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Summary

A rapid computational method has been developed to determine the equilibrium chemical composition of air to 15 000 K. Eleven chemically reacting species—O_2, N_2, O, NO, N, NO^+, e^-, N^+, O^+, Ar, and Ar^+—are included. The method involves the algebraic combination of the equilibrium, elemental mass-balance, and charge-neutrality equations and solves the resulting equation by an iterative method. Computational speeds for the determination of the equilibrium chemical composition are significantly faster than those of the often-used free-energy-minimization procedure. Data are also included from which the thermodynamic properties of air can be computed. Additionally, a listing of the computer program and a set of sample results are included.

Introduction

The application of computational fluid dynamics (CFD) techniques to hypersonic atmospheric flight vehicles requires methods that rapidly compute the composition of air over a wide range of temperatures and densities. Most of the available methods are very general in nature and employ the free-energy-minimization procedure. The generality of any method may be desirable if only a few calculations are to be carried out. But in a CFD code for hypersonic-flow-field computations for which the chemistry code is a subroutine executed a very large number of times, a large fraction of the computational time could be spent in executing the chemistry subroutine alone unless this subroutine is very efficient. For such an application it is evident that it would be beneficial to forego a certain amount of generality in favor of computational speed. The overall gain in the computational time, of course, depends on the particular application.

A method of combining the chemical equilibrium equations and the mass constraint equations algebraically and solving the resulting equation numerically was suggested by Erickson, Kemper, and Allison (ref. 1). Recently, Erickson and Prabhu (ref. 2) applied this method to hydrocarbon combustion products. Smith, Erickson, and Eastwood (ref. 3) also used a similar method for high-temperature equilibrium air. The present method, like that used by Smith et al., divides the temperature-density domain into four regions, each with a limited set of major species and a different computational scheme. Although the present work follows the same general approach used by Smith et al., it differs in that a different set and a smaller number of major species are selected to form the primary iteration equations, and

all the minor species are included in a series of secondary computations. The present approach leads to a more rapid computation and ensures continuity of results between adjacent regions. Eleven species are included, and air is assumed to be a reacting mixture of ideal gases.

The following sections describe the four models, their governing equations, and the solution procedures. A computer program to determine the equilibrium composition of air over a wide range of temperature and density conditions has been written with the present scheme. A listing of this code and a set of results are included. Computational speed for the present program is significantly faster than that of conventional free-energy-minimization routines.

Symbols

$a_{i,j}$	coefficients of the approximating polynomials for thermodynamic functions
b_n	coefficients of the polynomials
$c_{p,i}$	specific heat at constant pressure of ith species, J/mol-K
E_i^0	molar internal energy of ith species, J/mol
e	specific internal energy of the mixture, J/kg
G_i^0	molar Gibbs energy of ith species, J/mol
H_i^0	molar enthalpy of ith species, J/mol
h	specific enthalpy of the mixture, J/kg
K_j	equilibrium constants in terms of mole numbers $(j = 1, 2, ..., 7)$
$K_{p,j}$	equilibrium constants in terms of partial pressure $(j = 1, 2, ..., 7)$
$N(\varepsilon)$	number of iterations for an accuracy ε
p	pressure of the mixture, Pa
p^0	standard-state pressure, 101 325 Pa
R	universal gas constant, 8.314 J/mol-K
S_i^0	molar entropy of ith species, J/mol-K
s	specific entropy of the mixture, J/kg-K
T	temperature of the mixture, K
T_{ref}	reference temperature for enthalpy, 0 K
t	computational time, $t_0 + t_i N(\varepsilon)$, μs

t_i	time per iteration, μs
t_0	constant time outside the iteration loop, μs
ΔG^0	Gibbs energy for a reaction
$\Delta H^0_{f,i}$	enthalpy of formation of ith species at T_{ref}, J/mol
ΔN	increase in mole number in a reaction
ε	accuracy in mole fraction
ρ	density of the mixture, kg/m^3
σ	total mole number of the mixture, mol/kg
σ_i	mole number of ith species $(i = 1, 2, ..., 11)$, mol/kg
$\sigma_O, \sigma_N, \sigma_A$	equivalent mole numbers of oxygen, nitrogen, and argon, mol/kg

Analysis

In the present analysis, low-temperature air is assumed to consist of O_2, N_2, and Ar in molar proportions of 20.96 : 78.11 : 0.93. Eleven chemically reacting species are assumed to be present in equilibrium in air—O_2, N_2, O, NO, N, NO^+, e^-, N^+, O^+, Ar, and Ar^+—and are designated by the respective indices $i = 1, 2, ..., 11$.

Seven independent chemical reactions involving the 11 reacting chemical species are considered. These are as follows:

(1)	$O_2 = 2O$
(2)	$N_2 + O_2 = 2NO$
(3)	$N_2 = 2N$
(4)	$NO^+ + e^- = NO$
(5)	$N^+ + e^- = N$
(6)	$O^+ + e^- = O$
(7)	$Ar^+ + e^- = Ar$
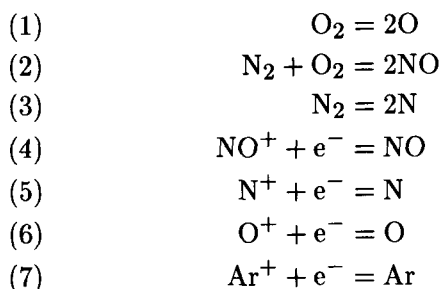
The corresponding 7 nonlinear equilibrium equations involving the unknown mole numbers of the 11 species and the 7 equilibrium constants are the following:

$$K_1 = \sigma_3^2/\sigma_1 \quad (1)$$
$$K_2 = \sigma_4^2/\sigma_1\sigma_2 \quad (2)$$
$$K_3 = \sigma_5^2/\sigma_2 \quad (3)$$
$$K_4 = \sigma_4/\sigma_6\sigma_7 \quad (4)$$

$$K_5 = \sigma_5/\sigma_8\sigma_7 \quad (5)$$
$$K_6 = \sigma_3/\sigma_9\sigma_7 \quad (6)$$
$$K_7 = \sigma_{10}/\sigma_{11}\sigma_7 \quad (7)$$

The equilibrium constants K_j in terms of mole numbers are related to the equilibrium constants $K_{p,j}$ in terms of partial pressures by the following relation:

$$K_j = K_{p,j}(p^0/\rho RT)^{\Delta N}$$

where ΔN is the increase in the number of moles when the reaction proceeds from reactants to products as written for reactions (1) to (7). Note that

$$\Delta N = 1 \text{ for reactions (1) and (3)}$$
$$= -1 \text{ for reactions (4), (5), (6), and (7)}$$
$$= 0 \text{ for reaction (2)}$$

Also, K_j has the units of moles per kilogram raised to the ΔN power, and $K_{p,j}$ has units of atmospheres raised to ΔN power. The equilibrium constants K_1 to K_7 are determined through the use of Gibbs energies of formation for each of the chemical species participating in the chemical reactions.

The mass-balance equations for oxygen, nitrogen, and argon provide three linear equations involving the unknown values of σ_i $(i = 1, 2, \ldots, 11)$ and the known values of σ_N, σ_O, and σ_A.

$$2\sigma_1 + \sigma_3 + \sigma_4 + \sigma_6 + \sigma_9 = \sigma_O \quad (8)$$
$$2\sigma_2 + \sigma_4 + \sigma_5 + \sigma_6 + \sigma_8 = \sigma_N \quad (9)$$
$$\sigma_{10} + \sigma_{11} = \sigma_A \quad (10)$$

In addition, the charge-neutrality condition of the mixture provides the following linear equation:

$$\sigma_6 + \sigma_8 + \sigma_9 + \sigma_{11} = \sigma_7 \quad (11)$$

In principle, it is possible to combine equations (1) to (11) into a single equation in one unknown and solve by some iteration procedure. The basic approach employed in the present analysis, however, is to identify 4 regions in the temperature-density domain such that in each of these regions, only some of the 11 species are found in abundance. These species are referred to as the major species and the rest as the minor species in that region. The nonlinear equations governing the major species and the appropriate linear equations are combined into a single equation, with the assumption that the minor species are adjustable constants. Such governing equations are solved by an iterative procedure updating the minor species at each iteration step. (This approach

is essentially a combination of Newton and fixed-point iteration schemes.) Although some of the species are treated as the major species and the others as the minor species, these models for the 4 regions compute the correct values of all the 11 reacting chemical species considered. These models also have some overlapping regions of applicability, and the choice of one model over the other for a given condition is entirely based on the criterion of minimum computational time.

The following sections discuss these four models. In each case the governing equations and the solution procedures are described.

Model I

At very low temperatures, the only major species are O_2, N_2, and Ar. Among the remaining species, those with a neutral charge (i.e., NO, N, and O) are small and are treated as minor species; the ionized species (i.e., NO^+, e^-, N^+, O^+, and Ar^+) are in very small quantities and hence are denoted trace species. Model I is a very simple model that considers this case. The mole numbers of the minor species and of the trace species are assumed to be zero to start with, and the major species, namely O_2, N_2, and Ar, are computed from the mass-balance equations. The equilibrium equations then determine the minor species, which are used to update the major species. The trace species are computed after this process has converged. The steps involved in this simple iteration scheme are given in the following:

1. Assume $\sigma_1' = \sigma_O/2$, $\sigma_2' = \sigma_N/2$, and $\sigma_{10} = \sigma_A$.

2. Compute the minor species:

$$\sigma_3 = \sqrt{K_1 \sigma_1'}$$
$$\sigma_5 = \sqrt{K_3 \sigma_2'}$$
$$\sigma_4 = K_e \sigma_5 \sigma_3$$

3. Update the major species:

$$\sigma_1 = (\sigma_O - \sigma_3 - \sigma_4)/2$$
$$\sigma_2 = (\sigma_N - \sigma_4 - \sigma_5)/2$$

4. Check and go to step 5 if the results have converged. If they have not converged, set $\sigma_1' = \sigma_1$ and $\sigma_2' = \sigma_2$ and go to step 2.

5. Compute the trace species:

$$\sigma_7 = \sqrt{(\sigma_4/K_4) + (\sigma_5/K_5) + (\sigma_3/K_6) + (\sigma_{10}/K_7)}$$
$$\sigma_6 = \sigma_4/(K_4 \sigma_7)$$
$$\sigma_8 = \sigma_5/(K_5 \sigma_7)$$
$$\sigma_9 = \sigma_3/(K_6 \sigma_7)$$
$$\sigma_{11} = \sigma_{10}/(K_7 \sigma_7)$$

As one might expect, this iteration scheme converges in a couple of iterations at low temperatures, where the minor species are present in extremely small quantities.

