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COMPUTER PROGRAM OF DATA REDUCTION PROCEDURES FOR FACILITIES USING CO_2-N_2-O_2-Ar EQUILIBRIUM REAL-GAS MIXTURES

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16. Abstract

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The data reduction procedures are based on combinations of three of the following flow parameters measured in the immediate vicinity of the test section:

(1) Stagnation pressure behind normal shock
(2) Free-stream static pressure
(3) Stagnation-point heat-transfer rate
(4) Free-stream velocity
(5) Free-stream density

Thus, these procedures do not depend explicitly upon measured or calculated upstream flow parameters. The procedures are incorporated into a single computer program written in FORTRAN IV language. A listing of this computer program is presented, along with a description of the inputs required and a sample of the data printout.

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SUMMARY

Data reduction procedures for determining free-stream and post-normal-shock flow conditions are presented. These procedures are applicable to flows of CO_2, N_2, O_2, Ar, or mixtures of these gases and include the effects of dissociation and ionization. The assumption of thermochemical equilibrium free-stream and post-normal-shock flow is made. Although derived primarily to meet the immediate needs of the expansion tube of the Langley hot gas radiation research facility, these procedures are applicable to any supersonic or hypersonic test facility using these gases or mixtures thereof.

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INTRODUCTION

As discussed in reference 1, significant differences between measured test-section flow quantities and predicted test-section flow quantities based on upstream flow conditions were observed in the Langley pilot model expansion tube. In order to provide a means for obtaining accurate test-section conditions, a computational scheme based on flow properties measured in the immediate vicinity of the test section was derived in reference 1.

This scheme eliminated an explicit dependence upon measured or calculated upstream flow properties, thereby resulting in a substantial reduction in the uncertainty in predicted test-section flow conditions. The study of reference 1 was, however, limited to thermochemical equilibrium, imperfect, real-air flows.

Experimental investigations made in test facilities for which the test gas will be representative of Mars and Venus atmospheres (CO_2 predominance) require accurate predictions of test-section flow conditions for such real-gas mixtures. Therefore, the purpose of this program is to provide a means for obtaining accurate test-section conditions for real gases CO_2, N_2, O_2, and Ar or mixtures of these gases. This is achieved by employing a computational scheme based on combinations of three flow parameters measured in the immediate vicinity of the test section. The measured flow properties serving as inputs to the data reduction procedures presented herein are as follows:

(1) Stagnation pressure behind normal shock

(2) Free-stream static pressure

(3) Stagnation-point heat-transfer rate

(4) Free-stream velocity

(5) Free-stream density

Of the 10 possible data reduction procedures from these inputs, seven are presented herein. (Data reduction procedures deemed less preferable in the error analysis study of ref. 1 are omitted.) The thermodynamic properties for CO_2, N_2, O_2, Ar, and mixtures of these gases are obtained from references 2 and 3. Although the data reduction procedures presented herein were derived to meet the immediate needs of the expansion tube of the Langley hot gas radiation research facility, these real-gas-mixture procedures are also applicable to supersonic or hypersonic test facilities using these gases or mixtures of these gases.

The procedures are incorporated into a single computer program written in FORTRAN IV language. A listing of this computer program is presented in appendix A and a description of the inputs required is presented in appendix B. Program output parameters for various gas mixtures are illustrated by sample data printouts presented in appendix C.

SYMBOLS

The International System of Units (SI) is used for all physical quantities in this study. Conversion factors relating the International System of Units to the U.S. Customary Units are given in reference 4.

a	speed of sound, m/sec
h	specific enthalpy, m^2/sec^2 (J/kg)
M	Mach number, U/a
N_{Pr}	Prandtl number
N_{Re}	Reynolds number, m^{-1}
p	pressure, N/m^2
$\dot{q}$	heat-transfer rate, W/m^2
R	universal gas constant, 8.31434×10^3 J/kmole-^oK
r	nose radius, m
sW_o/R	nondimensional specific entropy
T	temperature, ^oK
U	velocity, m/sec
W	molecular weight, kg/kmole
W_o	molecular weight of undissociated gas or gas mixture, kg/kmole
X	mole fraction, kmole of species i/kmole of mixture
Y_i	number of kmole of species i per mass of mixture, kmole of species i/kg of mixture
Z	compressibility factor, $pW_o/\rho RT$
γ_E	isentropic exponent, $\left(\frac{\partial \log p}{\partial \log \rho}\right)_{sW_o/R}$
η	parameter defined in equation (12), $kg/m^{3/2}$-sec-$(N/m^2)^{1/2}$

μ	viscosity, $N\text{-}sec/m^2$
ρ	density, kg/m^3

Subscripts:

c	calculated
g	geometric
i	individual species
m	measured
mix	mixture
prev	previous value of a parameter
t	stagnation conditions behind normal shock
w	model wall
1	free stream
2	static conditions immediately behind normal shock

Approximate value is denoted by $\sim$.

ANALYSIS

Before the discussion of the calculation procedures for determining free-stream and post-normal-shock flow quantities, the source of thermodynamic properties for CO_2-N_2-O_2-Ar gas mixtures in chemical equilibrium employed in this study is discussed. Next, the iterative methods for crossing the standing normal shock are discussed, since these methods are common to all calculation procedures. Finally, the relations used to predict stagnation-point heat-transfer rate are discussed.

Thermodynamic Properties for Arbitrary Gas Mixtures

Thermodynamic properties for CO_2-N_2-O_2-Ar gas mixtures are obtained from the results of references 2 and 3. These results include dissociation and ionization. Basic assumptions used in obtaining these results are as follows:

(1) The mixture is composed of ideal gases.

(2) For diatomic species the rigid-rotor harmonic oscillator model is used with vibrational-rotational corrections for each electronic configuration.

(3) Only electronic levels with principal quantum number less than or equal to five are included.

The procedure of references 2 and 3 is based upon the free-energy minimization method of reference 5. For a given pressure and temperature, the free energy for individual species are computed from the partition function of statistical mechanics. (The five components and 26 species considered in refs. 2 and 3 are tabulated in appendix B.) The equilibrium composition is then obtained by minimization of the free energy. After the composition for a given pressure and temperature is determined, the corresponding thermodynamic properties of interest are computed directly.

The program of references 2 and 3 is included in the present study as a subroutine and referred to herein as ROGO. The basic inputs to ROGO, other than the atomic energy level constants (which are tabulated in ref. 2), are pressure, temperature, and initial estimates of the species concentrations. For the free-energy minimization method to determine the composition of a gas mixture, the initial estimates of Y_i are somewhat arbitrary. In the present study, the partial pressures of the CO_2, N_2, O_2, and/or Ar test gases in the initial state (prior to addition of energy) are assumed known. The corresponding mole fractions for these gases are obtained from Dalton's law.

$$X_i = \frac{p_i}{p_{mix}} \tag{1}$$

and the molecular weight is given by

$$W_o = \sum_i X_i W_i \tag{2}$$

The initial estimates for the species concentrations for CO_2, N_2, O_2, and Ar are obtained from

$$Y_i = \frac{X_i}{W_o} \tag{3}$$

For the remaining 22 species, the initial estimates for the concentrations are set equal to 10^{-20}. Thermodynamic properties obtained from ROGO, for a given p and T, are a, h, sW_0/R, X_i, Z, γ_E, and ρ.

Combinations of input thermodynamic properties other than p and T are required in the present study. An iterative-interpolation scheme was derived to enable determination of thermodynamic properties from combinations of h, p, sW_0/R, and ρ. This iterative-interpolation scheme is referred to herein as FIND (I), and the inputs for a given I are as follows:

I	Inputs to FIND (I)
1	p, ρ
2	p, h
3	p, sW_0/R
4	h, ρ

In the iterative phase of FIND (1, 2, or 3), T is varied (for a given p) to bring the corresponding ρ, h, or sW_0/R from ROGO toward agreement with the known ρ, h, or sW_0/R. This iteration phase is terminated when the uncertainty in T is reduced to less than 250° K. ROGO is used to obtain the thermodynamic properties at the midpoint and ends of this region of uncertainty. An interpolation is performed over this region to obtain the desired thermodynamic properties. To assist in the reduction of computer time, the flow region (free stream or postshock) is identified in FIND (I). Upper and lower limits on T for these two regions are inputs. Hence, if the user of this program has a priori approximate values of T_1 and T_2 or T_t, a reduction in computer time can be realized by establishing these limits on T (see appendix B); if not, the limits are taken as 0° K to 8000° K for free-stream conditions and 0° K to $16\,000^\circ$ K for postshock conditions.

For FIND (4), where h and ρ are inputs, an initial value of p is assumed and the iteration-interpolation scheme for FIND (1) employed to determine the thermodynamic properties for this p (that is, with this $\tilde{p}$ and ρ, T is varied until the ρ from ROGO is within 0.1 percent of the input ρ). The calculated h is compared to the input h; if not within 0.1 percent, p is varied and the procedure repeated. This iterative scheme is continued until the condition on h is satisfied, or the Δp of the iteration becomes less than a given value. If the latter occurs, the iteration is terminated and an interpolation performed to obtain the desired thermodynamic quantities.

Iterative Procedure for Standing Normal Shock

The conservation relations for mass, momentum, and energy for a standing normal shock are

$$\rho_1 U_1 = \rho_2 U_2 \tag{4}$$

$$p_1 + \rho_1 U_1^2 = p_2 + \rho_2 U_2^2 \tag{5}$$

$$h_1 + \frac{1}{2} U_1^2 = h_2 + \frac{1}{2} U_2^2 \tag{6}$$

Both the direct solution and inverse solution to the conservation relations are used herein.

In the direct solution, the free-stream conditions appearing on the left side of equations (4) to (6) are considered known. The h_t can be determined from the energy relation (eq. (6))

$$h_t = h_1 + \frac{1}{2} U_1^2 \tag{7}$$

If measured p_t is not available, the relation (see ref. 1)

$$\tilde{p}_t = 0.97 \rho_1 U_1^2 \tag{8}$$

is used to obtain an accurate estimate of p_t. From a known p_t or estimated value from equation (8) and known value of h_t, a value of ρ_t is obtained from FIND (2). The initial estimate of ρ_2 is taken to be $0.955\rho_t$. This value of ρ_2 is used in equations (4) to (6) to obtain corresponding values of p_2, h_2, and U_2. The p_2 and h_2 are used as inputs to FIND (2) to obtain a value of ρ_2. This ρ_2 from FIND (2) is compared to the initial estimate of ρ_2. If these values are not within 0.1 percent, the ρ_2 obtained from FIND (2) is used in equations (4) to (6) to obtain upgraded values of p_2, h_2, and U_2. This method of successive approximations is repeated until successive values of ρ_2 from FIND (2) are within 0.1 percent.

The postshock stagnation conditions are determined by assuming that the flow region immediately behind the normal shock to the stagnation point is isentropic $\left(\text{that is, } \frac{s_t W_o}{R} = \frac{s_2 W_o}{R}\right)$. Now, the variation in conditions from immediately downstream of the shock to the stagnation point is relatively small $\left(\text{that is, } \gamma_{E,2} \approx \gamma_{E,t} \text{ and } Z_2 \approx Z_t\right)$. Thus, this region may be considered to behave as a calorically perfect gas. The p_t can be accurately estimated from the ideal-gas isentropic relation

$$\tilde{p}_t = p_2\left(1 + \frac{\gamma_{E,2} - 1}{2} M_2^2\right)^{\gamma_{E,2}/\gamma_{E,2}-1} \tag{9}$$

This $\tilde{p}_t$ is used as an input to FIND (2), in conjunction with h_t, to obtain a value of s_tW_o/R. If this s_tW_o/R is not within 0.05 percent of s_2W_o/R, the p_t is varied (upward or downward) 4 percent in 1-percent increments. The values of s_tW_o/R corresponding to each p_t and the h_t are obtained from FIND (2). The value of p_t resulting in $\frac{s_tW_o}{R} = \frac{s_2W_o}{R}$ is obtained by interpolation.

