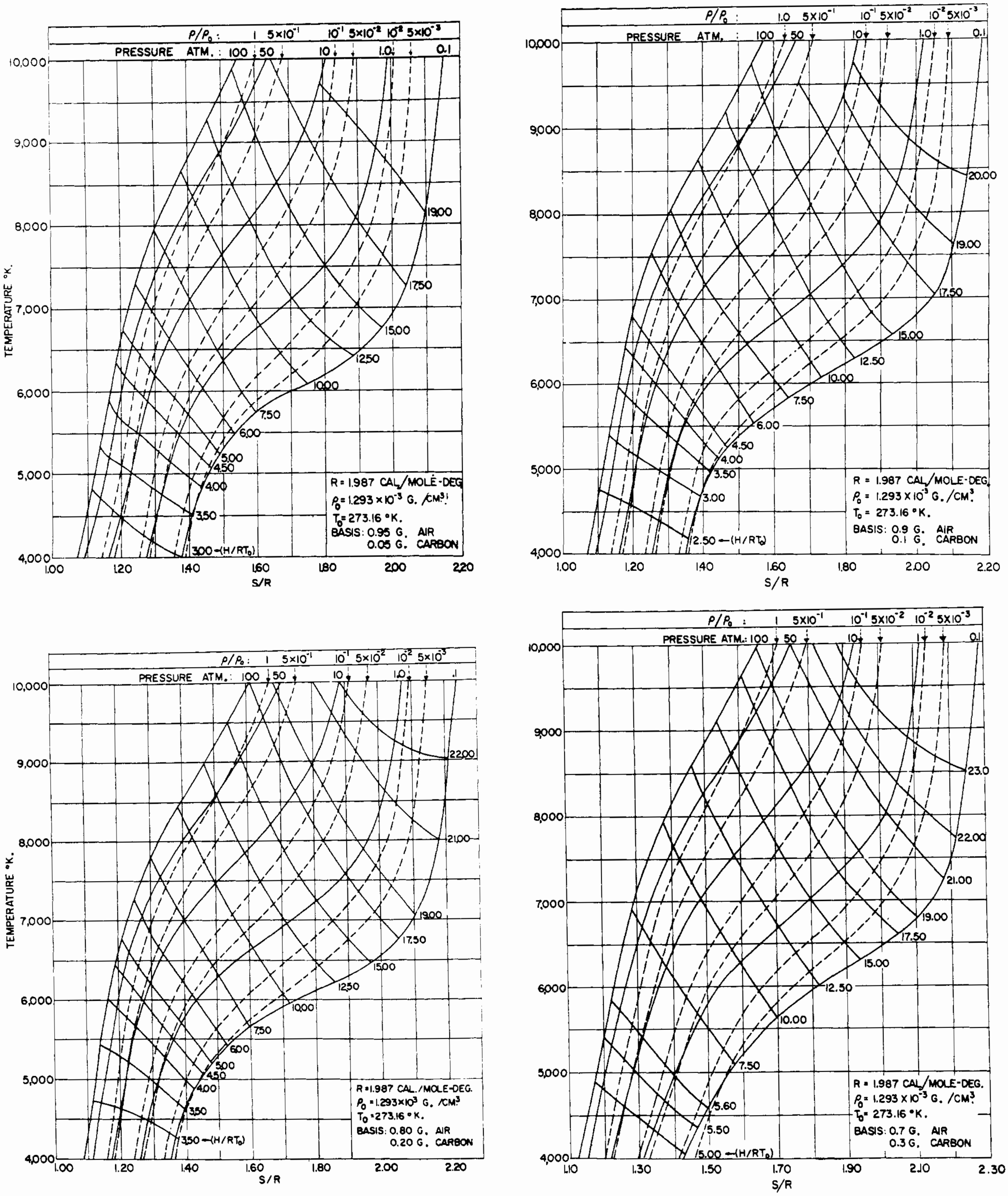

Figure 1. Plots of temperature vs. entropy functions in the 0.1 to 100 atm. for four air-carbon mixtures

Lines of constant enthalpy shown with labels on the right hand side of the 0.1 atmosphere isobar

Lines of constant density indicated by ρ/ρ_0, the ratios of the density of the mixture at the particular temperature and pressure to that of air at S.T.P.

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