Model II

This model is applicable for temperatures which are high enough for dissociation but not high enough for significant ionization. Under this condition, air is assumed to be a mixture of O_2, N_2, O, NO, N, and Ar, with the ionized species present only in small quantities. The derivation of the governing equation and the method employed in solving it are as follows. The equations governing the six major species are equations (1) to (3) and (8) to (10). With the mole numbers of the ionized species σ_6 to σ_9 and σ_{11} set equal to pseudo constants (equal to zero at the start), these equations are combined into a single equation involving one unknown, namely σ_3. The steps are as follows. Equations (1), (2), and (3) yield

$$\sigma_4/\sigma_3 \sigma_5 = \sqrt{K_2/K_1 K_3} = K_e$$

Therefore, $\sigma_4 = K_e \sigma_3 \sigma_5$. Equations (1) and (3) give

$$\sigma_1 = \sigma_3^2/K_1$$
$$\sigma_2 = \sigma_5^2/K_3$$

Substituting the above into equation (8) and solving for σ_5 in terms of σ_3 gives

$$\sigma_5 = \left[\sigma_O' - (2\sigma_3^2/K_1) - \sigma_3 \right]/K_e \sigma_3$$

Finally, upon substituting for σ_4, σ_2, and σ_5 in equation (9) and simplifying, we obtain the following quartic equation with σ_3 as the unknown:

$$\sum_{n=0}^{4} b_n \sigma_3^n = 0$$

where

$$b_4 = (8 - 2K_2)/K_1$$
$$b_3 = 8 - K_2 - 2K_3 K_e$$
$$b_2 = -8\sigma_O' + 2K_1 + (\sigma_O' - \sigma_N')K_2 - K_1 K_3 K_e$$
$$b_1 = (-4 + K_3 K_e)K_1 \sigma_O'$$

and

$$b_0 = 2K_1 \sigma_O'^2$$

Note that $\sigma_O' = \sigma_O - \sigma_6 - \sigma_9$ and $\sigma_N' = \sigma_N - \sigma_6 - \sigma_8$. The equation for σ_3 is solved by the Newton iteration scheme. The initial value for the unknown σ_3 is determined through solution of the following equations:

$$2\sigma_1 + \sigma_3 + \sigma_4' = \sigma_O$$
$$\sigma_1 = \sigma_3^2/K_1$$
$$\sigma_4'/\sigma_3 = \sqrt{2K_1/\sigma_N K_2}$$

where σ_4' is an approximate value of σ_4. These equations imply that all the oxygen is in the species O_2, O, and NO, which is a good approximation for the initial guess in this model.

The following steps are taken in the solution procedure:

1. Preset $\sigma_6 = \sigma_8 = \sigma_9 = 0$ and $\sigma_{10} = \sigma_A$.
2. Compute σ_3.
3. Determine $\sigma_O' = \sigma_O - \sigma_6 - \sigma_9$ and $\sigma_N' = \sigma_N - \sigma_6 - \sigma_8$.
4. Determine b_n $(n = 0, 1, \ldots, 4)$.
5. Compute $\Delta\sigma_3 = -F/F'$, where

$$F = \sum_{n=0}^{4} b_n \sigma_3^n$$

$$F' = \sum_{n=1}^{4} n \, b_n \sigma_3^{n-1}$$

6. Update σ_3 and compute the major species:

$$\sigma_3 = \sigma_3 + \Delta\sigma_3$$
$$\sigma_5 = \left[\sigma_O - (2\sigma_3^2/K_1) - \sigma_3\right]/K_e\sigma_3$$
$$\sigma_4 = K_e\sigma_3\sigma_5$$
$$\sigma_2 = (\sigma_N' - \sigma_4 - \sigma_5)/2$$
$$\sigma_1 = (\sigma_O' - \sigma_4 - \sigma_3)/2$$

7. Compute the minor species:

$$\sigma_7 = \sqrt{(\sigma_4/K_4) + (\sigma_5/K_5) + (\sigma_3/K_6) + (\sigma_{10}/K_7)}$$
$$\sigma_6 = \sigma_4/K_4\sigma_7$$
$$\sigma_8 = \sigma_5/K_5\sigma_7$$
$$\sigma_9 = \sigma_3/K_6\sigma_7$$
$$\sigma_{11} = \sigma_{10}/K_7\sigma_7$$
$$\sigma_{10} = \sigma_A - \sigma_{11}$$

8. Check and stop if the results are converged. If they are not converged, go to step 3.

As one might expect, the range of applicability of model II overlaps that of model I at the lower temperatures (at about 800 K). Similarly, the applicability of this model at higher temperatures overlaps that of model III, which is discussed in the next section.

Model III

This model is applicable under certain temperature and density conditions when oxygen is almost completely dissociated and not much ionization has taken place. The major species in this case are O, N_2, N, and Ar, and the remaining seven species are treated as minor species. The equations governing the major species (eqs. (3) and (8) to (10)) are combined into a single equation in one unknown, namely σ_5. This turns out to be a quadratic equation for which the coefficients involve the unknown mole numbers of the minor species. As in the previous case, these are treated as pseudo constants while the quadratic equation is solved. After the quadratic is solved for σ_5, the mole numbers of the minor species are determined and the coefficients of the quadratic equation are updated. This process is continued until a converged solution is obtained. The following steps describe this solution procedure:

1. Assume $\sigma_3' = \sigma_O$ and $\sigma_{10} = \sigma_A$ and set $\sigma_4 = \sigma_6 = \sigma_8 = 0$ initially.
2. Compute $\sigma_N' = \sigma_N - \sigma_4 - \sigma_6 - \sigma_8$.
3. Determine the coefficients b_n $(n = 0, 1, \text{ and } 2)$:

$$b_0 = -K_3\sigma_N'/2$$
$$b_1 = K_3/2$$
$$b_2 = 1$$

4. Solve the quadratic equation $b_2\sigma_5^2 + b_1\sigma_5 + b_0 = 0$ for σ_5.

5. Determine the unknown mole numbers:

$$\sigma_2 = (\sigma_N' - \sigma_5)/2$$
$$\sigma_1 = \sigma_3'^2/K_1$$
$$\sigma_4 = K_e\sigma_3'\sigma_5$$
$$\sigma_7 = \sqrt{(\sigma_3'/K_6) + (\sigma_4/K_4) + (\sigma_5/K_5) + (\sigma_{10}/K_7)}$$
$$\sigma_6 = \sigma_4/K_4\sigma_7$$
$$\sigma_8 = \sigma_5/K_5\sigma_7$$
$$\sigma_9 = \sigma_3'/K_6\sigma_7$$
$$\sigma_{11} = \sigma_{10}/K_7\sigma_7$$
$$\sigma_{10} = \sigma_A - \sigma_{11}$$

Finally,

$$\sigma_3 = \sigma_O - 2\sigma_1 - \sigma_4 - \sigma_6 - \sigma_9.$$

6. Check and stop if results are converged. If they are not converged, set $\sigma_3' = \sigma_3$ and go to step 2.

Model IV

This model considers the very-high-temperature case, which is dominated by atomic and ionic species. The major species in this model are O, N, e^-, N^+, O^+, and Ar, and the others are treated as minor species. When equations (5) to (11) governing the major species are combined, they reduce to a cubic equation involving one unknown, namely σ_7. The minor species mole numbers that appear in the coefficients of this cubic equation are treated as pseudo constants. Starting with a value of zero for the mole numbers of the minor species, we solve the cubic equation. Next the mole numbers of the remaining major and of all the minor species are computed, and the coefficients of the cubic equation are updated. This iteration process is continued until the results are converged. The following steps describe the iteration procedure:

1. Preset $\sigma_1 = \sigma_2 = \sigma_4 = \sigma_6 = \sigma_{11} = 0$.

2. Determine $\sigma_O' = \sigma_O - 2\sigma_1 - \sigma_4 - \sigma_6$ and $\sigma_N' = \sigma_N - 2\sigma_2 - \sigma_4 - \sigma_6$.

3. Determine b_n $(n = 0, 1, \ldots, 3)$:

$$b_0 = -\sigma_N' - \sigma_O' - \sigma_{11} - \sigma_6$$
$$b_1 = 1 - \sigma_N'K_6 - \sigma_O'K_5 - (\sigma_{11} + \sigma_6)(K_5 + K_6)$$
$$b_2 = K_5 + K_6 - (\sigma_{11} + \sigma_6)K_5K_6$$
$$b_3 = K_5K_6$$

4. Compute $\Delta\sigma_7 = -F/F'$, where

$$F = \sum_{n=0}^{3} b_n\sigma_7^n$$

$$F' = \sum_{n=1}^{3} nb_n\sigma_7^{n-1}$$

5. Update σ_7 and compute the major species:

$$\sigma_7 = \sigma_7 + \Delta\sigma_7$$
$$\sigma_3 = \sigma_O'\sigma_7K_6/(1 + K_6\sigma_7)$$
$$\sigma_5 = \sigma_N'\sigma_7K_5/(1 + K_5\sigma_7)$$
$$\sigma_{11} = \sigma_A/(1 + K_7\sigma_7)$$
$$\sigma_{10} = \sigma_A - \sigma_{11}$$
$$\sigma_9 = \sigma_3/K_6\sigma_6$$
$$\sigma_8 = \sigma_5/K_5\sigma_7$$

6. Compute the minor species:

$$\sigma_1 = \sigma_3^2/K_1$$
$$\sigma_2 = \sigma_5^2/K_1$$
$$\sigma_4 = K_e\sigma_3\sigma_5$$
$$\sigma_6 = \sigma_4/K_4\sigma_7$$

7. Check and stop if results are converged. If they are not converged, go to step 2.

Table I gives a summary of the major and minor species in the four temperature ranges considered here. As pointed out earlier, although these four models are developed assuming a certain set of major species in each, they have overlapping areas of applicability, and the choice of one model over the other for a given temperature and density is based strictly on minimum computational time. Figure 1 shows the regions in the temperature-density domain, where the four models are applicable and give results in minimum time.

Thermodynamic Data

Computation of thermodynamic properties for each of the 11 species as well as for the mixture has been included in the program. The data for the determination of the thermodynamic properties were obtained from several sources. The data for the molecular species were obtained directly from the tables of reference 4. The heat capacities for the monatomic species were computed by Bonnie J. McBride of NASA Lewis Research Center using the appropriate statistical-thermodynamic relations and

the data from references 5, 6, and 7. The specific heat data for all the species were processed, also by McBride, using the least-squares method of curve fitting employing the approximating polynomials of the following forms:

$$c_{p,i}/R = \sum_{j=1}^{5} a_{i,j} T^{j-1}$$

$$H_i^0/(RT) = \sum_{j=1}^{5} a_{i,j} T^{j-1}/j + a_{i,6}/T$$

$$S_i^0/R = \sum_{j=2}^{5} a_{i,j} T^{j-1}/(j-1) + a_{i,j} \ln T + a_{i,7}$$

$$G_i^0/(RT) = H_i^0/(RT) - S_i^0/R$$

The coefficients $a_{i,6}$ and $a_{i,7}$ ($i = 1, 2, \ldots, 11$) are the integration constants. The values of $a_{i,6}$ were determined from the enthalpy of formation (taken from the JANAF Thermochemical Tables published by Dow Chemical Co.) for all the species at the reference temperature of 0 K. The values of $a_{i,7}$ were determined from the values of entropy at $T = 298.15$ K.

The coefficients $a_{i,1}$ to $a_{i,7}$ ($i = 1, 2, \ldots, 11$) are given in table II. The entire temperature range from 200 to 15 000 K is divided into five smaller ranges; these ranges are 200 to 800 K, 800 to 3000 K, 3000 to 6000 K, 6000 to 10 000 K, and 10 000 to 15 000 K. The curves for the approximating least-squares polynomials are forced to pass through common points at the junctions between the five temperature ranges, thereby ensuring continuity in the values at the junction points.