In the inverse solution, the stagnation-point conditions are obtained from FIND (2) where inferred h_t from stagnation-point heat-transfer rate measurement and measured p_t serve as inputs. An estimate of p_2 is made and used with s_tW_o/R as inputs to FIND (3) to obtain ρ_2 and h_2. The corresponding U_2 is obtained from the energy relation (eq. (6))

$$U_2 = \sqrt{2\left(h_t - h_2\right)} \tag{10}$$

In the procedures using the inverse solution, either p_1 or ρ_1 is known. Thus, the free-stream quantities on the left side of equations (4) to (6) can be determined. The p_1 and ρ_1 are used in FIND (1) to obtain a value of h_1. This h_1 from FIND (1) is compared to the calculated h_1 from equation (6) and, if not within 0.1 percent, the p_2 is varied and the procedure repeated. This numerical iteration on p_2 is continued until the convergence criterion on h_1 is satisfied.

Prediction of Stagnation-Point Heat-Transfer Rates

Because measured $\dot{q}_t$ is a basic input datum, it is necessary that a relatively accurate means for predicting $\dot{q}_t$ in CO_2-N_2-O_2-Ar mixtures be available. Considerable effort has been directed toward obtainment of expressions for predicting $\dot{q}_t$ at high velocities in air. In comparison, the number of similar studies in arbitrary gas mixtures is relatively small.

Recently, however, an analytical study of stagnation-point convective heat transfer to an axisymmetric blunt body was performed for a number of gas mixtures in thermochemical equilibrium (ref. 6). This study demonstrated that the simple, empirical relation of reference 7 for predicting $\dot{q}_t$ in Ar-H_2-N_2-CO_2 gas mixtures yields results which are in good agreement with analytical results, provided the $N_{Pr,w}$ of the individual gases are approximately equal. For the gases considered herein, $N_{Pr,w}$ varies from approximately 0.67 for Ar to approximately 0.7 for N_2 and O_2 and to approximately 0.72 for CO_2 at the T_w of interest $\left(T_w \text{ from room temperature to } 1500^\circ \text{ K}\right)$. Hence, according to reference 6, the empirical relation of reference 7 should provide relatively accurate predictions of $\dot{q}_t$ for the present gas mixtures. This relation of reference 7, which was also employed in the air study of reference 1, is

$$\dot{q}_t = \eta\sqrt{\frac{p_t}{r_g}}\left(h_t - h_w\right) \tag{11}$$

where

$$\eta \equiv W_o\left(\sum_i \frac{X_i W_i}{\eta_i}\right)^{-1} \tag{12}$$

and the η_i are given in the following table:

Species i	η_i
CO_2	4.3102×10^{-4}
N_2	3.6285
O_2	4.8945
Ar	5.4788

(The value of η_i for O_2 is not presented in ref. 7. This value was deduced by comparison of the K_i of table I in ref. 7 for air to the K_i for an air mixture of CO_2, N_2, O_2, and Ar. The air-mixture composition was taken as 78.084 percent N_2, 20.946 percent O_2, 0.937 percent Ar, and 0.033 percent CO_2 by volume (ref. 1).) The h_w is obtained directly from ROGO, where the required temperature input to ROGO is T_w. For the range of T_w considered herein (300° K < T_w < 1500° K), h_w may be considered to be a function of T_w only and a precise knowledge of p_w is not necessary for obtaining h_w accurately. For procedures where $(p_t)_m$ is an input or $\tilde{p}_t$ can be obtained from equation (8), the p_w is equal to $(p_t)_m$ or $(p_t)_c$. (For the single procedure where $(p_t)_m$ is not an input, as well as $(\rho_1)_m$ and $(U_1)_m$ (that is, $\tilde{p}_t$ cannot be obtained from eq. (8)), p_w is simply set equal to 1.01325×10^5 N/m^2.)

Procedures for Determining Free-Stream and Postshock Conditions

The procedures for determining free-stream and post-normal-shock flow conditions are identified in the computer program by ITEST. For convenience, this method of identification is employed in the following discussion. The basic measured inputs and iterative procedure for crossing the normal shock are given in the following table:

ITEST	Measured inputs	Shock-crossing procedure
1	p_1, U_1, p_t	Direct
2	p_1, p_t, $\dot{q}_t$	Inverse
3	p_1, ρ_1, U_1	Direct
4	p_1, ρ_1, p_t	Direct
5	ρ_1, p_t, $\dot{q}_t$	Inverse
6	p_1, ρ_1, $\dot{q}_t$	Direct
7	ρ_1, U_1, $\dot{q}_t$	Direct

Of the 10 possible combinations of the input parameters p_1, ρ_1, U_1, p_t, and $\dot{q}_t$, three have been omitted from the present study. The procedure involving inputs ρ_1, U_1, and p_t was omitted because of the existence of a relatively accurate expression (eq. (8)) relating all three quantities. Omission of the other two procedures $\left(U_1,\ p_t,\ \dot{q}_t\right.$, and $\left.p_1,\ U_1,\ \dot{q}_t\right)$ was based on the error analysis performed in reference 1, which showed these procedures to be less acceptable than others.

The individual procedures are now discussed briefly.

ITEST = 1.- A value of $\tilde{\rho}_1$ is determined from the measured U_1 and p_t by using equation (8). The measured p_1 and this $\tilde{\rho}_1$ are used as inputs to FIND (1) to obtain the corresponding free-stream thermodynamic properties. The direct iterative shock-crossing procedure is performed. The calculated p_t is compared to the measured p_t and if not within a prescribed tolerance (TOLPT), $\tilde{\rho}_1$ is adjusted by using the relation

$$\tilde{\rho}_1 = \left(\tilde{\rho}_1\right)_{prev} \frac{\left(p_t\right)_m}{\left(p_t\right)_{c,prev}} \tag{13}$$

This new value of $\tilde{\rho}_1$ is used, in conjunction with $\left(p_1\right)_m$, as input into FIND (1). The corresponding value of h_1 obtained from FIND (1) is used in the direct shock-crossing solution. The $\left(p_t\right)_c$ is again compared to $\left(p_t\right)_m$. This procedure of upgrading

$\tilde{\rho}_1$ according to equation (13) is continued until $(p_t)_c$ is within TOLPT of $(p_t)_m$. (Note that $\tilde{\rho}_1$ from eq. (8) was used only to obtain a relatively accurate first estimate of h_1 and is not involved in the final phase of upgrading ρ_1.)

ITEST = 2.- Since p_t and $\dot{q}_t$ are measured quantities and r_g and T_w are considered known, the h_t is determined from equation (11). This h_t and the measured p_t are used as inputs to FIND (2) to obtain the postshock stagnation conditions. The inverse iterative shock-crossing procedure is performed, where $(p_1)_m$ is the known free-stream flow quantity, to obtain the corresponding static conditions immediately behind the normal shock and the free-stream conditions.

ITEST = 3.- The measured p_1 and ρ_1 are used as inputs to FIND (1) to obtain the corresponding free-stream conditions. After the free-stream thermodynamic properties are determined and U_1 known, the postshock conditions are obtained from the direct shock-crossing procedure.

ITEST = 4.- The $\tilde{U}_1$ is determined from equation (8) and the free-stream thermodynamic properties are obtained from FIND (1) with the measured p_1 and ρ_1 as inputs. The $(p_t)_c$ is obtained from the direct shock-crossing procedure and compared to $(p_t)_m$. If not within the desired tolerance (TOLPT), the $\tilde{U}_1$ is upgraded according to

$$\tilde{U}_1 = \left(\tilde{U}_1\right)_{prev}\sqrt{\frac{(p_t)_m}{(p_t)_{c,prev}}} \tag{14}$$

This new value of $\tilde{U}_1$ is used in the direct shock-crossing solution. The U_1 is upgraded according to equation (14) until $(p_t)_c$ is within TOLPT of $(p_t)_m$.

ITEST = 5.- The procedure of ITEST = 5 is similar to that of ITEST = 2, the only difference being that ρ_1 (instead of p_1) is used as the required known free-stream flow quantity in the inverse shock-crossing solution.

ITEST = 6.- The free-stream thermodynamic quantities are obtained from FIND (1) with inputs $(p_1)_m$ and $(\rho_1)_m$. A $\tilde{U}_1$ is obtained by combining equations (7), (8), and (11) to give

$$\tilde{U}_1^{\,3} + 2\left(h_1 - h_w\right)\tilde{U}_1 = \frac{2\left(\dot{q}_t\right)_m}{\eta}\sqrt{\frac{r_g}{0.97\left(\rho_1\right)_m}} \tag{15}$$

The $\tilde{U}_1$ from equation (15) is relatively accurate, the only uncertainty being in the value of 0.97 appearing in the last term. With a value of $\tilde{U}_1$, the postshock conditions are determined as discussed in ITEST = 3. The value of 0.97 appearing in equation (15) is compared with

$$C_1 = \frac{p_t}{\rho_1 U_1^2} \tag{16}$$

If not within 0.1 percent, the value 0.97 in equation (15) is replaced by C_1 of equation (16) and the calculation procedure repeated.

ITEST = 7.- In order to estimate a value of h_1, equation (15) is rearranged to give

$$\tilde{h}_1 = h_w + \frac{(\dot{q}_t)_m}{\eta}\sqrt{\frac{r_g}{0.97(\rho_1)_m (U_1)_m^2}} - \frac{1}{2}(U_1)_m^2 \tag{17}$$

Again, the value of 0.97 appearing under the square root is the only uncertainty in this expression. The free-stream thermodynamic quantities are obtained from FIND (4) with $(\rho_1)_m$ and $\tilde{h}_1$ as inputs. The postshock conditions are determined as discussed in ITEST = 3. The value of 0.97 appearing in equation (17) is compared with C_1 of equation (16). If not within 0.1 percent, the value 0.97 in equation (17) is replaced by C_1 of equation (16) and the procedure repeated.

In many flow studies, the parameters free-stream Mach number and free-stream unit Reynolds number are of interest. These two parameters are determined in each procedure. The M_1 is obtained simply by dividing U_1 by a_1. The $N_{Re,1}$ is defined as $\rho_1 U_1/\mu_1$; hence μ_1 must be determined. The viscosity of a gas mixture of n-components may be approximated by the relation (see ref. 8)

$$\mu = \sum_{i=1}^{n} \frac{\mu_i}{1 + \sum\limits_{\substack{j=1 \\ j \neq i}} \Phi_{ij} \frac{X_j}{X_i}} \tag{18}$$

where

$$\Phi_{ij} = \frac{\left[1 + \left(\frac{\mu_i}{\mu_j}\right)^{1/2}\left(\frac{W_j}{W_i}\right)^{1/4}\right]^2}{2\sqrt{2}\left(1 + \frac{W_i}{W_j}\right)^{1/2}} \tag{19}$$

In the present study, the number of components is taken to be four. These components correspond to the initial composition of Ar, CO_2, N_2, and O_2 (that is, the W_i and W_j of eq. (19) correspond to the W_o of the four gases under consideration).

The viscosity for Ar was obtained by applying a curve fit to the results of reference 9, which includes data from a number of sources. The resulting expression is

$$\mu = 3.33 \times 10^{-7} T^{0.739} \tag{20}$$

This expression yields values of μ within 10 percent of the results illustrated in reference 9, for the temperature range of 150° K to 5000° K.