The standard-state Gibbs energy for the 11 reacting species is required for the determination of the equilibrium constants for the 7 reactions. Equilibrium constants $K_{p,j}$ for reactions (1) to (7) are given by

$$K_{p,j} = \exp\left[-\Delta G_j^0/(RT)\right] \quad (j = 1, 2, \ldots, 7)$$

where $\Delta G_j^0 = \sum_i \nu_i G_i^0 - \sum_i \nu_i' G_i^0$, ν_i, and ν_i' are the stoichiometric coefficients, and ΔG_i^0 is the standard-state Gibbs energy of formation of the ith species. For example, for reaction (2) ($N_2 + O_2 = 2NO$),

$$\Delta G_2^0 = 2(G^0)_{NO} - (G^0)_{N_2} - (G^0)_{O_2}$$

and

$$K_{p,2} = \exp(-\Delta G_2^0/RT)$$

The enthalpy of the mixture in terms of the enthalpies of the constituent species and their mole numbers is given by

$$h = \sum_{i=1}^{11} H_i^0 \sigma_i$$

Because the reference temperature is 0 K, internal energy of each species is simply given by

$$E_i^0 = H_i^0 - RT \quad (i = 1, 2, \ldots, 11)$$

and the internal energy of the mixture is given by

$$e = \sum_{i=1}^{11} E_i^0 \sigma_i$$
$$= h - RT\sigma$$

The entropy of the mixture is determined from the expression

$$s = -R\sigma \ln(p/p^0) + \sum_{i=1}^{11} \sigma_i \left[S_i^0 - R \ln(\sigma_i)\right]$$

where p^0 is the standard-state pressure (101 325 Pa) and p is the pressure of the mixture given by

$$p = \rho RT\sigma$$

Results and Discussion

A computer code has been written to implement the computational scheme. The thermodynamic data in the form of coefficients $a_{i,j}$ ($j = 1, 2, \ldots, 7$) for the 11 chemical species ($i = 1, 2, \ldots, 11$) are included in the code. The program has four subroutines, one for each model. This program reads a set of values for temperature, density, and convergence criterion and computes the chemical equilibrium composition and the thermodynamic properties of air. The appendix gives a listing of the computer code and a set of sample results.

The total time t for the computation of chemical equilibrium composition for any iterative method is given by the expression

$$t = t_0 + t_i N(\varepsilon)$$

where t_0 is a constant time required to compute the terms outside the iteration loop and includes the time for computation of equilibrium constants and estimates of initial values to be used for the

iteration, t_i is the time required per iteration, and $N(\varepsilon)$ is the number of iterations required for the desired accuracy ε.

A series of cases were run on the CDC CYBER 170/750 to determine the three quantities t_0, t_i, and $N(\varepsilon)$ for the present computational scheme. Sample results are shown in table III. The constant time is essentially the same for all four models. However, the time per iteration and the number of iterations required for convergence are different for the four models. The number of iterations for convergence depends on the desired accuracy. Over the wide range of conditions explored, one or two iterations were required for a mole fraction accuracy of $\varepsilon = 0.001$, and in most cases two or three iterations were sufficient for an accuracy of $\varepsilon = 0.0001$. Results for points along the boundaries between various models are indicated with an asterisk.

Computations have been carried out with the computer code to obtain equilibrium chemical composition for air over a temperature range of 200 to 15 000 K and for density values of 1×10^{-5}, 1×10^{-2}, and 1×10^{2} kg/m^3. These results are presented in figures 2(a), 2(b), and 2(c).

Concluding Remarks

The computational scheme presented provides a means for rapidly computing the equilibrium chemical composition of air to 15 000 K. This scheme was developed for the purpose of providing a relatively rapid computer code for use with computational fluid dynamics programs that deal with high-temperature air. A computer code and a thermodynamic data base are also included from which the thermodynamic properties of air to 15 000 K may be computed.

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Appendix
Computer Code Listing and Sample Results

Computer Code

```
      PROGRAM AIRNEW(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
C*****************************************************************************C
C
C     THIS PROGRAM COMPUTES THE EQUILIBRIUM CHEMICAL COMPOSITION OF AIR ASSUMING
C        (1) THE DENSITY IS CONSTANT.
C        (2) THE ELEVEN SPECIES: O2, N2, O, NO, N, NO+, E-, N+, O+, AR, AND AR+.
C        (3) CURVE FITTED DATA RECEIVED FROM BONNIE J. MCBRIDE.
C        (4) REFERENCE TEMPERATURE IS ZERO KELVIN.
C     ALSO COMPUTES ENTHALPY, INTERNAL ENERGY, AND ENTROPY.
C
C*****************************************************************************C
      REAL AA(11,7,5),C(11),H(11),EN(11),S(11),E(11)
      REAL K1,K2,K3,K4,K5,K6,K7,KE
      COMMON  / A /  K1,K2,K3,K4,K5,K6,K7,KE
      COMMON  / B /  SN,SO,SR,EPS
      COMMON  / C /  S
      COMMON  / D /  NITER
      EQUIVALENCE (S1,S(1)),(S2,S(2)),(S3,S(3)),(S4,S(4)),(S5,S(5)),
     1            (S6,S(6)),(S7,S(7)),(S8,S(8)),(S9,S(9)),(SA,S(10)),
     2            (SB,S(11))
C
      GBYRT(I,K,T)=(   AA(I,1,K)*(1.-ALOG(T))-AA(I,2,K)*T/2.-AA(I,3,K)
     1*T**2/6.-AA(I,4,K)*T**3/12.0-AA(I,5,K)*T**4/20.0+AA(I,6,K)/T
     1-AA(I,7,K)   )
C
      HBYRT(I,K,T)=AA(I,1,K)            +AA(I,2,K)*T   /2.+AA(I,3,K)*T**2/3.
     1             +AA(I,4,K)*T**3/4.+AA(I,5,K)*T**4/5.
     2             +AA(I,6,K)/T
C
      SBYR (I,K,T)=AA(I,2,K)*T          +AA(I,3,K)*T**2/2.+AA(I,4,K)*T**3/3.
     1             +AA(I,5,K)*T**4/4.+AA(I,1,K)*ALOG(T)+AA(I,7,K)
C
C     THE FOLLOWING CONSTANTS ARE OBTAINED FROM B. J. MCBRIDE,
C     THE BASIC DATA SOURCES ARE:
C     (1) TABULATED DATA FROM: THERMODYNAMIC PROPERTIES OF
C         INDIVIDUAL SUBSTANCES, ACADEMY OF SCIENCES, MOSCOW, USSR,
C         1978, VOL.1, PART 2. (FOR MOLECULAR SPECIES,
C         AND FORMATION VALUES OF ALL SPECIES.)
C     (2) VALUES COMPUTED (BY MCBRIDE) USING STATISTICAL DATA
C         FOR MONATOMIC SPECIES.
C         SOURCE OF BASIC STATISTICAL DATA:
C         (A) NSRDS NBS VOLUME 35, 1971
C         (B)       NBS 3, SECTION 5, 1975
C         (C)       NBS 3, SECTION 7, 1976
C
C.....      NEUTRAL MOLECULAR OXYGEN O2.
      DATA ((AA(1,J,K),J=1,7),K=1,5)/
     * .37703733E+01,-.28952206E-02, .95332231E-05,-.92469913E-08,
     * .30191908E-11,-.18859751E+02, .36933495E+01,
     * .28969178E+01, .23736545E-02,-.14917097E-05, .46603392E-09,
     *-.53945166E-13, .82240429E+02, .75019384E+01,
     * .28421112E+01, .13320561E-02,-.33915853E-06, .44652178E-10,
     *-.22914824E-14, .58350386E+03, .86255038E+01,
     * .56821087E+01,-.75300588E-03, .22980075E-06,-.23955920E-10,
     * .80048472E-15,-.24700372E+04,-.98740054E+01,
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      *-.27258966E+00,  .20115141E-02,-.24547714E-06,  .12025200E-10,
      *-.21389859E-15,  .76117740E+04,  .31631739E+02/
C.....      NEUTRAL MOLECULAR NITROGEN N2
       DATA ((AA(2,J,K),J=1,7),K=1,5)/
      * .34622648E+01,  .58202350E-03,-.30525456E-05,  .62280057E-08,
      *-.33755957E-11,  .87951739E+00,  .32192648E+01,
      * .27022403E+01,  .19443933E-02,-.89300044E-06,  .19739206E-09,
      *-.16967813E-13,  .20180222E+03,  .72040846E+01,
      * .39143506E+01,  .31537108E-03,-.56481043E-07,  .36012299E-11,
      * .52359433E-16,-.53551958E+03,  .21671998E-01,
      * .12657466E+01,  .18269791E-02,-.37583896E-06,  .33033716E-10,
      *-.93651108E-15,  .31426960E+04,  .17943292E+02,
      * .27715943E+02,-.74173486E-02,  .82395970E-06,-.35285300E-10,
      * .49671195E-15,-.56942692E+05,-.17402873E+03/
C.....      NEUTRAL MONATOMIC OXYGEN O
       DATA ((AA(3,J,K),J=1,7),K=1,5)/
      * .32167143E+01,-.37822689E-02,  .84746788E-05,-.88658246E-08,
      * .35365597E-11,  .29640462E+05,  .18526415E+01,
      * .26045368E+01,-.17235464E-03,  .11574138E-06,-.36417858E-10,
      * .46011536E-14,  .29728962E+05,  .45865262E+01,
      * .28101683E+01,-.29039910E-03,  .90833347E-07,-.99427817E-11,
      * .37704361E-15,  .29536612E+05,  .32536467E+01,
      * .19209266E+01,  .21776554E-03,-.18288405E-07,  .49050959E-12,
      * .28507296E-17,  .30783423E+05,  .92748629E+01,
      * .19209266E+01,  .21776554E-03,-.18288405E-07,  .49050959E-12,
      * .28507296E-17,  .30783423E+05,  .92748629E+01/
C.....      NEUTRAL NITRIC OXIDE, NO
       DATA ((AA(4,J,K),J=1,7),K=1,5)/
      * .42064360E+01,-.45098354E-02,  .10557385E-04,-.85919382E-08,
      * .24047097E-11,  .10888965E+05,  .23137934E+01,
      * .27543778E+01,  .23093284E-02,-.12823359E-05,  .34043524E-09,
      *-.34807544E-13,  .11134325E+05,  .90789671E+01,
      * .38015418E+01,  .49857546E-03,-.12531319E-06,  .14093893E-10,
      *-.44820194E-15,  .10666566E+05,  .31619390E+01,
      * .49133164E+01,  .61755267E-06,-.55222382E-07,  .11686489E-10,
      *-.54642492E-15,  .88453776E+04,-.45786900E+01,
      * .20456654E+02,-.61498079E-02,  .86914275E-06,-.50877512E-10,
      * .10624157E-14,-.22955242E+05,-.11561956E+03/
C.....      NEUTRAL MONATOMIC NITROGEN N
       DATA ((AA(5,J,K),J=1,7),K=1,5)/
      * .25000000E+01,0.            ,0.            ,0.            ,
      *0.            , .56626706E+05,  .41807280E+01,
      * .25075109E+01,-.24797882E-04,  .29641517E-07,-.15288108E-10,
      * .28913714E-14,  .56624949E+05,  .41431864E+01,
      * .26376051E+01,-.87373323E-05,-.64772651E-07,  .23473436E-10,
      *-.17396164E-14,  .56452267E+05,  .32232104E+01,
      * .33720620E+01,-.88554639E-03,  .25293270E-06,-.23187896E-10,
      * .70471420E-15,  .56270151E+05,-.10563976E+01,
      *-.10205642E+02,  .42931347E-02,-.49310664E-06,  .24951067E-10,
      *-.46969943E-15,  .84933779E+05,  .96403744E+02/
C.....      UNIPOSITIVE NITRIC OXIDE, NO+
       DATA ((AA(6,J,K),J=1,7),K=1,5)/
      * .35659323E+01,-.27420307E-03,-.52284273E-06,  .30228201E-08,
      *-.19112702E-11,  .11841356E+06,  .35935691E+01,
      * .27152625E+01,  .18998146E-02,-.85346216E-06,  .18390288E-09,
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     *-.15328469E-13, .11862129E+06, .79369146E+01,
     * .39310989E+01, .30660785E-03,-.56705942E-07, .45573508E-11,
     *-.77762022E-16, .11786296E+06, .70198182E+00,
     * .10656163E+01, .17917961E-02,-.33077778E-06, .25052719E-10,
     *-.54540127E-15, .12214242E+06, .20328302E+02,
     * .31376951E+02,-.78170663E-02, .75437124E-06,-.24734142E-10,
     * .15952361E-15, .48124504E+05,-.20218492E+03/
C.....      ELECTRON, E-
     DATA ((AA(7,J,K),J=1,7),K=1,5)/
     * .25000000E+01,0.            ,0.            ,0.             ,
     *0.            ,-.42498957E-01,-.11733917E+02,
     * .25000000E+01,0.            ,0.            ,0.             ,
     *0.            ,-.42498957E-01,-.11733917E+02,
     * .25000000E+01,0.            ,0.            ,0.             ,
     *0.            ,-.42498957E-01,-.11733917E+02,
     * .25000000E+01,0.            ,0.            ,0.             ,
     *0.            ,-.42498957E-01,-.11733917E+02,
     * .25000000E+01,0.            ,0.            ,0.             ,
     *0.            ,-.42498957E-01,-.11733917E+02/
C.....      UNIPOSITIVE MONATOMIC NITROGEN, N+
     DATA ((AA(8,J,K),J=1,7),K=1,5)/
     * .30816977E+01,-.37737512E-02, .96771466E-05,-.11099460E-07,
     * .47248633E-11, .22532807E+06, .24315936E+01,
     * .25347005E+01,-.55067384E-04, .36440013E-07,-.12313199E-10,
     * .19224650E-14, .22539524E+06, .47895586E+01,
     * .28005551E+01,-.29566365E-03, .96649663E-07,-.11053590E-10,
     * .44145151E-15, .22518494E+06, .31305296E+01,
     * .20047667E+01, .19189730E-03,-.15499136E-07, .41165940E-12,
     * .26287640E-17, .22622600E+06, .84634959E+01,
     * .20598363E+01, .18875424E-03,-.18075532E-07, .80284344E-12,
     *-.13089587E-16, .22602766E+06, .80254371E+01/
C.....      UNIPOSITIVE MONATOMIC OXYGEN, O+
     DATA ((AA(9,J,K),J=1,7),K=1,5)/
     * .25000000E+01,0.            ,0.            ,0.             ,
     *0.            , .18771321E+06, .43801998E+01,
     * .25013354E+01,-.40431297E-05, .43271450E-08,-.19527702E-11,
     * .31632791E-15, .18771288E+06, .43734240E+01,
     * .22258863E+01, .29650143E-03,-.11561144E-06, .18461192E-10,
     *-.89249152E-15, .18791159E+06, .60576133E+01,
     * .41210991E+01,-.86786175E-03, .15337469E-06,-.92260135E-11,
     * .17842049E-15, .18543702E+06,-.66388864E+01,
     * .17349474E+01,-.80710732E-04, .59806317E-07,-.45998476E-11,
     * .10295182E-15, .19107440E+06, .10791908E+02/
C.....      NEUTRAL ARGON, A.
     DATA ((AA(10,J,K),J=1,7),K=1,5)/
     * .25000000E+01,0.            ,0.            ,0.             ,
     *0.            ,-.42498957E-01, .43664979E+01,
     * .25000000E+01,0.            ,0.            ,0.             ,
     *0.            ,-.42498957E-01, .43664979E+01,
     * .25000000E+01,0.            ,0.            ,0.             ,
     *0.            ,-.42498957E-01, .43664979E+01,
     * .26303545E+01,-.77393441E-04, .17219729E-07,-.17028231E-11,
     * .63198847E-16,-.17548010E+03, .34890096E+01,
     *-.91423987E+01, .38508169E-02,-.46800440E-06, .24506918E-10,
     *-.45646899E-15, .27751915E+05, .89461765E+02/
```

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C.....      UNIPOSITIVE MONATOMIC  ARGON, A.
      DATA ((AA(11,J,K),J=1,7),K=1,5)/
     * .26818797E+01,-.20720300E-02, .74786002E-05,-.87672013E-08,
     * .34484189E-11, .18287091E+06, .50764556E+01,
     * .24220646E+01, .86346979E-03,-.78459395E-06, .26673998E-09,
     *-.31850590E-13, .18285266E+06, .59236280E+01,
     * .25588416E+01, .89736230E-04,-.50091586E-07, .88298198E-11,
     *-.52371930E-15, .18301380E+06, .55313033E+01,
     * .25014164E+01, .29446558E-04,-.80471729E-08, .77535785E-12,
     *-.25780935E-16, .18325162E+06, .60544022E+01,
     * .25706058E+01,-.20621051E-04, .29786013E-08,-.21101899E-12,
     * .57476758E-17, .18322322E+06, .56165023E+01/
      RR=8.31441
      P0=1.01325E+05
C
C..... ASSUME AIR TO HAVE O2 : N2 : A = 20.96 : 78.11 : 0.93
C
      SO = 14.4802
      SN = 53.9620
      SR =  0.3212
C***********************************************************************C
C
C      INPUT DATA:
C
C             TKEL    =   TEMPERATURE (KELVIN)
C            RKGM3    =   DENSITY (KG/M**3)
C              EPS    =   CONVERGENCE CRITERION
C
C***********************************************************************C
   60 WRITE(6,66)
   66 FORMAT(/,2X,*INPUT:-   TKEL, RKGM3, EPS*,
     1       /,2X,*         ENTER <RETURN> TO STOP*)
      READ (5,*) TKEL,RKGM3,EPS
      IF(EOF(5)) 62,5,62
    5 CONTINUE
C
C.....CHOOSE APPROPRIATE CONSTANTS DEPENDING UPON THE TEMPERATURE.
C
      K=1
      IF(TKEL .GT.  800.) K=2
      IF(TKEL .GT. 3000.) K=3
      IF(TKEL .GT. 6000.) K=4
      IF(TKEL .GT.10000.) K=5
C
C.....COMPUTE DG/RT, H/RT, AND S/R FOR ALL THE ELEVEN SPECIES.
C
      DO 8 I=1,11
      C(I)=DGBYRT(I,K,TKEL)
      H(I)=(HBYRT (I,K,TKEL)*TKEL)*RR
      EN(I)=SBYR  (I,K,TKEL) *RR
C     WRITE(6,50) I,K,TKEL,C(I),H(I),EN(I)
   50 FORMAT(2I2,7E12.5)
    8 CONTINUE
C***********************************************************************C
C
```

```
C.....COMPUTE THE EQUILIBRIUM CONSTANTS FOR THE GIVEN TEMPERATURE
C.....AND DENSITY CONDITIONS.
C.....THE REACTIONS ARE:
C
C                       O2 = 2 O                          (1)
C
C                  N2 + O2 = 2 NO                         (2)
C
C                       N2 = 2 N                          (3)
C
C            (NO+) + E- = NO                              (4)
C
C             (N+) + E- = N                               (5)
C
C             (O+) + E- = O                               (6)
C
C            (AR+) + E- = AR                              (7)
C
C*********************************************************************************C
      K1=C(3)+C(3)-C(1)
      K2=C(4)+C(4)-C(1)-C(2)
      K3=C(5)+C(5)-C(2)
      K4=C(4)-C(6)-C(7)
      K5=C(5)-C(8)-C(7)
      K6=C(3)-C(9)-C(7)
      K7=C(10)-C(11)-C(7)
      K1=EXXP(-K1)    $    K2=EXXP(-K2)    $    K3=EXXP(-K3)
      K4=EXXP(-K4)    $    K5=EXXP(-K5)    $    K6=EXXP(-K6)
      K7=EXXP(-K7)
      POBYRT=PO/(RR*TKEL*RKGM3)
      K1=K1*POBYRT
      K3=K3*POBYRT
      K4=K4/POBYRT
      K5=K5/POBYRT
      K6=K6/POBYRT
      K7=K7/POBYRT
      KE = SQRT(K2/(K1*K3))
C
C.....CALL APPROPRIATE SUBROUTINE DEPENDING UPON THE TEMPERATURE
C.....TO COMPUTE THE COMPOSITION.
C
      IF(TKEL .LE. 1600.0) GO TO 151
      RLOG = ALOG10(RKGM3)
      TEMP1 = 1000.0*(3.5+10.0*((RLOG+6.0)/7.0)**2.5)
      IF(TKEL .LE. TEMP1) GO TO 154
      TEMP2=1000.*(5.4+3.2*(RLOG+6.)/6.+5.55*(ABS(RLOG+6.)/6.)**3.35)
      IF(TKEL .LE. TEMP2) GO TO 152
  153 MODEL = 3
      CALL CUBIC
      GO TO 156
  152 MODEL = 2
      CALL QUDRATC
      GO TO 156
  154 MODEL = 4
      CALL QUARTIC
```