Simple expressions for the viscosity, in the form

$$\mu = \left(a_0 + a_1 T + a_2 T^2\right) \times 10^{-7} \tag{21}$$

were obtained for CO_2, N_2, and O_2 for temperature ranges of 150° K to 1000° K and 1000° K to 5000° K. The constants $\left(a_0,\ a_1, \text{ and } a_2\right)$ of equation (21) are presented in the following table, along with the source used in obtaining these constants:

Gas	ΔT	a_0	a_1	a_2	Ref.
CO_2	150 to 1000	-9.7303×10^{-1}	5.5222×10^{-1}	-1.6139×10^{-4}	10
CO_2	1000 to 5000	1.5029×10^{2}	2.4890×10^{-1}	-6.1747×10^{-6}	10, 11
N_2	150 to 1000	2.2992×10^{1}	5.5586×10^{-1}	-1.8436×10^{-4}	10, 12
N_2	1000 to 5000	1.6388×10^{2}	2.4601×10^{-1}	-7.7388×10^{-6}	10, 13
O_2	150 to 1000	1.9939×10^{1}	6.6236×10^{-1}	-2.0410×10^{-4}	10
O_2	1000 to 5000	2.3030×10^{2}	2.5597×10^{-1}	-2.2643×10^{-6}	10, 14

Viscosities for temperatures from 150° K to 5000° K were calculated for air $\left(X_{Ar} = 9.37 \times 10^{-3},\ X_{CO_2} = 3.3 \times 10^{-4},\ X_{N_2} = 7.8084 \times 10^{-1}, \text{ and } X_{O_2} = 2.0946 \times 10^{-1}\right)$ by using equation (18) and compared to values from reference 1. This comparison showed that the values of μ from equation (18) were within 3 percent of those of reference 1 for this temperature range. For mixtures where Ar or N_2 predominate, equation (18) should provide reasonably accurate values of μ for temperatures up to 5000° K. For mixtures where CO_2 or O_2 predominate, the μ of equation (18) will contain somewhat larger uncertainties at $T \gtrsim 2000°$ K because of dissociation of the CO_2 or O_2. For example, reference 11 shows that for $T \gtrsim 1700°$ K, the μ_{CO_2} has a pressure dependence because of dissociation of CO_2. However, variation in pressure from 10^2 to 10^6 N/m^2, for a given temperature, results in a maximum uncertainty in μ_{CO_2} of less than 10 percent for temperatures less than 5000° K (ref. 11). Thus, equation (18) should provide values of μ, for mixtures where CO_2 or O_2 predominate, of sufficient accuracy for many flow studies. (Eq. (18) was employed for the Mars model of ref. 11 ($X_{Ar} = 0.32$, $X_{CO_2} = 0.43$, and $X_{N_2} = 0.25$) and a temperature range of 1000° K to 5000° K. These μ from eq. (18) were within 6 percent of those presented in ref. 11 for $p = 10^5$ N/m^2 for this temperature range.)

DISCUSSION

Because of the greater simplicity associated with procedure ITEST = 3, this procedure was the first to be examined. A check case was run with air (78.084 percent N_2, 20.946 percent O_2, 0.937 percent Ar, and 0.033 percent CO_2 by volume) as the test gas. The inputs p_1, ρ_1, and U_1 were the same values as used in obtaining the sample printout of reference 1. Comparison of these results for ITEST = 3 to the sample printout case of reference 1 showed excellent agreement. The 15.24-km/sec entry trajectory cases presented in reference 1 were run with the present ITEST = 3 procedure and the preceding air model. For this trajectory, which encompassed a range of T_t from 1500° K to 12 000° K, excellent agreement was observed between the present results and those of reference 1. Following the successful check of ITEST = 3, the remaining six procedures were run with a common check case. These check cases used the same free-stream inputs as ITEST = 3, but used the calculated postshock outputs p_t and $\dot{q}_t$ of ITEST = 3 as inputs. For these check cases, TOLPT = 0.001 and TOLQT = 0.005. The computed flow quantities for all six procedures were observed to be in agreement with those of ITEST = 3.

Additional cases were run with ITEST = 3 for mixtures of 95 percent CO_2 and 5 percent N_2 (representative of Venus) and 85 percent CO_2, 1 percent N_2, and 14 percent Ar (representative of Mars). The free-stream inputs were the same as those employed in the check case for ITEST = 3 and are representative of an expansion tube test in air with heated helium driver. The results of these additional cases are presented in the sample printouts of appendix C.

In order to examine the relative total computer time (computational and peripheral) required by the various procedures, each procedure was run on a Control Data 6600 computer system. The representative expansion-tube test case for air used in the computer time study of reference 1 was also used in the present time study. The limits on temperature for FIND (I) (see appendix B) were as follows:

TMAX1 = 1500° K

TMAX2 = 8000° K

TMIN1 = 200° K

TMIN2 = 5000° K

The total computer times for each procedure were obtained for the case where all 26 species (see appendix B) were considered and for the case where the air model was simplified to 10 species $\left(e^-, Ar, N, N^+, N_2, O, O^+, O_2, NO, NO^+\right)$. The times for these two cases are given in the following table:

ITEST	Total computer time, sec	
	26-species model	10-species model
1	125	70
2	250	120
3	80	45
4	110	65
5	300	125
6	80	45
7	125	70

The reduction in computer time for the simplified air model is illustrated by this table. For the test case used in this time study, elimination of the 16 species between the two air models did not introduce significant variations (greater than 0.5 percent) in calculated free-stream and postshock conditions. (See printout of appendix C for 26-species air model and 10-species air model.) This result is not surprising since the percent by volume of CO_2 in the initial air composition for the 26-species model was relatively small (0.033 percent); hence elimination of CO_2 from the initial composition should not significantly influence the calculated flow quantities. (Elimination of CO_2 from the initial air composition corresponds to a reduction of eight species, since the C-element is eliminated.) Examination of the mole fractions at the stagnation-point conditions for the 26-species air model shows that the dependence on doubly ionized species along with O^-, Ar^+, $N_2{}^+$, $O_2{}^+$, and $O_2{}^-$ is much less than the remaining species; thus, elimination of these species should also not significantly influence the calculated flow quantities for the test case being considered. Therefore, judicious selection of species can result in a substantial reduction in computer time without appreciable loss in accuracy. (See appendix B for discussion of variation in the number of species as required in the present computer program.)

CONCLUDING REMARKS

Data reduction procedures for determining free-stream and post-normal-shock flow conditions are presented. These procedures are applicable to flows of CO_2, N_2, O_2, Ar, or mixtures of these gases and include the effects of dissociation and ionization. The assumption of thermochemical equilibrium flow is made. Although derived primarily to meet the immediate needs of the expansion tube of the Langley hot gas radiation research facility, these procedures are applicable to any supersonic or hypersonic test facility using these gases or mixtures thereof.

These procedures are based on the following flow parameters measured in the immediate vicinity of the test section:

(1) Stagnation pressure behind normal shock

(2) Free-stream static pressure

(3) Stagnation-point heat-transfer rate

(4) Free-stream velocity

(5) Free-stream density

The various combinations of measured flow parameters are identified herein as ITEST and are:

ITEST	Measured flow parameter
1	(1), (2), (4)
2	(1), (2), (3)
3	(2), (4), (5)
4	(1), (2), (5)
5	(1), (3), (5)
6	(2), (3), (5)
7	(3), (4), (5)

These seven procedures are incorporated into a single computer program written in FORTRAN IV language.

Cases run with procedure ITEST = 3 for an air mixture were observed to be in good agreement with the results of the real-air study of NASA TN D-6618 for stagnation temperatures from 1500° K to $12\ 000^\circ$ K.

A computer time study for each procedure showed that a substantial reduction in computer time, without appreciable loss in accuracy, may be realized in many cases by judicious selection of the number of species.

Langley Research Center,
National Aeronautics and Space Administration,
Hampton, Va., February 2, 1972.

APPENDIX A

LISTING OF COMPUTER PROGRAM

The data reduction procedures for determining free-stream and post-normal-shock flow conditions for CO_2, N_2, O_2, Ar, or mixtures of these gases are incorporated into a single computer program. This program is written in FORTRAN IV language for the Control Data 6600 computer system. Machine requirements are 70 000-octal locations of core storage. A listing of the main program (MILLER) and subroutines FIND (I) and ROGO, with comments, is reproduced in the following pages.

```
JOB,1,1000,070000,500.                A3238    RGK143                        1247A      CENT
USER.MILLER, CHARLES G   III               000605575N 34540
RUN(S),
SETINDF. ,
LGO.    ,
- ,
      PROGRAM MILLER(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)                   A   1
C     DATA REDUCTION PROCEDURE FOR CO2-N2-O2-AR MIXTURES                      A   2
C     THERMODYNAMIC PROPERTIES OBTAINED FROM PROGRAM OF ALLISON               A   3
C     THERMOCHEMICAL EQUILIBRIUM ASSUMED                                      A   4
C                                                                             A   5
      COMMON NUMSP,JINDX,IAR,IN2,IO2,ICO2,BOZ,XAR,XN2,XO2,XCO2                A   6
      COMMON TMAX1,TMAX2,TMIN1,TMIN2                                          A   7
      COMMON XMOLE(30),SPECIE(30)                                             A   8
      DIMENSION TABP(5), TABR(5), TABSR(5), TABT(5), TABA(5), TABZ(5), T      A   9
     1ABG(5)                                                                  A  10
      DIMENSION COEFFS(4), ROOTS(6), TEMP(14)                                 A  11
      DIMENSION VIS(4), W(4), XMF(4), PHI(4,4), SUM(4,4), SUMM(4)             A  12
      DIMENSION RESULT(2)                                                     A  13
      REAL M1,M2,MU                                                           A  14
      NAMELIST /INP/ PTM,P1M,U1M,QTM,RHO1M,RN,ITEST,TWE,PCO2,PN2,PO2,PAR      A  15
     1,PMIX,RUN,TOLPT,TMAX1,TMAX2,TMIN1,TMIN2,TOLQT,NUMSP,JINDX,IAR,IN2,      A  16
     2IO2,ICO2                                                                A  17
      BOZ=0.                                                                  A  18
      CALL DAYTIM (RESULT)                                                    A  19
1     PCO2=PN2=PO2=PAR=PTM=P1M=U1M=QTM=RHO1M=QTHOS=0.0                        A  20
      TMAX1=TMAX2=TMIN1=TMIN2=0.0
      IAR=IN2=IO2=ICO2=0
      TOLPT=.001
      TOLQT=.005
      TWE=300.
      RN=.01
      READ (5,INP)                                                            A  21
      IF (ENDFILE 5) 49,2                                                     A  22
2     PRINT 50, RESULT(1)                                                     A  23
      PRINT 51                                                                A  24
      PRINT 52                                                                A  25
      PRINT 53                                                                A  26
      XCO2=PCO2/PMIX                                                          A  27
      XN2=PN2/PMIX                                                            A  28
      XO2=PO2/PMIX                                                            A  29
      XAR=PAR/PMIX                                                            A  30
      MU=44.011*XCO2+28.016*XN2+32.*XO2+39.944*XAR                            A  31
      PRINT 54                                                                A  32
```

```
      PRINT 55, RUN,P1M,U1M,PTM,QTM,RHO1M,MU,XCO2,XN2,XO2,XAR           A  33
      P1=P1M                                                            A  34
      U1=U1M                                                            A  35
      PT=PTM                                                            A  36
      QT=QTM                                                            A  37
      RHO1=RHO1M                                                        A  38
      ZMIX=1.E+4*(7.2906*XAR+10.2109*XCO2+7.7211*XN2+6.53795*XO2)/MU    A  39
      TW=TWE                                                            A  40
      GO TO (4,4,5,4,4,3,5), ITEST                                      A  41
    3 PWR=1.                                                            A  42
      GO TO 6                                                           A  43
    4 PWR=PTM/1.01325E+5                                                A  44
      GO TO 6                                                           A  45
    5 PWR=(.97*RHO1M*U1M**2)/1.01325E+5                                 A  46
    6 CALL ROGO (PWR,RHOW,HW,SWR,TW,AW,ZW,GAMEW,MU)                     A  47
C                                                                       A  48
C     INPUTS FOR ITEST=1 ARE P1M,U1M, AND PTM                           A  49
C     INPUTS FOR ITEST=2 ARE P1M,PTM, AND QTM                           A  50
C     INPUTS FOR ITEST=3 ARE P1M,U1M, AND RHO1M                         A  51
C     INPUTS FOR ITEST=4 ARE P1M,PTM, AND RHO1M                         A  52
C     INPUTS FOR ITEST=5 ARE PTM,QTM, AND RHO1M                         A  53
C     INPUTS FOR ITEST=6 ARE P1M,RHO1M, AND QTM                         A  54
C     INPUTS FOR ITEST=7 ARE QTM,RHO1M, AND U1M                         A  55
C                                                                       A  56
      GO TO (7,8,15,24,8,15,22), ITEST                                  A  57
C                                                                       A  58
C     ESTIMATING PRE-SHOCK CONDITIONS FOR ITEST=1                       A  59
C                                                                       A  60
    7 RHOEST=PTM/(.97*U1M**2)                                           A  61
      CALL FIND (P1M,RHOEST,H1,S1R,T1,A1,Z1,GAME1,MU,1,1)               A  62
      RHO1=RHOEST                                                       A  63
      GO TO 25                                                          A  64
C                                                                       A  65
C     ESTIMATING POST-SHOCK STAGNATION CONDITIONS FOR ITEST=2 AND 5     A  66
C                                                                       A  67
C     ESTIMATING HT USING ZOBY RELATION(NASA TN D-4799)                 A  68
C                                                                       A  69
    8 HT=ZMIX*QT*SQRT(RN/PT)+HW                                         A  70
      CALL FIND (PT,RHOT,HT,STR,TT,AT,ZT,GAMET,MU,2,2)                  A  71
      GO TO 44                                                          A  72
C                                                                       A  73
C     PERFORMING STANDING NORMAL SHOCK CROSSING, POST-TO-PRE            A  74
C                                                                       A  75
    9 MM=0                                                              A  76
```

```
      MN=0
      S2R=STR
      PLOW=.84*PT
      PUP=.98*PT
      P2=(PUP-PLOW)/2.+PLOW
   10 DELP=(PUP-PLOW)/2.
      IF (MM.EQ.0.AND.MN.EQ.0) GO TO 11
      P2=PUP-DELP
   11 CALL FIND (P2,RHO2,H2,STR,T2,A2,Z2,GAME2,MU,3,2)
      U2=SQRT(2.*(HT-H2))
      M2=U2/A2
      BINV=RHO2*U2
      CINV=P2+BINV*U2
      IF (ITEST.EQ.2) GO TO 14
C
C     CASE WHEN RHO1 IS AN INPUT
C
      U1=BINV/RHO1
      P1=CINV-BINV*U1
      IF (P1.LT.1.) GO TO 13
      H1=HT-.5*U1**2
   12 CALL FIND (P1,RHO1,H1E,S1R,T1,A1,Z1,GAME1,MU,1,1)
      IF (MM.EQ.20) GO TO 46
      MM=MM+1
C
C     CONVERGENCE TEST ON H1
C
      IF (ABS(1.-H1/H1E).LE..0015) GO TO 33
      IF (H1.GT.H1E) GO TO 13
      PUP=P2
      PLOW=P2-DELP
      MN=MN+1
      GO TO 10
   13 PLOW=P2
      PUP=P2+DELP
      MN=MN+1
      GO TO 10
C
C     CASE WHEN P1 IS AN INPUT
C
   14 U1=(CINV-P1)/BINV
      RHO1=BINV/U1
      H1=HT-.5*U1**2
      GO TO 12
```

```
C
C     DETERMINING PRE-SHOCK CONDITIONS FOR ITEST=3 AND 6
C
15    CALL FIND (P1M,RHO1M,H1,S1R,T1,A1,Z1,GAME1,MU,1,1)
      IF (ITEST.EQ.3) GO TO 25
      CON6=.97
      NNN=0
      COEFFS(1)=1.
      COEFFS(2)=0.
      COEFFS(3)=2.*(H1-HW)
16    COEFFS(4)=-2.*QTM*ZMIX*SQRT(RN/(CON6*RHO1M))
      CALL FALG (COEFFS,3,0,ROOTS,TEMP,IERR)
      IF (IERR.NE.0) GO TO 21
      NNN=NNN+1
      IF (ABS(ROOTS(2)).LT.1.E-20) GO TO 17
      IF (ABS(ROOTS(4)).LT.1.E-20) GO TO 19
      IF (ABS(ROOTS(6)).LT.1.E-20) GO TO 20
      PRINT 56
      GO TO 1
17    U1=ROOTS(1)
      IF (ABS(ROOTS(4)).GT.1.E-20.AND.ABS(ROOTS(6)).GT.1.E-20) GO TO 25
18    PRINT 57
      GO TO 1
19    U1=ROOTS(3)
      IF (ABS(ROOTS(6)).GT.1.E-20) GO TO 25
      GO TO 18
20    U1=ROOTS(5)
      GO TO 25
21    PRINT 58
      GO TO 1
C
C     ESTIMATING PRE-SHOCK CONDITIONS FOR ITEST=7
C
22    CON7=.97
      MMM=0
23    H1EST=ZMIX*QTM*SQRT(RN/(CON7*RHO1M*U1M**2))+HW-.5*U1M**2
      H1=H1EST
      CALL FIND (P1,RHO1M,H1,S1R,T1,A1,Z1,GAME1,MU,4,1)
      MMM=MMM+1
      GO TO 25
C
C     DETERMINING PRE-SHOCK CONDITIONS FOR ITEST=4
C
24    CALL FIND (P1M,RHO1M,H1,S1R,T1,A1,Z1,GAME1,MU,1,1)
```

```
      U1=SQRT(PT/(.97*RHO1))                                            A 165
C                                                                       A 166
C     PERFORMING STANDING NORMAL SHOCK CROSSING, PRE-TO-POST            A 167
C                                                                       A 168
25    BSNS=RHO1*U1                                                      A 169
      CSNS=P1+BSNS*U1                                                   A 170
      DSNS=H1+.5*U1**2                                                  A 171
      HT=DSNS                                                           A 172
      PTEST=.965*RHO1*U1**2                                             A 173
      CALL FIND (PTEST,RHOT,HT,STR,TT,AT,ZT,GAMET,MU,2,2)               A 174
      RHO2=.955*RHOT                                                    A 175
26    U2=BSNS/RHO2                                                      A 176
      P2=CSNS-BSNS*U2                                                   A 177
      H2=DSNS-.5*U2**2                                                  A 178
      CALL FIND (P2,RNEW,H2,S2R,T2,A2,Z2,GAME2,MU,2,2)                  A 179
      IF (ABS(1.-RHO2/RNEW).LE..001) GO TO 27                           A 180
      RHO2=RNEW                                                         A 181
      GO TO 26                                                          A 182
27    RHO2=RNEW                                                         A 183
      M2=U2/A2                                                          A 184
      PTCAL=P2*(1.+((GAME2-1.)/2.)*M2**2)**(GAME2/(GAME2-1.))           A 185
      CALL FIND (PTCAL,RHOT,HT,STR,TT,AT,ZT,GAMET,MU,2,2)               A 186
      IF (ABS(1.-S2R/STR).LE..0005) GO TO 31                            A 187
      TABP(1)=PTCAL                                                     A 188
      TABR(1)=RHOT                                                      A 189
      TABSR(1)=STR                                                      A 190
      TABT(1)=TT                                                        A 191
      TABA(1)=AT                                                        A 192
      TABZ(1)=ZT                                                        A 193
      TABG(1)=GAMET                                                     A 194
      IF (STR.LT.S2R) GO TO 28                                          A 195
      CON=.01                                                           A 196
      N=-2                                                              A 197
      GO TO 29                                                          A 198
28    CON=-.01                                                          A 199
      N=2                                                               A 200
29    YX=1.+CON                                                         A 201
      DO 30 I=2,5                                                       A 202
      TABP(I)=XX*PTCAL                                                  A 203
      PTIN=TABP(I)                                                      A 204
      CALL FIND (PTIN,RHOT,HT,STR,TT,AT,ZT,GAMET,MU,2,2)                A 205
      TABR(I)=RHOT                                                      A 206
      TABSR(I)=STR                                                      A 207
      TABT(I)=TT                                                        A 208
```

```
      TABA(I)=AT                                                        A 209
      TABZ(I)=ZT                                                        A 210
      TABG(I)=GAMET                                                     A 211
      XX=XX+CON                                                         A 212
   30 CONTINUE                                                          A 213
      CALL FTLUP (S2R,PTCAL,N,5,TABSR,TABP)                             A 214
      CALL FTLUP (S2R,RHOT,N,5,TABSR,TABR)                              A 215
      CALL FTLUP (S2R,TT,N,5,TABSR,TABT)                                A 216
      CALL FTLUP (S2R,AT,N,5,TABSR,TABA)                                A 217
      CALL FTLUP (S2R,ZT,N,5,TABSR,TABZ)                                A 218
      CALL FTLUP (S2R,GAMET,N,5,TABSR,TABG)                             A 219
      STR=S2R                                                           A 220
C                                                                       A 221
   31 PT=PTCAL                                                          A 222
      IF (ITEST.EQ.3.OR.ITEST.EQ.6) GO TO 33                            A 223
      IF (ITEST.EQ.7) GO TO 33                                          A 224
      IF (ABS(1.-PTM/PT).LE.TOLPT) GO TO 33                             A 225
      IF (ITEST.EQ.4) GO TO 32                                          A 226
      RHO1=RHO1*PTM/PT                                                  A 227
      CALL FIND (P1M,RHO1,H1,S1R,T1,A1,Z1,GAME1,MU,1,1)                 A 228
      GO TO 25                                                          A 229
   32 U1=U1*SQRT(PTM/PT)                                                A 230
      GO TO 25                                                          A 231
   33 M1=U1/A1                                                          A 232
      QTZO=SQRT(PT/RN)*(HT-HW)/ZMIX                                     A 233
      IF (ITEST.NE.6.OR.ITEST.NE.7) GO TO 36                            A 234
      IF (ITEST.EQ.6) GO TO 34                                          A 235
      CON77=PT/(RHO1*U1**2)                                             A 236
      IF (ABS(1.-CON7/CON77).LE..001) GO TO 35                          A 237
      CON7=CON77                                                        A 238
      IF (MMM.EQ.3) GO TO 47                                            A 239
      GO TO 23                                                          A 240
   34 CON66=PT/(RHO1*U1**2)                                             A 241
      IF (ABS(1.-CON6/CON66).LE..001) GO TO 35                          A 242
      CON6=CON66                                                        A 243
      IF (NNN.EQ.3) GO TO 47                                            A 244
      GO TO 16                                                          A 245
   35 IF (ABS(1.-QTZO/QTM).GE.TOLQT) GO TO 48                           A 246
C                                                                       A 247