```
          GO TO 156
      151 MODEL = 1
          CALL LOWTEMP
C
C.....TOTAL MOL NUMBER.
C
      156 SUM = S1+S4+S2+S3+S5+S6+S7+S8+S9+SA+SB
C
C.....COMPUTE PRESSURE
C
          PBAR = RKGM3*8.314*SUM*TKEL/100000.
          PATM = PBAR/1.01325
C
C.....COMPUTE RESIDUES....
C
          R1 = S3*S3/K1/S1-1.0
          R2 = S4*S4/K2/S1/S2-1.0
          R3 = S5*S5/K3/S2-1.0
          R4 = S4/K4/S6/S7-1.0
          R5 = S5/K5/S8/S7-1.0
          R6 = S3/K6/S9/S7-1.0
          R7 = SO-2.0*S1-S3-S4-S6-S9
          R8 = SN-2.0*S2-S4-S5-S6-S8
          R9 = S7-S6-S8-S9-SB
          RA = SR - SA -SB
          RB = SA - K7*SB*S7
          IF(SB .EQ. 0.0) RB = 0.0
C************************************************************************C
C
C.....COMPUTE THE ENTHALPY, INT. ENERGY, AND ENTROPY  OF THE MIXTURE.
C.....NOTE: ENTHALPY AND INT. ENERGY ARE IN JOULES/KG.
C.....      ENTROPY IS IN JOULES/KG.KELVIN
C
C************************************************************************C
          H0 = 0.0
          E0 = 0.0
          ENTO = -RR*SUM*ALOG(PATM/SUM)
          DO 96 I=1,11
          H0 = H0+S(I)*H(I)
          E(I) = H(I)-RR*TKEL
          E0=E0+S(I)*E(I)
          IF(S(I) .EQ. 0.0) GO TO 96
          ENTO = ENTO+S(I)*(EN(I)-RR*ALOG(S(I)))
       96 CONTINUE
C
C.....WRITE OUT THE RESULTS.
C
          WRITE(6,101) TKEL,RKGM3,EPS
          WRITE(6,100) SO,SN,SR
          WRITE(6,102) K1,K2,K3,K4,K5,K6,K7,KE
          IF(MODEL .EQ. 1) WRITE(6,304) NITER
          IF(MODEL .EQ. 2) WRITE(6,307) NITER
          IF(MODEL .EQ. 3) WRITE(6,306) NITER
          IF(MODEL .EQ. 4) WRITE(6,305) NITER
          WRITE(6,303) S1,S2,S3,S4,S5,S6,S7,S8,S9,SA,SB
```

```
      WRITE(6,318) (H(I),I =1,11)
      WRITE(6,316) (E(I),I =1,11)
      WRITE(6,319) (EN(I),I =1,11)
      WRITE(6,317) SUM,H0,ENT0,E0,PBAR
      WRITE(6,204) R1,R2,R3,R4,R5,R6,R7,R8,R9,RA,RB
  303 FORMAT(/,2X,38HMOLE NUMBERS OF THE SPECIES (MOL/KG):-,
     1/, 9X,2HO2, 11X,2HN2,11X,2HO ,11X,2HNO,11X,2HN ,10X,3HNO+,
     1/, 9X,2HE-,11X,2HN+,11X,2HO+,11X,2HAR,11X,3HAR+,//,
     1 2X,6E13.5,/,2X,5E13.5)
  304 FORMAT(/,2X,43HSOLUTION BY THE SIMPLE ITERATION PROCEDURE;,
     1  I3,11H ITERATIONS)
  305 FORMAT(/,2X,33HSOLUTION OF THE QUARTIC EQUATION;,
     1  I3,11H ITERATIONS)
  306 FORMAT(/,2X,31HSOLUTION OF THE CUBIC EQUATION:,
     1  I3,11H ITERATIONS)
  307 FORMAT(/,2X,35HSOLUTION OF THE QUADRATIC EQUATION;,
     1  I3,11H ITERATIONS)
  100 FORMAT(/,2X,*OXYGEN = *,F8.4,2X,*NITROGEN = *,F8.4,2X,
     1          *ARGON = *,F6.4,*   MOLS/KG.*)
  101 FORMAT(/,2X,*T (KELVIN) = *,F8.2,2X,*DENSITY (KG/M**3) = *,E12.6
     1 ,2X,*EPS = *,E10.4)
  204 FORMAT(/,2X,*RESIDUES:-*,3(/,2X,6E13.5))
  102 FORMAT(/,2X,*EQUILIBRIUM CONSTANTS K(I):-*,
     1       /,2X,6E13.5,/,2X,6E13.5)
  317 FORMAT(
     1/,2X,29HTOTAL MOL NUMBER            = ,F12.4,11H MOLS/KG.  ,
     1/,2X,29HENTHALPY OF THE MIXTURE     = ,E12.6,11H JOULES/KG.,
     1/,2X,29HENTROPY OF THE MIXTURE      = ,E12.6,18H JOULES/KG./KELVIN,
     1/,2X,29HINT. ENERGY OF THE MIXTURE = ,E12.6,11H JOULES/KG.,
     1   /,2X,29HPRESSURE                 = ,E12.6,6H (BAR))
  318 FORMAT(/,2X,39HENTHALPY OF EACH SPECIES (JOULES/MOL):-,/,
     1       3(2X,6E13.5,/,))
  316 FORMAT(/,2X,46HINTERNAL ENERGY OF EACH SPECIES (JOULES/MOL):-,/,
     1       3(2X,6E13.5,/,))
  319 FORMAT(/,2X,45HENTROPY OF EACH SPECIES (JOULES/MOL/KELVIN):-,/,
     1       3(2X,6E13.5,/,))
      GO TO 60
   62 STOP
      END
```

```
      SUBROUTINE LOWTEMP
C****************************************************************************C
C
C.....THIS SUBROUTINE COMPUTES THE COMPOSITION OF AIR
C.....AT LOW TEMPERATURES WHERE THERE IS SOME DISSOCIATION
C.....BUT VERY LITTLE IONIZATION.
C.....THE MAJOR SPECIES ARE O2, N2, AND AR.
C.....(MODEL I)
C
C****************************************************************************C
      COMMON  / A /  K1,K2,K3,K4,K5,K6,K7,KE
      COMMON  / B /  SN,SO,SR,EPS
      COMMON  / C /  S1,S2,S3,S4,S5,S6,S7,S8,S9,SA,SB
      COMMON  / D /  ITER
      REAL K1,K2,K3,K4,K5,K6,K7,KE
C
C.....INITIALIZE AND START ITERATING.
C
      S1P = SO / 2.0   $   S2 = SN / 2.0   $   SA = SR
      DO 200 ITER = 1,20
C
C.....COMPUTE THE MINOR SPECIES.
C
      S3 = SQRT(K1*S1P)   $   S5=SQRT(K3*S2)   $   S4 = KE*S3*S5
C
C.....UPDATE THE MAJOR SPECIES.
C
      S1 = (SO - S4 - S3) / 2.0   $   S2 = (SN - S4 - S5) / 2.0
C
C.....CHECK FOR CONVERGENCE.
C
      DS1 = S1 - S1P
      IF(ABS(DS1) .LE. EPS) GO TO 201
      S1P = S1
  200 CONTINUE
  201 CONTINUE
C
C.....COMPUTE THE TRACE SPECIES.
C
      C3 = S3/K6   $   C4 = S4/K4   $   C5 = S5/K5   $   C6 = SA/K7
      S7 = SQRT(C3 + C4 + C5 + C6)
      S6 = C4/S7   $   S8 = C5/S7   $   S9 = C3/S7   $   SB = C6/S7
      RETURN
      END
```

```
      SUBROUTINE QUARTIC
C****************************************************************************C
C
C.....THIS SUBROUTINE COMPUTES THE COMPOSITION OF AIR
C.....AT MODERATE TEMPERATURES WHERE THERE IS DISSOCIATION
C.....BUT NOT MUCH IONIZATION.
C.....THE MAJOR SPECIES ARE O2, N2, O, NO, AND N.
C.....(MODEL II)
C
C****************************************************************************C
      COMMON  / A /  K1,K2,K3,K4,K5,K6,K7,KE
      COMMON  / B /  SN,SO,SR,EPS
      COMMON  / C /  S1,S2,S3,S4,S5,S6,S7,S8,S9,SA,SB
      COMMON  / D /  ITER
      REAL K1,K2,K3,K4,K5,K6,K7,KE
C
C.....INITIALIZE, DETERMINE THE INITIAL GUESS, AND START ITERATION.
C
      S6 = 0.0   $   S8 = 0.0   $   S9 = 0.0    $    SA = SR
      B4 = (8.0 - K2 - K2) / K1
      B3 = 8.0 - K2 - 2.0*K3*KE
      BB= K1*(1.0 + SQRT(K2*SN / (K1 + K1)))
      S3 = ( - BB + SQRT(BB*BB + 8.0*SO*K1)) / 4.0
      C1=K1*K3*KE
      DO 200 ITER = 1,20
      SO1 = SO - S6 - S9
      SN1 = SN - S6 - S8
      B2 = - 8.0*SO1 + K1 + K1 + (SO1 - SN1)*K2 - C1
      B1 = SO1*( - K1 - K1 - K1 - K1 + C1)
      B0 = 2.0*SO1*SO1*K1
      F  = B0 + S3*(B1 + S3*(B2 + S3*(B3 + S3*B4)))
      FP = B1 + S3*(B2 + B2 + S3*(B3 + B3 + B3 + S3*(B4+B4+B4+B4)))
      D3 = - F / FP
      S3 = S3 + D3
C
C.....UNRAVEL THE REST OF THE MAJOR SPECIES
C
      S5 = (SO1 - S3 - 2.0*S3*S3 / K1) / (KE*S3)
      S4 = KE*S5*S3
      S2 = (SN1 - S4 - S5) / 2.0
      S1 = (SO1 - S4 - S3) / 2.0
C
C.....COMPUTE THE MINOR SPECIES.
C
      C3 = S3/K6    $   C4 = S4/K4   $   C5 = S5/K5   $   C6 = SA/K7
      S7 = SQRT(C3 + C4 + C5 + C6)
      S6 = C4/S7    $   S8 = C5/S7   $   S9 = C3/S7   $   SB = C6/S7
      SA = SR - SB
C
C.....CHECK FOR CONVERGENCE
C
      IF(ABS(D3) .LE. EPS) GO TO 201
  200 CONTINUE
  201 CONTINUE
     ·RETURN
      END
```