C        CALCULATING FREE-STREAM REYNOLDS NUMBER                        A 248
C                                                                       A 249
   36 VIS(1)=3.33E-7*T1**.739                                           A 250
      IF (T1.GT.950.) GO TO 37                                          A 251
      VIS(2)=(-.973034+.5522198*T1-1.613866E-4*T1**2)*1.E-7             A 252
```

```
      VIS(3)=(22.99167+.5558644*T1-1.84356E-4*T1**2)*1.E-7              A 253
      VIS(4)=(19.93933+.6623589*T1-2.04096E-4*T1**2)*1.E-7              A 254
      GO TO 38                                                          A 255
   37 VIS(2)=(150.2874+.248903*T1-6.174675E-6*T1**2)*1.E-7              A 256
      VIS(3)=(163.8798+.2460075*T1-7.738745E-6*T1**2)*1.E-7             A 257
      VIS(4)=(230.3+.2559657*T1-2.264286E-6*T1**2)*1.E-7                A 258
   38 W(1)=39.944                                                       A 259
      W(2)=44.011                                                       A 260
      W(3)=28.016                                                       A 261
      W(4)=32.                                                          A 262
      XMF(1)=XAR                                                        A 263
      XMF(2)=XCO2                                                       A 264
      XMF(3)=XN2                                                        A 265
      XMF(4)=XO2                                                        A 266
      DO 40 I=1,4                                                       A 267
      DO 40 J=1,4                                                       A 268
      PHI(I,J)=(((1.+SQRT(VIS(I)/VIS(J))*(W(J)/W(I))**.25)**2)/(2.8284*S A 269
     1QRT(1.+W(I)/W(J))))                                               A 270
      IF (XMF(I).EQ.0.) GO TO 39                                        A 272
      SUM(I,J)=PHI(I,J)*XMF(J)/XMF(I)                                   A 273
      GO TO 40                                                          A 274
   39 SUM(I,J)=0.                                                       A 275
   40 CONTINUE                                                          A 276
      DO 41 I=1,4                                                       A 277
      SUMM(I)=SUM(I,1)+SUM(I,2)+SUM(I,3)+SUM(I,4)                       A 278
      IF (SUMM(I).NE.0.) GO TO 41                                       A 279
      SUMM(I)=1.                                                        A 280
      VIS(I)=0.                                                         A 281
   41 CONTINUE                                                          A 282
      VISMIX=(VIS(1)/SUMM(1))+(VIS(2)/SUMM(2))+(VIS(3)/SUMM(3))+(VIS(4)/ A 283
     1SUMM(4))                                                          A 284
      RE1=RHO1*U1/VISMIX                                                A 285
C                                                                       A 286
C        CALCULATING QT FROM-HOSHIZAKI, SCALA, MARVIN(NASA TR R-224)    A 287
C                                                                       A 288
      IF (XCO2.LT..9) GO TO 42                                          A 289
      BO=(1./RN)*SQRT(2.*(PT-P1)/RHOT)                                  A 290
      QTHOS=5.9647E-5*SQRT(BO*RHO1)*(U1**2.69)*(1.-HW/HT)               A 291
   42 IF (XAR.GT..05) GO TO 43                                          A 292
      QTSCAL=8.4681E-6*SQRT(PT/RN)*(HT-HW)*(12.+.866*MU)                A 293
   43 QTAVCO=3.2675E+5*(1.1+.075*MU)*SQRT(P1/RN)*(U1/3.048E+3)**(3.909-. A 294
     10229*MU)*(P1/PT)**.535                                            A 295
      CON1=XAR*118.6+XCO2*90.4+XN2*78.8+XO2*115.5                       A 296
      CON2=XAR*2.11+XCO2*2.04+XN2*2.03+XO2*1.838                        A 297
```

```
      QTMARV=19.569640*CON1*SQRT(PT/RN)*(1.-HW/HT)*(U1/3.048E+3)**CON2        A 298
      PRINT 59                                                                A 299
      PRINT 60                                                                A 300
      PRINT 55, P1,RHO1,T1,H1,S1R,Z1,GAME1,A1,U1,M1,RE1                       A 301
      PRINT 62                                                                A 302
      PRINT 63                                                                A 303
      PRINT 55, P2,RHO2,T2,H2,S2R,Z2,GAME2,A2,U2,M2                           A 304
      PRINT 64                                                                A 305
      PRINT 65                                                                A 306
      PRINT 55, PT,RHOT,TT,HT,STR,ZT,GAMET,AT,QTZO,HW,RN                      A 307
      IF (ITEST.EQ.2.OR.ITEST.EQ.5) GO TO 1                                   A 308
   44 PRINT 67                                                                A 309
      PRINT 68                                                                A 310
      DO 45 I=1,NUMSP                                                         A 311
      PRINT 69, SPECIE(I),XMOLE(I)                                            A 312
   45 CONTINUE                                                                A 313
      IF (ITEST.EQ.2.OR.ITEST.EQ.5) GO TO 9                                   A 314
      GO TO 1                                                                 A 315
   46 PRINT 71                                                                A 318
      GO TO 1                                                                 A 319
   47 PRINT 72                                                                A 320
      PRINT 73                                                                A 321
      GO TO 36                                                                A 322
   48 PRINT 74                                                                A 323
      GO TO 1                                                                 A 324
   49 STOP                                                                    A 325
C                                                                             A 326
   50 FORMAT (1H1,A10//)                                                      A 327
   51 FORMAT (46H  GAS MIXTURE DATA REDUCTION PROGRAM OF MILLER)              A 328
   52 FORMAT (51H  ALL PHYSICAL QUANTITIES IN MKS UNITS-NASA SP-7012)         A 329
   53 FORMAT (//17H  MEASURED INPUTS)                                         A 330
   54 FORMAT (/107H    RUN          P1          U1          PT          QT    A 331
     1 RHO1        WO          XCO2        XN2         XO2         XAR)       A 332
   55 FORMAT (11E10.3)                                                        A 333
   56 FORMAT (//38H ALL 3 ROOTS COMPLEX FOR U1 IN ITEST=6)                    A 334
   57 FORMAT (//40H MORE THAN 1 REAL ROOT FOR U1 IN ITEST=6)                  A 335
   58 FORMAT (//26H ERROR IN FALG FOR ITEST=6)                                A 336
   59 FORMAT (//24H  FREE-STREAM CONDITIONS)                                  A 337
   60 FORMAT (/107H    P           RHO         T           H           S/R   A 338
     1  Z          GAME        A           U           M           NRE)       A 339
   62 FORMAT (//39H  STATIC CONDITIONS BEHIND NORMAL SHOCK)                   A 341
   63 FORMAT (/96H     P           RHO         T           H           S/R   A 342
     1 Z          GAME        A           U           M)                      A 343
   64 FORMAT (//43H  STAGNATION CONDITIONS BEHIND NORMAL SHOCK)               A 344
```

```
65    FORMAT (/106H      P          RHO          T          H          S/R         A 345
     1 Z          GAME          A          QTZO          HW          RN)           A 346
67    FORMAT (//40H MOLE FRACTIONS AT STAGNATION CONDITIONS)                        A 348
68    FORMAT (/29H  SPECIE          MOLE FRACTION/)                                 A 349
69    FORMAT (A10,E16.4)                                                            A 350
71    FORMAT (///46H ITERATIONS ON P2 EXCEED LIMIT IN ITEST=2 OR 5)                 A 352
72    FORMAT (//46H MAJOR ITERATION FOR ITEST=6 OR 7 EXCEED LIMIT)                  A 353
73    FORMAT (//29H VALUES BELOW MAY BE IN ERROR)                                   A 354
74    FORMAT (//37H QTZO NOT WITHIN TOLQT OF QTM-TROUBLE)                           A 355
      END                                                                           A 356-
      SUBROUTINE FIND (P,RHO,H,SR,T,AM,ZM,GAME,MU,K,L)                              B   1
C                                                                                   B   2
C     FIND OBTAINS THERMODYNAMIC PROPERTIES FROM SUBROUTINE ROGO WITH-              B   3
C             (1) PRESSURE AND DENSITY (K=1)                                        B   4
C             (2) PRESSURE AND ENTHALPY (K=2)                                       B   5
C             (3) PRESSURE AND ENTROPY (K=3)                                        B   6
C             (4) DENSITY AND ENTHALPY (K=4)                                        B   7
C                                                                                   B   8
C                                                                                   B   9
C     UPPER LIMIT ON T AS REQUIRED IN ITERATION DENOTED BY L                        B  10
C          L=1 DENOTES TUP=TMAX1 FOR FREESTREAM CONDITIONS                          B  11
C          L=2 DENOTES TUP=TMAX2 FOR STATIC CONDITIONS BEHIND SHOCK                 B  12
C                                                                                   B  13
C     IF TMAX1=0, THEN TUP=8000 DEG K                                               B  14
C     IF TMAX2=0, THEN TUP=16,000 DEG K                                             B  15
C                                                                                   B  16
      DIMENSION TABT(3), TAPR(3), TABH(3), TABSR(3), TABAM(3), TABZM(3),            B  17
     1 TABG(3), TABXM(3,30), TABXMO(80), TABFIT(30)                                 B  18
      DIMENSION TABPM(3), TABHM(3), TABSRM(3), TABTM(3), TABAMM(3), TABZ            B  19
     1MM(3), TABGM(3)                                                               B  20
      COMMON NUMSP,JINDX,IAR,IN2,IO2,ICO2,BOZ,XAR,XN2,XO2,XCO2                      B  21
      COMMON TMAX1,TMAX2,TMIN1,TMIN2                                                B  22
      COMMON XMOLE(30),SPECIE(30)                                                   B  23
      REAL MU                                                                       B  24
      NN=0                                                                          B  25
      IF (K.NE.4) GO TO 10                                                          B  26
      II=0                                                                          B  27
      MN=0                                                                          B  28
      PLOW=.01*RHO*ABS(H)                                                           B  29
      PPP=PLOW                                                                      B  30
      PUP=.51*RHO*ABS(H)                                                            B  31
      P=(PUP-PLOW)/2.+PLOW                                                          B  32
1     DELP=(PUP-PLOW)/2.                                                            B  33
      IF (MN.EQ.0) GO TO 2                                                          B  34
```

```
      P=PUP-DELP
 2    PN=P/1.01325E+5
      TLOW=0.
      IF (L.EQ.1) GO TO 3
      TUP=1.6E+4
      GO TO 4
 3    TUP=8.E+3
 4    MN=MN+1
      NN=0
      GO TO 16
 5    IF (ABS(1.-H/HK).LE..001) GO TO 41
      IF (HK.LT.H) GO TO 6
      PUP=P
      PLOW=P-DELP
      IF (DELP.GT.PPP) GO TO 1
      TABPM(1)=PUP
      TABPM(3)=PLOW
      NNN=-2
      GO TO 7
 6    PLOW=P
      PUP=P+DELP
      IF (DELP.GT.PPP) GO TO 1
      TABPM(1)=PLOW
      TABPM(3)=PUP
      NNN=2
 7    TABHM(1)=HK
      TABSRM(1)=SR
      TABTM(1)=T
      TABAMM(1)=AM
      TABZMM(1)=ZM
      TABGM(1)=GAME
      DELP=(TABPM(3)-TABPM(1))/2.
      TABPM(2)=TABPM(1)+DELP
      DO 9 JK=2,3
      P=TABPM(JK)
      II=1
      GO TO 2
 8    TABHM(JK)=HK
      TABSRM(JK)=SR
      TABTM(JK)=T
      TABAMM(JK)=AM
      TABZMM(JK)=ZM
      TABGM(JK)=GAME
 9    CONTINUE
```

```
      CALL FTLUP (H,SR,NNN,3,TABHM,TABSRM)
      CALL FTLUP (H,AM,NNN,3,TABHM,TABAMM)
      CALL FTLUP (H,ZM,NNN,3,TABHM,TABZMM)
      CALL FTLUP (H,T,NNN,3,TABHM,TABTM)
      CALL FTLUP (H,P,NNN,3,TABHM,TABPM)
      CALL FTLUP (H,GAME,NNN,3,TABHM,TABGM)
      GO TO 41
   10 PN=P/1.01325E+5
      IF (L.EQ.2) GO TO 12
      IF (TMAX1.EQ.0.) GO TO 11
      TUP=TMAX1
      GO TO 14
   11 TUP=8.E+3
      GO TO 14
   12 IF (TMAX2.EQ.0.) GO TO 13
      TUP=TMAX2
      GO TO 14
   13 TUP=1.6E+4
   14 IF (L.EQ.2) GO TO 15
      TLOW=TMIN1
      GO TO 16
   15 TLOW=TMIN2
   16 T=(TUP-TLOW)/2.+TLOW
   17 DELT=(TUP-TLOW)/2.
      IF (NN.EQ.0) GO TO 18
      T=TUP-DELT
   18 CALL ROGO (PN,RHOA,HA,SAR,T,AM,ZM,GAME,MU)
      NN=NN+1
      IF (K.EQ.2) GO TO 23
      IF (K.EQ.3) GO TO 24
C
C     CONVERGENCE TEST FOR K=1
C
      IF (ABS(1.-RHO/RHOA).LE..001) GO TO 36
      IF (RHO.LT.RHOA) GO TO 21
   19 TUP=T
      TLOW=T-DELT
      IF (DELT.GT.250.) GO TO 17
      TABT(1)=TUP
      TABT(3)=TLOW
      IF (K.EQ.1.OR.K.EQ.4) GO TO 20
      N=-2
      GO TO 25
   20 N=2
```

```
      GO TO 25
   21 TLOW=T
      TUP=T+DELT
      IF (DELT.GT.250.) GO TO 17
      TABT(1)=TLOW
      TABT(3)=TUP
      IF (K.EQ.1.OR.K.EQ.4) GO TO 22
      N=2
      GO TO 25
   22 N=-2
      GO TO 25
C
C     CONVERGENCE TEST FOR K=2
C
   23 IF (ABS(1.-H/HA).LE..001) GO TO 37
      IF (HA.LT.H) GO TO 21
      GO TO 19
C
C     CONVERGENCE TEST FOR K=3
C
   24 IF (ABS(1.-SR/SAR).LE..001) GO TO 38
      IF (SAR.LT.SR) GO TO 21
      GO TO 19
C
C     INTERPOLATION FOR DELT LESS THAN 250 DEG K
C
   25 TABR(1)=RHOA
      TABH(1)=HA
      TABSR(1)=SAR
      TABAM(1)=AM
      TABZM(1)=ZM
      TABG(1)=GAME
      DO 26 J=1,NUMSP
      TABXM(1,J)=XMOLE(J)
   26 CONTINUE
      DELT=(TABT(3)-TABT(1))/2.
      TABT(2)=TABT(1)+DELT
      DO 28 I=2,3
      T=TABT(I)
      CALL ROGO (PN,RHOA,HA,SAR,T,AM,ZM,GAME,MU)
      DO 27 J=1,NUMSP
      TABXM(I,J)=XMOLE(J)
   27 CONTINUE
      TABR(I)=RHOA
```

```
      TABH(I)=HA                                                        B 167
      TABSR(I)=SAR                                                      B 168
      TABAM(I)=AM                                                       B 169
      TABZM(I)=ZM                                                       B 170
      TABG(I)=GAME                                                      B 171
   28 CONTINUE                                                          B 172
      IJK=0                                                             B 173
      DO 29 I=1,3                                                       B 174
      DO 29 J=1,NUMSP                                                   B 175
      IJK=IJK+1                                                         B 176
      TABXMO(IJK)=TABXM(I,J)                                            B 177
   29 CONTINUE                                                          B 178
      DO 30 J=1,NUMSP                                                   B 179
      TABFIT(J)=J                                                       B 180
   30 CONTINUE                                                          B 181
      IY=3*NUMSP                                                        B 182
      IF (K.EQ.2) GO TO 32                                              B 183
      IF (K.EQ.3) GO TO 34                                              B 184
      CALL FTLUP (RHO,T,N,3,TABR,TABT)                                  B 185
      CALL FTLUP (RHO,HK,N,3,TABR,TABH)                                 B 186
      CALL FTLUP (RHO,SR,N,3,TABR,TABSR)                                B 187
      CALL FTLUP (RHO,AM,N,3,TABR,TABAM)                                B 188
      CALL FTLUP (RHO,ZM,N,3,TABR,TABZM)                                B 189
      CALL FTLUP (RHO,GAME,N,3,TABR,TABG)                               B 190
      DO 31 JJ=1,NUMSP                                                  B 191
      FIT=JJ                                                            B 192
      CALL DISCOT (FIT,RHO,TABFIT,TABXMO,TABR,02,IY,3,XMOLE(JJ))        B 193
   31 CONTINUE                                                          B 194
      IF (K.EQ.1) GO TO 40                                              B 195
      IF (II.EQ.1) GO TO 8                                              B 196
      GO TO 5                                                           B 197
   32 CALL FTLUP (H,T,N,3,TABH,TABT)                                    B 198
      CALL FTLUP (H,RHO,N,3,TABH,TABR)                                  B 199
      CALL FTLUP (H,SR,N,3,TABH,TABSR)                                  B 200
      CALL FTLUP (H,AM,N,3,TABH,TABAM)                                  B 201
      CALL FTLUP (H,ZM,N,3,TABH,TABZM)                                  B 202
      CALL FTLUP (H,GAME,N,3,TABH,TABG)                                 B 203
      DO 33 JJ=1,NUMSP                                                  B 204
      FIT=JJ                                                            B 205
      CALL DISCOT (FIT,H,TABFIT,TABXMO,TABH,02,IY,3,XMOLE(JJ))          B 206
   33 CONTINUE                                                          B 207
      GO TO 41                                                          B 208
   34 CALL FTLUP (SR,RHO,N,3,TABSR,TABR)                                B 209
      CALL FTLUP (SR,H,N,3,TABSR,TABH)                                  B 210
```

```
      CALL FTLUP (SR,T,N,3,TABSR,TABT)                                  B 211
      CALL FTLUP (SR,AM,N,3,TABSR,TABAM)                                B 212
      CALL FTLUP (SR,ZM,N,3,TABSR,TABZM)                                B 213
      CALL FTLUP (SR,GAME,N,3,TABSR,TABG)                               B 214
      DO 35 JJ=1,NUMSP                                                  B 215
      FIT=JJ                                                            B 216
      CALL DISCOT (FIT,SR,TABFIT,TABXMO,TABSR,02,IY,3,XMOLE(JJ))        B 217
   35 CONTINUE                                                          B 218
      GO TO 41                                                          B 219
   36 IF (K.EQ.4) GO TO 39                                              B 220
      H=HA                                                              B 221
      SR=SAR                                                            B 222
      GO TO 41                                                          B 223
   37 RHO=RHOA                                                          B 224
      SR=SAR                                                            B 225
      GO TO 41                                                          B 226
   38 H=HA                                                              B 227
      RHO=RHOA                                                          B 228
      GO TO 41                                                          B 229
   39 HK=HA                                                             B 230
      SR=SAR                                                            B 231
      GO TO 5                                                           B 232
   40 H=HK                                                              B 233
   41 RETURN                                                            B 234
      END                                                               B 235-
      SUBROUTINE ROGO (PN,RHOAN,HA,SOR,T,AM,XZ,GAMMAE,MU)               C   1
C                                                                       C   2
C     PROGRAM OF ALLISON(NASA TN D-3538) AND NEWMAN(NASA TN D-3540)     C   3
C     COMPUTES THERMOCHEMICAL EQUILIBRIUM PROPERTIES OF GAS MIXTURES    C   4
C     REQUIRES INPUTS OF P AND T                                        C   5
C                                                                       C   6
      COMMON NUMSP,JINDX,IAR,IN2,IO2,ICO2,BOZ,XAR,XN2,XO2,XCO2          C   7
      COMMON TMAX1,TMAX2,TMIN1,TMIN2                                    C   8
      COMMON XMOLE(30),SPECIE(30)                                       C   9
      REAL NO,M,LAMB,LAMBDA,MU,NE,NEGFRT,LOGNE,MASSFR,LMIN              C  10
      REAL INTENE,LGEORT,LGRORE                                         C  11
      INTEGER F(30),V(30,10)                                            C  12
      DIMENSION LB(30), M(30), DELHF(30), BETA(30), NDEBUG(30), IPIVOT(1C  13
     10), R(10,10), SUMAY(10,1), G(30,30), E(30,30), BE(30,10), ALPHAE(3C  14
     20,10), OMEGA(30,10), OMEGAX(30,10), XOMEG(30,4), XOMEGX(30,4), Z(3C  15
     30), SIGMA(10), U(10), DELTA(10), GAMMA(10), XX(10), Q(30), Y(30), C  16
     4X(30), A(30,9), HORT(30), FORT(30), NEGFRT(30), PI(9,2), XPRIME(30C  17
     5), MASSFR(30), CAPX(50), YINT(30,5), CSUBP(30), PSI(30,2), CON(10,C  18
     62), DXDT(30), RR(10,10), O(10,10)                                 C  19
```

```
      DIMENSION HEPG(30), DMSFRDT(30)                                   C  20
      H=6.62517E-27                                                     C  21
      XK=1.38044E-16                                                    C  22
      PREF=1.013250E+6                                                  C  23
      NO=6.02322E+23                                                    C  24
      C=2.99793E+10                                                     C  25
      IF (BOZ.EQ.1.) GO TO 3                                            C  26
      BOZ=1.                                                            C  27
      EA=1.E-12                                                         C  28
      ER=1.E-1                                                          C  29
      DO 2 I=1,NUMSP                                                    C  30
      READ (5,74) SPECIE(I),LB(I),F(I),NDEBUG(I),M(I),DELHF(I),BETA(I)  C  31
      IL=LB(I)                                                          C  32
C     IF NDEBUG EQUALS 0, DEBUG                                         C  33
      READ (5,75) (G(I,L),F(I,L),L=1,IL)                                C  34
      IF (F(I).EQ.0) GO TO 2                                            C  35
      IF (F(I).EQ.2) GO TO 1                                            C  36
      READ (5,76) (BE(I,L),ALPHAE(I,L),OMEGA(I,L),OMEGAX(I,L),V(I,L),L=1 C  37
     1,IL)                                                              C  38
      GO TO 2                                                           C  39
    1 READ (5,75) BE(I,1),ALPHAE(I,1)                                   C  40
      READ (5,75) (XOMEG(I,LW),XOMEGX(I,LW),LW=1,4)                     C  41
    2 CONTINUE                                                          C  42
      READ (5,77) ((A(I,J),J=1,JINDX),I=1,NUMSP)                        C  43
    3 DO 4 I=1,NUMSP                                                    C  44
    4 YINT(I,1)=1.E-20                                                  C  45
      YINT(IO2,1)=1.E-5                                                 C  46
      IF (XAR.EQ.0.) GO TO 5                                            C  47
      YINT(IAR,1)=XAR/MU                                                C  48
    5 IF (XN2.EQ.0.) GO TO 6                                            C  49
      YINT(IN2,1)=XN2/MU                                                C  50
    6 IF (XO2.EQ.0.) GO TO 7                                            C  51
      YINT(IO2,1)=XO2/MU                                                C  52
    7 IF (XCO2.EQ.0.) GO TO 8                                           C  53
      YINT(ICO2,1)=XCO2/MU                                              C  54
    8 RHOO=PREF*MU/(NO*XK*273.15)                                       C  55
      DO 9 I=1,NUMSP                                                    C  56
    9 IF (YINT(I,1).EQ.0.) YINT(I,1)=1.E-20                             C  57
      AO=SQRT(1.4*(PREF/RHOO))                                          C  58
      NUMT=NCAPX=1                                                      C  59
      LEEBOB=INDEP=0                                                    C  60
      IF (INDEP.NE.0) GO TO 11                                          C  61
      DO 10 KP=1,NCAPX                                                  C  62
   10 CAPX(KP)=ALOG10(PN)                                               C  63
```

```
 11    DO 73 KI=1,NUMT                                                    C  64
       IF (LEEBOB.EQ.1) PUNCH 81, T                                       C  65
       NY=1                                                               C  66
       PART=H*C/(XK*T)                                                    C  67
       DO 19 I=1,NUMSP                                                    C  68
       IL=LR(I)                                                           C  69
       IF (F(I).EQ.1) GO TO 13                                            C  70
       IF (F(I).EQ.2) GO TO 16                                            C  71
       QSUM=0.                                                            C  72
       FPQSUM=0.                                                          C  73
       SPQSUM=0.                                                          C  74
       DO 12 L=1,IL                                                       C  75
       Z(L)=PART*E(I,L)                                                   C  76
       GEZ=G(I,L)*EXP(-Z(L))                                              C  77
       QSUM=QSUM+GEZ                                                      C  78
       FPQSUM=FPQSUM+GEZ*Z(L)                                             C  79
 12    SPQSUM=SPQSUM+(Z(L)-2.)*GEZ*Z(L)                                   C  80
       FPQSUM=FPQSUM/T                                                    C  81
       SPQSUM=SPQSUM/T**2                                                 C  82
       QI=(M(I)*T*.32807618)**1.5*QSUM*.13623883*T                        C  83
       GO TO 18                                                           C  84
 13    QSUM=0.                                                            C  85
       FPQSUM=0.                                                          C  86
       SPQSUM=0.                                                          C  87
       DO 15 L=1,IL                                                       C  88
       Z(L)=PART*E(I,L)                                                   C  89
       SIGMA(L)=PART*(BE(I,L)-.5*ALPHAE(I,L))                             C  90
       U(L)=PART*(OMEGA(I,L)-2.*OMEGAX(I,L))                              C  91
       DELTA(L)=ALPHAE(I,L)*1./(BE(I,L)-.5*ALPHAE(I,L))                   C  92
       GAMMA(L)=(BE(I,L)/OMEGA(I,L))**2*1./(1.-.5*ALPHAE(I,L)/BE(I,L))    C  93
       XX(L)=OMEGAX(I,L)/(OMEGA(I,L)-2.*OMEGAX(I,L))                      C  94
       THREF=0.                                                           C  95
       FOUR=0.                                                            C  96
       FIVE=0.                                                            C  97
       NV=V(I,L)+1                                                        C  98
       DO 14 IV=1,NV                                                      C  99
       W=IV-1                                                             C 100
       CC=(1.-W*DELTA(L))                                                 C 101
       AA=SIGMA(L)*CC                                                     C 102
       BB=U(L)*(W-XX(L)*W*(W-1.))                                         C 103
       ONE1=1./AA+8.*GAMMA(L)/(AA**2*CC)+.33333333+AA/12.                 C 104
       TWO2=1./AA+16.*GAMMA(L)/(AA**2*CC)-AA/12.-384.*GAMMA(L)**2/(AA**3* C 105
      1CC**2)                                                             C 106
       THREE=THREE+ONE1*EXP(-BB)                                          C 107
```

```
      FOUR=FOUR+(BB*ONE1+TWO2)*EXP(-BB)                                 C 108
   14 FIVE=FIVE+((BB**2*ONE1+2.*BB*TWO2+GAMMA(L)/(AA**2*CC)*(48.-3456.*G C 109
     1AMMA(L)/(AA*CC)+46080.*GAMMA(L)**2/(AA**2*CC**2))+2./AA)*EXP(-BB)) C 110
      GEZ=G(I,L)*EXP(-Z(L))                                             C 111
      Q(L)=THREE/BETA(I)*GEZ                                            C 112
      QSUM=QSUM+Q(L)                                                    C 113
      FPQSUM=FPQSUM+(FOUR+THREE*Z(L))*GEZ                               C 114
   15 SPQSUM=SPQSUM+(Z(L)*(Z(L)-2.)*THREE+2.*(Z(L)-1.)*FOUR+FIVE)*GEZ   C 115
      FPQSUM=FPQSUM/(T*BETA(I))                                         C 116
      SPQSUM=SPQSUM/(T**2*BETA(I))                                      C 117
      QI=(M(I)*T*.32807618)**1.5*QSUM*.13623883*T                       C 118
      GO TO 18                                                          C 119
   16 SIGMA(1)=PART*(BE(I,1)-.5*ALPHAE(I,1))                            C 120
      PROD=1.                                                           C 121
      SUM1=0.                                                           C 122
      SUM2=0.                                                           C 123
      DO 17 LW=1,4                                                      C 124
      U(LW)=PART*(XOMEG(I,LW)-XOMEGX(I,LW))                             C 125
      PROD=PROD*(1.-EXP(-U(LW)))                                        C 126
      BTM=EXP(U(LW))-1.                                                 C 127
      SUM1=SUM1+U(LW)/BTM                                               C 128
   17 SUM2=SUM2+U(LW)**2*EXP(U(LW))/BTM**2                              C 129
      QSUM=G(I,1)/(BETA(I)*SIGMA(1)*PROD)                               C 130
      FPQSUM=(1.+SUM1)*QSUM/T                                           C 131
      SPQSUM=(SUM1**2+SUM2)*QSUM/T**2                                   C 132
      QI=(M(I)*T*.32807618)**1.5*QSUM*.13623883*T                       C 133
   18 HORT(I)=2.5+T/QSUM*FPQSUM+DELHF(I)/(NO*XK*T)                      C 134
      HEPG(I)=HORT(I)*NO*XK*T/M(I)                                      C 135
      FORT(I)=DELHF(I)/(NO*XK*T)-ALOG(QI)                               C 136
      NEGFRT(I)=-FORT(I)                                                C 137
   19 CSUBP(I)=2.5+2.*T/QSUM*FPQSUM-(T*FPQSUM/QSUM)**2+T**2*SPQSUM/QSUM C 138
      IF (LEEBOB.EQ.1) PUNCH 81, (CSUBP(I),HORT(I),I=1,NUMSP)           C 139
      NNN=1                                                             C 140
      DO 72 KP=1,NCAPX                                                  C 141
      IF (INDEP.EQ.2) SAVERHO=CAPX(KP)                                  C 142
      P=(10.**CAPX(KP))*PREF                                            C 143
      POPO=P/PREF                                                       C 144
      DO 20 I=1,NUMSP                                                   C 145