```
      SUBROUTINE CUBIC
C****************************************************************************C
C
C.....THIS SUBROUTINE COMPUTES THE COMPOSITION OF AIR
C.....AT VERY HIGH TEMPERATURES WHERE NOT MANY DIATOMIC PARTICLES ARE FOUND.
C.....THE MAJOR SPECIES ARE O, N, E- , N+ , AND O+.
C.....(MODEL IV)
C
C****************************************************************************C
      COMMON   / A /   K1,K2,K3,K4,K5,K6,K7,KE
      COMMON   / B /   SN,SO,SR,EPS
      COMMON   / C /   S1,S2,S3,S4,S5,S6,S7,S8,S9,SA,SB
      COMMON   / D /   ITER
      REAL  K1,K2,K3,K4,K5,K6,K7,KE
C
C.....INITIALIZE, DETERMINE THE INITIAL GUESS, AND START ITERATION.
C
      S1 = 0.0   $  S2 = 0.0  $  S4 = 0.0  $  S6 = 0.0
      SA = SR       $  SB = 0.0
      S7 = ( SQRT(1.0 + 4.0*SN*K5)-1.0 ) / (K5 + K5)
      S9 = SO / (1.0 + K6*S7)
      SB = SR / (1.0 + K7*S7)
      S7 = S7 + S9 + SB
      B3 = K5*K6
      C2 = K5 + K6
      DO 200 ITER = 1,20
      SO1 = SO - S1 - S1 - S4 - S6
      SN1 = SN - S2 - S2 - S4 - S6
      S6P = S6 + SB
      B2 =   C2 - B3*S6P
      B1 = 1.0 - SN1*K6 - SO1*K5 - S6P*C2
      B0 = - SN1 - SO1 - S6P
      F  = B0 + S7*(B1 + S7*(B2 + S7*B3))
      FP = B1 + S7*(B2 + B2 + S7*3.0*B3)
      D7 = - F / FP
      S7 = S7 + D7
C
C.....UNRAVEL THE REST OF THE MAJOR SPECIES
C
      S3 = SO1*S7*K6 / (1.0 + K6*S7)
      S5 = SN1*S7*K5 / (1.0 + K5*S7)
      SB = SR / (1.0 + K7*S7)
      SA = SR - SB
      S9 = S3 / (K6*S7)
      S8 = S5 / (K5*S7)
C
C.....COMPUTE THE MINOR SPECIES.
C
      S1 = S3*S3 / K1
      S2 = S5*S5 / K3
      S4 = KE*S3*S5
      S6 = S4 / (K4*S7)
C
C.....CHECK FOR CONVERGENCE
C
      IF(ABS(D7) .LE. EPS) GO TO 201
  200 CONTINUE
  201 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE QUDRATC
C**********************************************************************C
C
C.....THIS SUBROUTINE COMPUTES THE COMPOSITION OF AIR AT INTERMEDIATE
C.....TEMPERATURES WHERE OXYGEN IS ALMOST FULLY DISSOCIATED,
C.....BUT NOT MUCH IONIZATION HAS TAKEN PLACE.
C.....THE MAJOR SPECIES ARE N2, O, AND N.
C.....(MODEL III)
C
C**********************************************************************C
      COMMON  / A /  K1,K2,K3,K4,K5,K6,K7,KE
      COMMON  / B /  SN,SO,SR,EPS
      COMMON  / C /  S1,S2,S3,S4,S5,S6,S7,S8,S9,SA,SB
      COMMON  / D /  ITER
      REAL K1,K2,K3,K4,K5,K6,K7,KE
C
C.....INITIALIZE, DETERMINE THE INITIAL GUESS, AND START ITERATION.
C
      S4 = 0.0   $   S6 = 0.0   $   S8 = 0.0   $   SA = SR
C
      B1 = K3 / 2.0     $    B2 = K1 / 2.0
      S5  = ( - B1 + SQRT(B1*B1 + 4.0*B1*SN )) / 2.0
      S3P = ( - B2 + SQRT(B2*B2 + 4.0*B2*SO )) / 2.0
      DO 200 ITER = 1,20
      SN1 = SN - S4 - S6 - S8
      F = - B1*SN1 + S5*(B1 + S5)
      FP = B1 + S5 + S5
      S5 = S5 - F / FP
      S2 = (SN1 - S5) / 2.0
C
C.....UNRAVEL THE REMAINING SPECIES
C
      S1 = S3P*S3P / K1
      S4 = KE*S3P*S5
      C3 = S3P/K6   $   C4 = S4/K4   $   C5 = S5/K5   $   C6 = SA/K7
      S7 = SQRT(C3 + C4 + C5 + C6)
      S6 = C4/S7   $   S8 = C5/S7   $   S9 = C3/S7   $   SB = C6/S7
      SA = SR - SB
      S3 = SO - S1 - S1 - S4 - S6 - S9
C
C.....CHECK FOR CONVERGENCE.
C
      D3 = S3P - S3
      S3P = S3
      IF(ITER .EQ. 1) GO TO 200
      IF( ABS(D3) .LE. EPS) GO TO 201
  200 CONTINUE
  201 CONTINUE
      RETURN
      END
      FUNCTION EXXP(X)
      EXXP=0.0
      IF(X .LT. - 670.0) RETURN
      EXXP=EXP(X)
      RETURN
      END
```

Sample Results

```
/lgo

   INPUT:-    TKEL, RKGM3, EPS
           ENTER <RETURN> TO STOP
 ? 10000.,1.e-6,1.e-10

   T (KELVIN) = 10000.00  DENSITY (KG/M3) =  .100000E-05  EPS =   .1000E-09

   OXYGEN =  14.4802  NITROGEN =  53.9620  ARGON =  .3212   MOLS/KG.

   EQUILIBRIUM CONSTANTS K(I):-
       .29508E+11   .19149E+01   .23078E+09   .34684E-04   .13169E-02   .20269E-02
       .19413E-02   .53027E-09

   SOLUTION OF THE CUBIC EQUATION;  5 ITERATIONS

   MOLE NUMBERS OF THE SPECIES (MOL/KG):-
           O2           N2           O            NO           N            NO+
           E-           N+           O+           AR           AR+

       .91003E-10   .73958E-07   .16387E+01   .35900E-08   .41314E+01   .16440E-05
       .62958E+02   .49831E+02   .12841E+02   .34983E-01   .28622E+00

   ENTHALPY OF EACH SPECIES (JOULES/MOL):-
       .41091E+06   .38016E+06   .46617E+06   .48132E+06   .71628E+06   .13623E+07
       .20786E+06   .20934E+07   .17866E+07   .20790E+06   .17334E+07

   INTERNAL ENERGY OF EACH SPECIES (JOULES/MOL):-
       .32776E+06   .29702E+06   .38303E+06   .39817E+06   .63313E+06   .12792E+07
       .12472E+06   .20103E+07   .17035E+07   .12476E+06   .16502E+07

   ENTROPY OF EACH SPECIES (JOULES/MOL/KELVIN):-
       .33620E+03   .31386E+03   .23614E+03   .33631E+03   .23135E+03   .32018E+03
       .93886E+02   .23460E+03   .23013E+03   .22776E+03   .24261E+03

   TOTAL MOL NUMBER          =     131.7218 MOLS/KG.
   ENTHALPY OF THE MIXTURE   =   .144573E+09 JOULES/KG.
   ENTROPY OF THE MIXTURE    =   .332118E+05 JOULES/KG./KELVIN
   INT. ENERGY OF THE MIXTURE =  .133621E+09 JOULES/KG.
   PRESSURE                  =   .109513E-03 (BAR)