   20 Y(I)=YINT(I,NY)                                                   C 146
      NUMIT=0                                                           C 147
      NUMITF=0                                                          C 148
      MM=JINDX+1                                                        C 149
      DO 22 J=1,JINDX                                                   C 150
      O(J,MM)=0.                                                        C 151
```

```
      DO 21 I=1,NUMSP                                               C 152
   21 O(J,MM)=O(J,MM)+A(I,J)*Y(I)                                   C 153
      O(MM,J)=O(J,MM)                                               C 154
   22 CONTINUE                                                      C 155
      O(MM,MM)=0.                                                   C 156
   23 CONTINUE                                                      C 157
      YBAR=Y(1)                                                     C 158
      NUMIT=NUMIT+1                                                 C 159
      IF (NUMIT.EQ.201) GO TO 59                                    C 160
      DO 24 I=2,NUMSP                                               C 161
   24 YBAR=YBAR+Y(I)                                                C 162
      IF (INDEP.EQ.2) P=NO*XK*T*YBAR*CAPX(KP)                       C 163
      DO 26 K=1,JINDX                                               C 164
      R(1,K)=0.                                                     C 165
      DO 25 I=1,NUMSP                                               C 166
   25 R(1,K)=R(1,K)+A(I,1)*A(I,K)*Y(I)                              C 167
   26 CONTINUE                                                      C 168
      ICOUNT=1                                                      C 169
      JJ=2                                                          C 170
      DO 30 J=JJ,JINDX                                              C 171
      DO 28 K=J,JINDX                                               C 172
      R(J,K)=0.                                                     C 173
      DO 27 I=1,NUMSP                                               C 174
   27 R(J,K)=R(J,K)+A(I,J)*A(I,K)*Y(I)                              C 175
   28 CONTINUE                                                      C 176
      DO 29 K=1,ICOUNT                                              C 177
   29 R(J,K)=R(K,J)                                                 C 178
      ICOUNT=ICOUNT+1                                               C 179
   30 JJ=1+ICOUNT                                                   C 180
      DO 31 J=1,MM                                                  C 181
      R(J,MM)=O(J,MM)                                               C 182
   31 R(MM,J)=O(J,MM)                                               C 183
      DO 32 J=1,MM                                                  C 184
      DO 32 K=1,MM                                                  C 185
   32 RR(J,K)=R(J,K)                                                C 186
      PYBAR=PREF*YBAR                                               C 187
      DO 34 J=1,JINDX                                               C 188
      SUMAY(J,1)=0.                                                 C 189
      DO 33 I=1,NUMSP                                               C 190
      THIS=P*Y(I)/PYBAR                                             C 191
      IF (THIS.LE.0.) GO TO 33                                      C 192
      SUMAY(J,1)=SUMAY(J,1)+A(I,J)*Y(I)*(FORT(I)+ALOG(THIS))        C 193
   33 CONTINUE                                                      C 194
   34 CONTINUE                                                      C 195
```

```
      SUMAY(MM,1)=0.                                              C 196
      DO 35 I=1,NUMSP                                             C 197
      THIS=P*Y(I)/PYBAR                                           C 198
      IF (THIS.LE.0.) GO TO 35                                    C 199
      SUMAY(MM,1)=SUMAY(MM,1)+Y(I)*(FORT(I)+ALOG(THIS))           C 200
   35 CONTINUE                                                    C 201
      MN=1                                                        C 202
      NMAX=10                                                     C 203
      CALL SIMEQ (R,MM,SUMAY,MN,DETERM,IPIVOT,NMAX,ISCALE)        C 204
      DO 36 J=1,JINDX                                             C 205
   36 PI(J,1)=SUMAY(J,1)                                          C 206
      U=SUMAY(MM,1)                                               C 207
      LMIN=1.                                                     C 208
      LCOUNT=0                                                    C 209
      DO 43 I=1,NUMSP                                             C 210
      API=0.                                                      C 211
      DO 37 J=1,JINDX                                             C 212
   37 API=API+A(I,J)*PI(J,1)                                      C 213
      THIS=P*Y(I)/PYBAR                                           C 214
      IF (THIS.LE.0.) GO TO 38                                    C 215
      X(I)=Y(I)*(NEGFRT(I)-ALOG(THIS)+U+1.+API)                   C 216
      GO TO 39                                                    C 217
   38 X(I)=0.                                                     C 218
   39 IF (X(I)) 40,42,43                                          C 219
   40 LAMB=-Y(I)/(X(I)-Y(I))                                      C 220
      IF (LAMB.GT.0.) GO TO 41                                    C 221
      Y(I)=0.                                                     C 222
      GO TO 23                                                    C 223
   41 LCOUNT=1                                                    C 224
      LMIN=AMIN1(LMIN,LAMB)                                       C 225.
      GO TO 43                                                    C 226
   42 IF (Y(I).EQ.0.) GO TO 43                                    C 227
      LCOUNT=1                                                    C 228
      LAMB=1.                                                     C 229
      LMIN=AMIN1(LMIN,LAMB)                                       C 230
   43 CONTINUE                                                    C 233
      IF (LCOUNT.EQ.0) GO TO 45                                   C 234
      LAMBDA=.999999999999*LMIN                                   C 235
      DO 44 I=1,NUMSP                                             C 236
      Y(I)=(1.-LAMBDA)*Y(I)+LAMBDA*X(I)                           C 237
   44 IF (Y(I).LT.1.E-100) Y(I)=0.                                C 238
      GO TO 23                                                    C 239
   45 DO 46 I=1,NUMSP                                             C 240
      IF (Y(I).EQ.0.) GO TO 46                                    C 241
```

```
      IF (ABS(X(I)-Y(I))/Y(I).GE.ER.OR.ABS(X(I)-Y(I)).GE.EA) GO TO 47      C 242
46    CONTINUE                                                              C 243
      GO TO 54                                                              C 244
47    XBAR=0.                                                               C 245
      LAMBDA=1.                                                             C 246
      LASTCT=0                                                              C 247
48    DO 49 I=1,NUMSP                                                       C 248
      XPRIME(I)=(1.-LAMBDA)*Y(I)+LAMBDA*X(I)                                C 249
49    XBAR=XBAR+XPRIME(I)                                                   C 250
      DFLAMB=0.                                                             C 251
      DO 50 I=1,NUMSP                                                       C 252
      THIS=P*XPRIME(I)/(PREF*XBAR)                                          C 253
      IF (THIS.LE.1.E-38) GO TO 50                                          C 254
      DFLAMB=DFLAMB+(X(I)-Y(I))*(FORT(I)+ALOG(THIS))                        C 255
50    CONTINUE                                                              C 256
      IF (DFLAMB.GT.0.) GO TO 53                                            C 257
51    DO 52 I=1,NUMSP                                                       C 258
52    Y(I)=XPRIME(I)                                                        C 259
      GO TO 23                                                              C 260
53    LASTCT=LASTCT+1                                                       C 261
      IF (LASTCT.EQ.4) GO TO 51                                             C 262
      LAMBDA=.9*LAMBDA                                                      C 263
      XBAR=0.                                                               C 264
      GO TO 48                                                              C 265
54    IF (NUMITF.EQ.1) GO TO 56                                             C 266
      NUMITO=0                                                              C 267
      IF (INDEP.NE.2) GO TO 56                                              C 268
      NUMITF=1                                                              C 269
      NUMITO=NUMIT                                                          C 270
      INDEP=1                                                               C 271
      DO 55 I=1,NUMSP                                                       C 272
55    Y(I)=X(I)                                                             C 273
      GO TO 23                                                              C 274
56    XBAR=0.                                                               C 275
      ONE=0.                                                                C 276
      TWO=0.                                                                C 277
      DO 57 I=1,NUMSP                                                       C 278
      XBAR=XBAR+X(I)                                                        C 279
      ONE=ONE+X(I)*HORT(I)                                                  C 280
      MASSFR(I)=X(I)*M(I)                                                   C 281
      IF (Y(I).EQ.0.) GO TO 57                                              C 282
      TWO=TWO+X(I)*(FORT(I)+ALOG(X(I)))                                     C 283
57    CONTINUE                                                              C 284
      RECIPZ=1./(MU*XBAR)                                                   C 285
```

```
      IF (NUMITF.EQ.1) CAPX(KP)=ALOG10(P/PREF)                         C 286
      IF (NUMITF.EQ.1) INDFP=2                                         C 287
      CAPU=CAPX(KP)+ALOG10(RECIPZ*273.15/T)                            C 288
      CHORT=MU*ONE                                                     C 289
      SOR=CHORT-MU*(XBAR*ALOG(P/(PREF*XBAR))+TWO)                      C 290
      RHO=P/(XBAR*NO*XK*T)                                             C 291
      NE=X(1)*RHO*NO                                                   C 292
      IF (X(1).GT.10.**-20) GO TO 58                                   C 293
      LOGNE=-0.                                                        C 294
      GO TO 60                                                         C 295
   58 LOGNE=ALOG10(NE)                                                 C 296
      GO TO 60                                                         C 297
   59 WRITE (6,78) P                                                   C 298
      GO TO 72                                                         C 299
   60 CONTINUE                                                         C 300
      DO 62 I=1,NUMSP                                                  C 301
      TEST=X(I)*P/(XBAR*PREF)                                          C 302
      IF (TEST.LT.10.**(-20)) GO TO 61                                 C 303
      PSI(I,1)=X(I)/T*(HORT(I)-FORT(I)-ALOG(TEST))                     C 304
      PSI(I,2)=-X(I)                                                   C 305
      GO TO 62                                                         C 306
   61 PSI(I,1)=0.                                                      C 307
      PSI(I,2)=0.                                                      C 308
   62 CONTINUE                                                         C 309
      DO 64 J=1,JINDX                                                  C 310
      CON(J,1)=A(1,J)*PSI(1,1)                                         C 311
      CON(J,2)=A(1,J)*PSI(1,2)                                         C 312
      DO 63 I=2,NUMSP                                                  C 313
      CON(J,1)=CON(J,1)+A(I,J)*PSI(I,1)                                C 314
   63 CON(J,2)=CON(J,2)+A(I,J)*PSI(I,2)                                C 315
   64 CONTINUE                                                         C 316
      CON(MM,1)=PSI(1,1)                                               C 317
      CON(MM,2)=PSI(1,2)                                               C 318
      DO 65 I=2,NUMSP                                                  C 319
      CON(MM,1)=CON(MM,1)+PSI(I,1)                                     C 320
   65 CON(MM,2)=CON(MM,2)+PSI(I,2)                                     C 321
      NC=2                                                             C 322
      CALL SIMEQ (RR,MM,CON,NC,DETERM,IPIVOT,NMAX,ISCALE)              C 323
      DO 66 J=1,MM                                                     C 324
      PI(J,1)=CON(J,1)                                                 C 325
   66 PI(J,2)=CON(J,2)                                                 C 326
      DHDT=0.                                                          C 327
      DO 68 I=1,NUMSP                                                  C 328
      SUMAP=A(I,1)*PI(1,1)                                             C 329
```

```
      DO 67 J=2,JINDX
   67 SUMAP=SUMAP+A(I,J)*PI(J,1)
      DXDT(I)=PSI(I,1)-X(I)*(PI(MM,1)+SUMAP)
      DMSFRDT(I)=M(I)*DXDT(I)
   68 DHDT=DHDT+(X(I)*CSUBP(I)+T*HORT(I)*DXDT(I))
      DRHODT=T*PI(MM,1)-1.
      DRHODP=1.+PI(MM,2)
      CPOR=MU*DHDT
      XZ=XBAR*MU
      CVOR=CPOR-DRHODT**2/DRHODP*XZ
      XGAMMA=CPOR/CVOR
      GAMMAE=XGAMMA/DRHODP
      RHOR=1./(10.**CAPU)
      HPGRAM=CHORT*NO*XK*T/MU
      TEST=(GAMMAE/1.4*P/PREF*RHOR)
      IF (TEST.LE.0.) WRITE (6,80) CAPX(KP),CAPU,XZ,CHORT,SOR,LOGNE,DRHO
     1DT,DRHODP,CPOR,CVOR,XGAMMA,GAMMAE,AOAO
      AOAO=SQRT(TEST)
      AM=AOAO*AO*.01
      RHOAN=(10.**CAPU)*RHOO*1.E+3
      HA=CHORT*8.31469E+3*T/MU
      INTENE=((CHORT-XZ)*NO*XK*T+3.93146E+12)/MU
      GAMBAR=(INTENE+(P/RHO))/INTENE
      EORTO=INTENE*28.9672/(NO*XK*273.15)
      LGEORT=ALOG10(EORTO)
      RORHOE=RHO/1.29233666E-3
      LGRORE=ALOG10(RORHOE)
      DO 69 I=1,NUMSP
   69 XMOLE(I)=MASSFR(I)*MU/(XZ*M(I))
      IF (NNN.EQ.10) GO TO 70
      GO TO 71
   70 WRITE (6,79)
      NNN=0
   71 NNN=NNN+1
      IF (INDEP.EQ.2) CAPX(KP)=SAVERHO
      IF (LEEBOB.EQ.0) GO TO 72
      IF (KP.EQ.1) PUNCH 82, NCAPX
      PUNCH 81, POPO,CPOR
      PUNCH 83, (XMOLE(I),I=1,NUMSP)
   72 CONTINUE
   73 CONTINUE
      RETURN
C
   74 FORMAT (A6,3I5,3E14.8)
```

```
 75   FORMAT (5E14.8)
 76   FORMAT (4E14.8,I5)
 77   FORMAT (15E5.0)
 78   FORMAT (1X,2HP=E15.8,2X,28H200 ITERATIONS-NONCONVERGENT)
 79   FORMAT (/)
 80   FORMAT (/F9.4,F10.4,F9.4,F11.4,F10.4,F9.3,F10.3,F10.3,F10.3,F10.3,
     1F8.3,F8.3,F9.3)
 81   FORMAT (2E16.8)
 82   FORMAT (I5)
 83   FORMAT (5E16.8)
      END
```