   RESIDUES:-
     0.            -.71054E-14  0.           0.          0.           0.
       .56843E-13   .22737E-12   .58797E-12  0.          -.35527E-13
```

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Table I. Major and Minor Species in the Present Air Model

Model I*	Model II	Model III	Model IV
Major species			
O_2	O_2	N_2	O
N_2	N_2	O	N
Ar	O	N	e^-
	NO	Ar	N^+
	N		O^+
	Ar		Ar
Minor species			
O	NO^+	O_2	O_2
NO	e^-	NO	N_2
N	N^+	NO^+	NO
NO^+	O^+	e^-	NO^+
e^-	Ar^+	N^+	Ar^+
N^+		O^+	
O^+		Ar^+	
Ar^+			

* The species NO^+, e^-, N^+, and Ar^+ are considered as trace species in model I.

Table II. Coefficients of Approximating Polynomials for Thermodynamic Functions

$$[T_{\text{ref}} = 0 \text{ K}]$$

TEMP. RANGE	a(1,1)	a(1,2)	a(1,3)	a(1,4)	a(1,5)	a(1,6)	a(1,7)
i=1; Neutral Diatomic Oxygen (O2)						$\Delta H^0_{f,1} = 0$ J/mol	
200. - 800.	.377037E+01	-.289522E-02	.953322E-05	-.924699E-08	.301919E-11	-.188598E+02	.369335E+01
800. - 3000.	.289692E+01	.237365E-02	-.149171E-05	.466034E-09	-.539452E-13	.822404E+02	.750194E+01
3000. - 6000.	.284211E+01	.133206E-02	-.339159E-06	.446522E-10	-.229148E-14	.583504E+03	.862550E+01
6000. - 10000.	.568211E+01	-.753006E-03	.229801E-06	-.239559E-10	.800485E-15	-.247004E+04	-.987401E+01
10000. - 15000.	-.272590E+00	.201151E-02	-.245477E-06	.120252E-10	-.213899E-15	.761177E+04	.316317E+02
i=2; Neutral Diatomic Nitrogen (N2)						$\Delta H^0_{f,2} = 0$ J/mol	
200. - 800.	.346226E+01	.582024E-03	-.305255E-05	.622801E-08	-.337560E-11	.879517E+00	.321926E+01
800. - 3000.	.270224E+01	.194439E-02	-.893000E-06	.197392E-09	-.169678E-13	.201802E+03	.720408E+01
3000. - 6000.	.391435E+01	.315371E-03	-.564810E-07	.360123E-11	-.523594E-16	-.535520E+03	.216720E-01
6000. - 10000.	.126575E+01	.182698E-02	-.375839E-06	.330337E-10	-.936511E-15	.314270E+04	.179433E+02
10000. - 15000.	.277159E+02	-.741735E-02	.823960E-06	-.352853E-10	.496712E-15	-.569427E+05	-.174029E+03
i=3; Neutral Monatomic Oxygen (O)						$\Delta H^0_{f,3} = 246\ 783$ J/mol	
200. - 800.	.321671E+01	-.378227E-02	.847468E-05	-.886582E-08	.353656E-11	.296405E+05	.185264E+01
800. - 3000.	.260454E+01	-.172355E-03	.115741E-06	-.364179E-10	.460115E-14	.297290E+05	.458653E+01
3000. - 6000.	.281017E+01	-.290399E-03	.908333E-07	-.994278E-11	.377044E-15	.295366E+05	.325365E+01
6000. - 10000.	.192093E+01	.217766E-03	-.182884E-07	.490510E-12	.285073E-17	.307834E+05	.927486E+01
10000. - 15000.	.192093E+01	.217766E-03	-.182884E-07	.490510E-12	.285073E-17	.307834E+05	.927486E+01
i=4; Neutral Nitric Oxide (NO)						$\Delta H^0_{f,4} = 90\ 671$ J/mol	
200. - 800.	.420644E+01	-.450984E-02	.105574E-04	-.859194E-08	.240471E-11	.108890E+05	.231379E+01
800. - 3000.	.275438E+01	.230933E-02	-.128234E-05	.340435E-09	-.348075E-13	.111343E+05	.907897E+01
3000. - 6000.	.380154E+01	.498575E-03	-.125313E-06	.140939E-10	-.448202E-15	.106666E+05	.316194E+01
6000. - 10000.	.491332E+01	.617553E-06	-.552224E-07	.116865E-10	-.546425E-15	.884538E+04	-.457869E+01
10000. - 15000.	.204567E+02	-.614981E-02	.869143E-06	-.508775E-10	.106242E-14	-.229552E+05	-.115620E+03
i=5; Neutral Monatomic Nitrogen (N)						$\Delta H^0_{f,5} = 470\ 818$ J/mol	
200. - 800.	.250000E+01	0.	0.	0.	0.	.566267E+05	.418073E+01
800. - 3000.	.250751E+01	-.247979E-04	.296415E-07	-.152881E-10	.289137E-14	.566249E+05	.414319E+01
3000. - 6000.	.263761E+01	-.873733E-05	-.647727E-07	.234734E-10	-.173962E-14	.564523E+05	.322321E+01
6000. - 10000.	.337206E+01	-.885546E-03	.252933E-06	-.231879E-10	.704714E-15	.562702E+05	-.105640E+01
10000. - 15000.	-.102056E+02	.429313E-02	-.493107E-06	.249511E-10	-.469699E-15	.849338E+05	.964037E+02
i=6; Unipositive Nitric Oxide (NO+)						$\Delta H^0_{f,6} = 984\ 611$ J/mol	
200. - 800.	.356593E+01	-.274203E-03	-.522843E-06	.302282E-08	-.191127E-11	.118414E+06	.359357E+01
800. - 3000.	.271526E+01	.189981E-02	-.853462E-06	.183903E-09	-.153285E-13	.118621E+06	.793691E+01
3000. - 6000.	.393110E+01	.306608E-03	-.567059E-07	.455735E-11	-.777620E-16	.117863E+06	.701982E+00
6000. - 10000.	.106562E+01	.179180E-02	-.330778E-06	.250527E-10	-.545401E-15	.122142E+06	.203283E+02
10000. - 15000.	.313770E+02	-.781707E-02	.754371E-06	-.247341E-10	.159524E-15	.481245E+05	-.202185E+03

Table II. Concluded

TEMP. RANGE	a(i,1)	a(i,2)	a(i,3)	a(i,4)	a(i,5)	a(i,6)	a(i,7)
i=7; Electron (E-)						$\Delta H^0_{f,7} = 0$ J/mol	
200. - 800.	.250000E+01	0.	0.	0.	0.	-.424990E-01	-.117339E+02
800. - 3000.	.250000E+01	0.	0.	0.	0.	-.424990E-01	-.117339E+02
3000. - 6000.	.250000E+01	0.	0.	0.	0.	-.424990E-01	-.117339E+02
6000. - 10000.	.250000E+01	0.	0.	0.	0.	-.424990E-01	-.117339E+02
10000. - 15000.	.250000E+01	0.	0.	0.	0.	-.424990E-01	-.117339E+02
i=8; Unipositive Monatomic Nitrogen (N+)						$\Delta H^0_{f,8} = 1\,873\,124$ J/mol	
200. - 800.	.308170E+01	-.377375E-02	.967715E-05	-.110995E-07	.472486E-11	.225328E+06	.243159E+01
800. - 3000.	.253470E+01	-.550674E-04	.364400E-07	-.123132E-10	.192247E-14	.225395E+06	.478956E+01
3000. - 6000.	.280056E+01	-.295664E-03	.966497E-07	-.110536E-10	.441452E-15	.225185E+06	.313053E+01
6000. - 10000.	.200477E+01	.191897E-03	-.154991E-07	.411659E-12	.262876E-17	.226226E+06	.846350E+01
10000. - 15000.	.205984E+01	.188754E-03	-.180755E-07	.802843E-12	-.130896E-16	.226028E+06	.802544E+01
i=9; Unipositive Monatomic Oxygen (O+)						$\Delta H^0_{f,9} = 1\,560\,726$ J/mol	
200. - 800.	.250000E+01	0.	0.	0.	0.	.187713E+06	.438020E+01
800. - 3000.	.250134E+01	-.404313E-05	.432715E-08	-.195277E-11	.316328E-15	.187713E+06	.437342E+01
3000. - 6000.	.222589E+01	.296501E-03	-.115611E-06	.184612E-10	-.892492E-15	.187912E+06	.605761E+01
6000. - 10000.	.412110E+01	-.867862E-03	.153375E-06	-.922601E-11	.178420E-15	.185437E+06	-.663889E+01
10000. - 15000.	.173495E+01	-.807107E-04	.598063E-07	-.459985E-11	.102952E-15	.191074E+06	.107919E+02
i=10; Neutral Argon (Ar)						$\Delta H^0_{f,10} = 0$ J/mol	
200. - 800.	.250000E+01	0.	0.	0.	0.	-.424990E-01	.436650E+01
800. - 3000.	.250000E+01	0.	0.	0.	0.	-.424990E-01	.436650E+01
3000. - 6000.	.250000E+01	0.	0.	0.	0.	-.424990E-01	.436650E+01
6000. - 10000.	.263035E+01	-.773934E-04	.172197E-07	-.170282E-11	.631988E-16	-.175480E+03	.348901E+01
10000. - 15000.	-.914240E+01	.385082E-02	-.468004E-06	.245069E-10	-.456469E-15	.277519E+05	.894618E+02
i=11; Unipositive Argon (Ar+)						$\Delta H^0_{f,11} = 1\,520\,581$ J/mol	
200. - 800.	.268188E+01	-.207203E-02	.747860E-05	-.876720E-08	.344842E-11	.182871E+06	.507646E+01
800. - 3000.	.242206E+01	.863470E-03	-.784594E-06	.266740E-09	-.318506E-13	.182853E+06	.592363E+01
3000. - 6000.	.255884E+01	.897362E-04	-.500916E-07	.882982E-11	-.523719E-15	.183014E+06	.553130E+01
6000. - 10000.	.250142E+01	.294466E-04	-.804717E-08	.775358E-12	-.257809E-16	.183252E+06	.605440E+01
10000. - 15000.	.257061E+01	-.206211E-04	.297860E-08	-.211019E-12	.574768E-17	.183223E+06	.561650E+01

Table III. Computational Time and Number of Iterations for Sample Cases

| Model	t_0, μs	t_i, μs	ρ, kg/m^3	T, K	$N(\varepsilon)$ ($\varepsilon = 0.001$)	$N(\varepsilon)$ ($\varepsilon = 0.0001$)
I	286	20	1×10^1	800	1	1
			1×10^{-2}	800	1	1
			1×10^{-5}	800	1	1
			1×10^1	1 600*	2	2
			1×10^{-2}	1 600*	2	2
			1×10^{-5}	1 600*	2	2
II	294	40	1×10^1	1 600*	1	1
			1×10^{-2}	1 600*	1	1
			1×10^{-5}	1 600*	1	1
			1×10^1	7 000	1	2
			1×10^{-2}	3 000	1	1
			1×10^{-5}	2 000	1	1
			1×10^1	13 500*	2	3
			1×10^{-2}	5 968*	1	1
			1×10^{-5}	3 577*	1	1
III	286	31	1×10^1	13 500*	2	4
			1×10^{-2}	5 968*	1	3
			1×10^{-5}	3 577*	1	3
			1×10^1	13 000	2	3
			1×10^{-2}	10 000	1	2
			1×10^{-5}	7 000	1	2
			1×10^1	15 000	2	3
			1×10^{-2}	8 960*	2	2
			1×10^{-5}	5 950*	1	2
IV	293	31	1×10^{-2}	8 960*	2	3
			1×10^{-5}	5 950*	2	3
			1×10^{-2}	14 000	1	2
			1×10^{-5}	13 000	1	2
			1×10^{-2}	15 000	1	2
			1×10^{-5}	15 000	1	1

*Point on boundary between models.
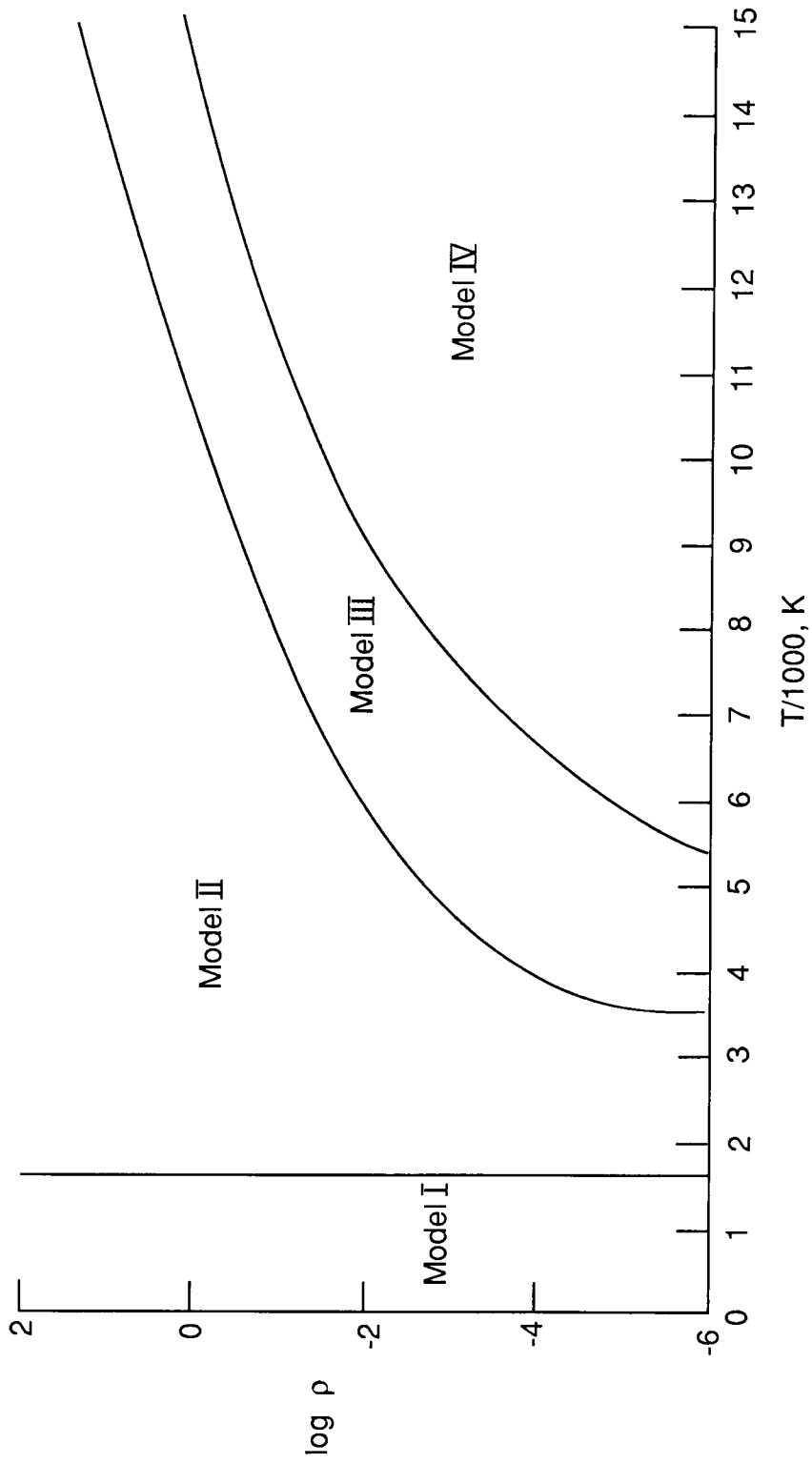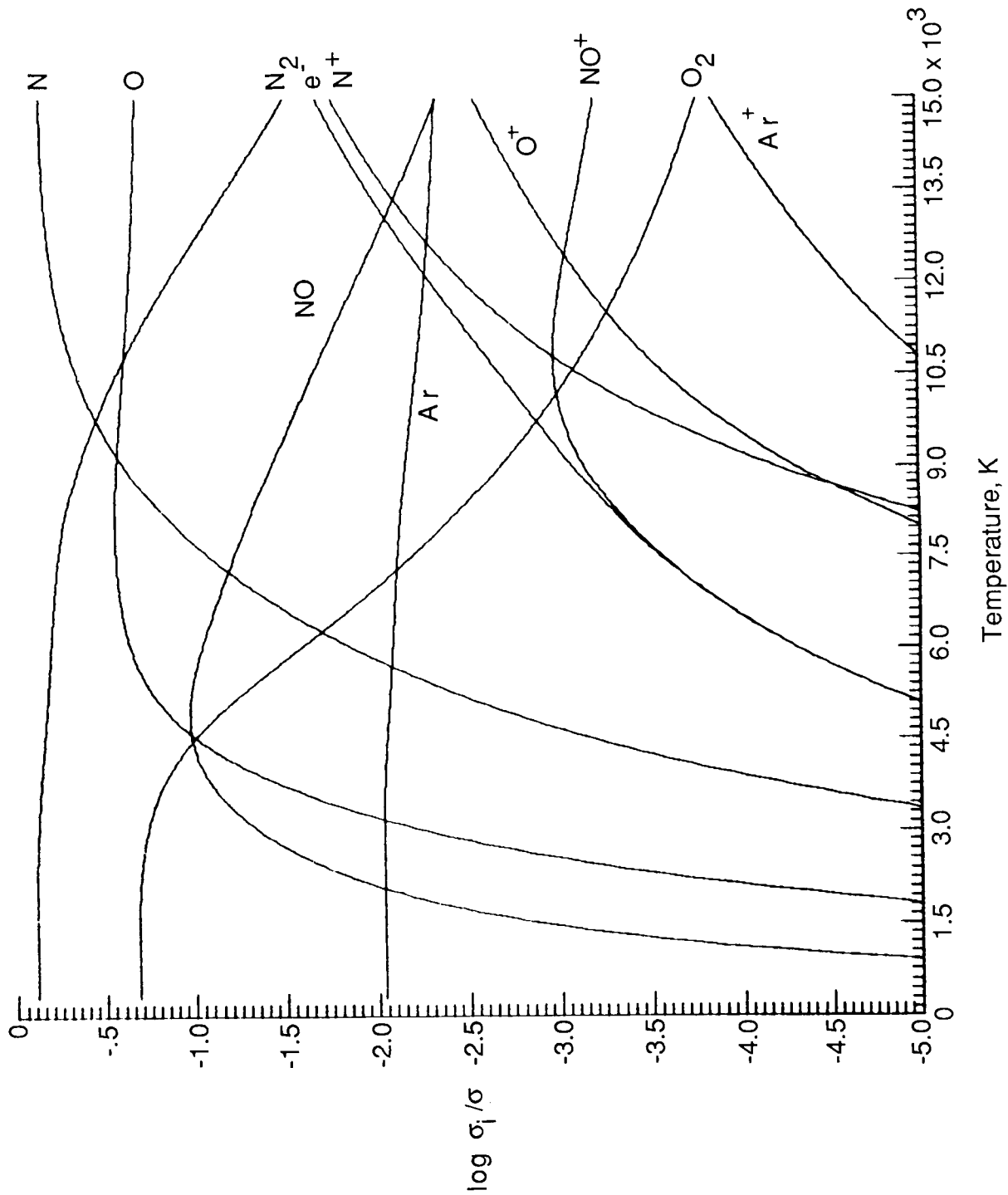
Figure 1. Regions of applicability of various models.
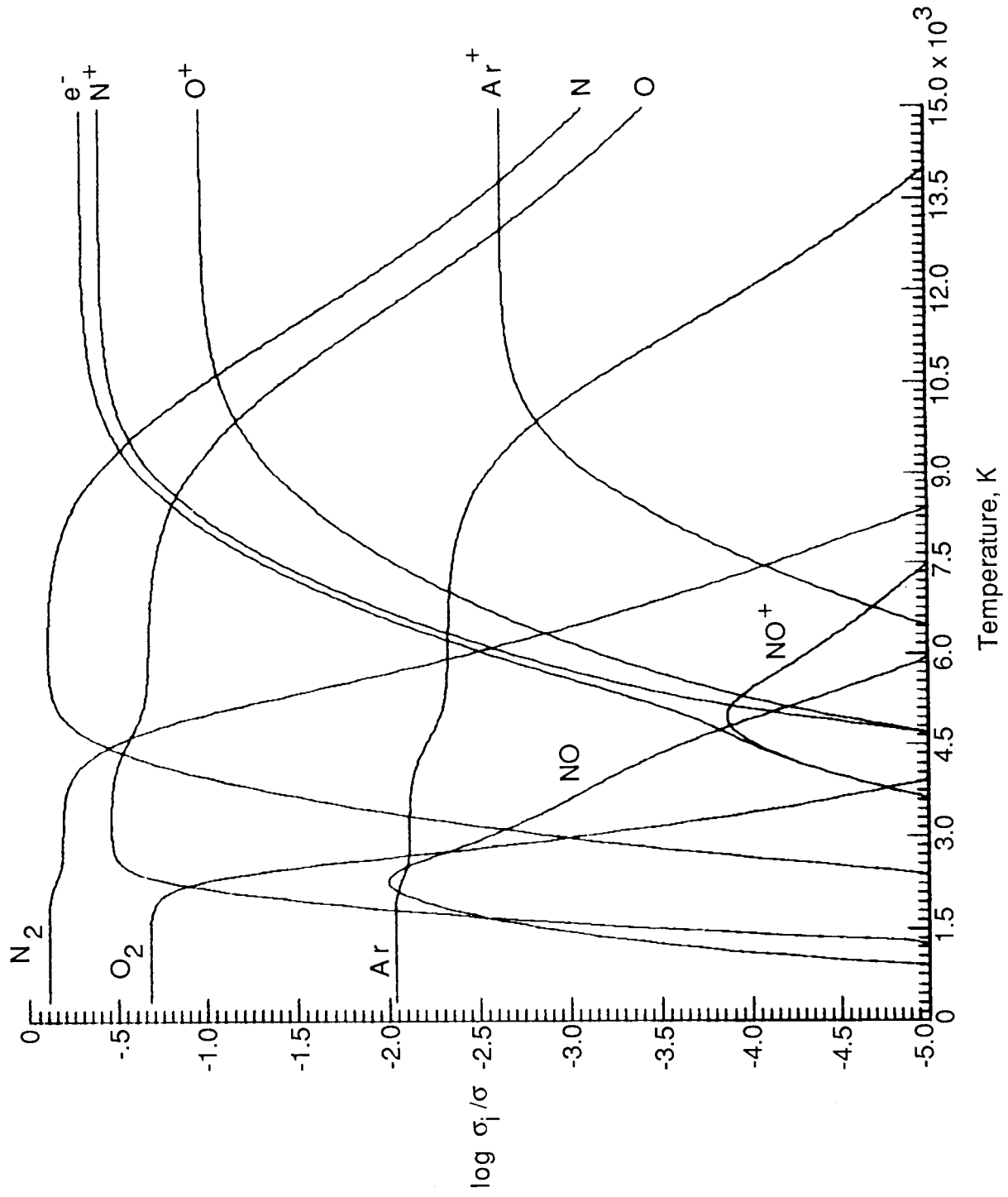
Figure 2. Log σ_i/σ as function of temperature.

(a) $\rho = 1 \times 10^{-5}$ kg/m^3.
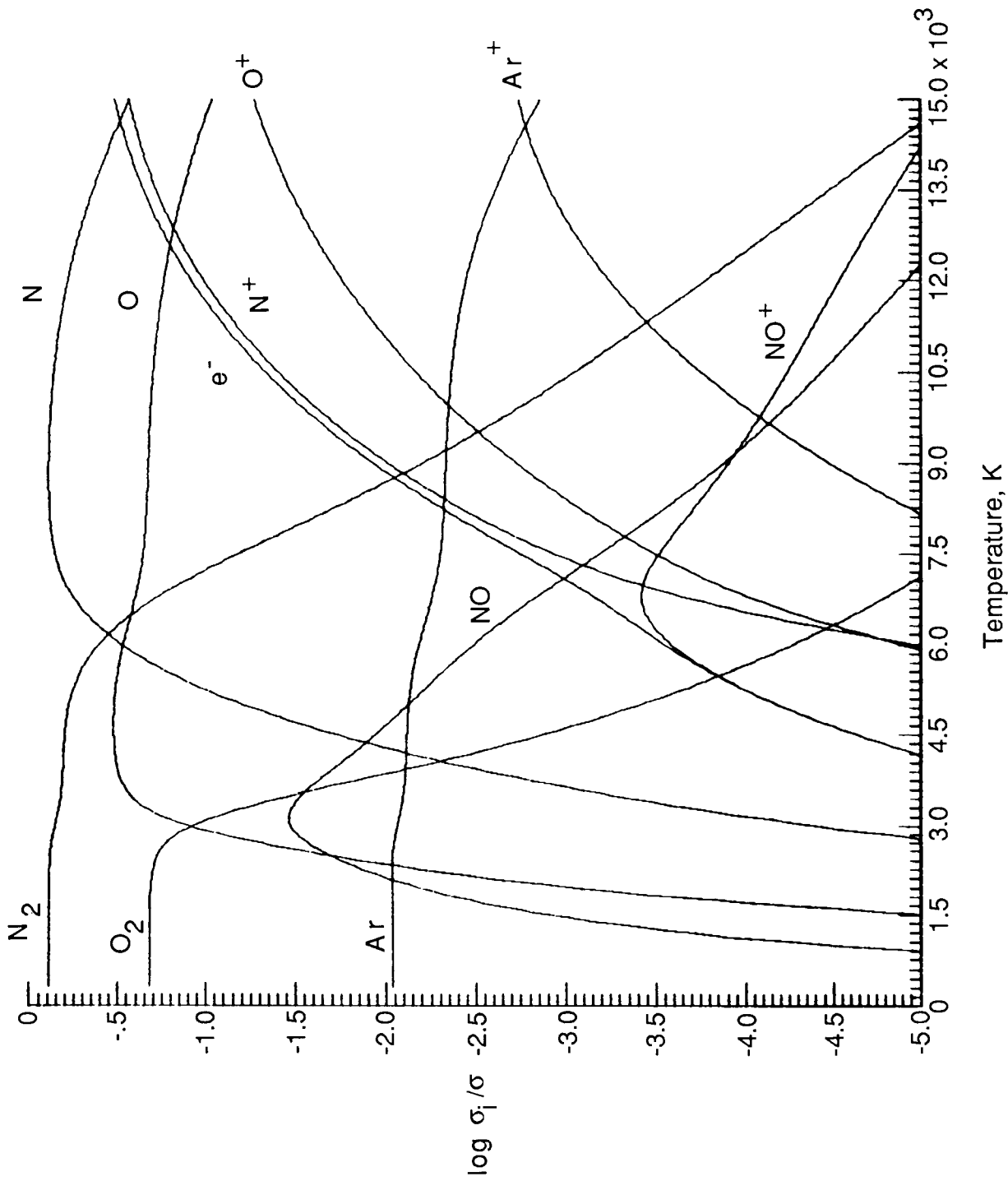
(b) $\rho = 1 \times 10^{-2}$ kg/m^3.

Figure 2. Continued.

(c) $\rho = 1 \times 10^1$ kg/m^3.

Figure 2. Concluded.

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15. Supplementary Notes

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16. Abstract

A rapid computational method has been developed to determine the equilibrium chemical composition of air to 15 000 K. Eleven chemically reacting species—O_2, N_2, O, NO, N, NO^+, e^-, N^+, O^+, Ar, and Ar^+—are included. The method involves the algebraic combination of seven nonlinear equilibrium equations and four linear elemental mass-balance and charge-neutrality equations. Computational speeds for determining the equilibrium chemical composition are significantly faster than those of the often-used free-energy-minimization procedure. Data are also included from which the thermodynamic properties of air can be computed. Additionally, a listing of the computer program and a set of sample results are included.

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