APPENDIX B

COMPUTER PROGRAM INPUTS

The inputs necessary to utilize the included computer program are presented in the following table:

Program (FORTRAN) symbol	Description
ITEST	Data reduction procedure to be used
RUN	Facility test number
TØLPT	Convergence criteria for iteration involving p_t
TØLQT	Convergence criteria for iteration involving $\dot{q}_t$
TWE	T_w
RN	r_g
PCØ2	Measured partial pressure of CO_2
PN2	Measured partial pressure of N_2
PØ2	Measured partial pressure of O_2
PAR	Measured partial pressure of Ar
PMIX	Measured pressure of mixture
P1M	$(p_1)_m$
PTM	$(p_t)_m$
QTM	$(\dot{q}_t)_m$
RHØ1M	$(\rho_1)_m$
U1M	$(U_1)_m$
TMAX1	Maximum T_1 expected
TMAX2	Maximum T_t expected
TMIN1	Minimum T_1 expected
TMIN2	Minimum T_2 expected
NUMSP	Number of species considered
JINDX	Number of components considered
IAR	Position in species array of Ar
IN2	Position in species array of N_2
IØ2	Position in species array of O_2
ICØ2	Position in species array of CO_2

The FORTRAN NAMELIST capability is used for the input data with INP as the NAMELIST name. A sample listing of the input cards for the 26-species air test case (ITEST = 3) is as follows:

```
$INP  ITEST=3,RUN=1,P1M=1040,U1M=6100,RHO1M=.00485,RN=.0127,PMIX=1,
 PCO2=.00033,PN2=.78084,PO2=.20946,PAR=.00937,NUMSP=26,JINDX=5,IAR=2,
 IN2=8,IO2=14,ICO2=26$
```

The units for the inputs which are physical quantities are given in the section entitled "SYMBOLS." In using a specific ITEST, only those three measured inputs (combinations of P1M, U1M, RHØ1M, PTM, and QTM) associated with this ITEST need be included. (The required measured inputs corresponding to a specific ITEST are given in the section entitled "Procedures for Determining Free-Stream and Postshock Conditions.") It should be noted that the condition

$$PMIX = PAR + PN2 + PØ2 + PCØ2$$

must be satisfied. If Ar, N_2, O_2, or CO_2 is not included in the test gas, then the partial pressure (PAR, PN2, PØ2, and PCØ2, respectively) need not be included as input. The IAR, IN2, IØ2, and ICØ2 need be included as input only if Ar, N_2, O_2, or CO_2, respectively, is included in the species deck. (The computer cards containing the thermodynamic data for the various species are denoted as the species deck and are discussed subsequently.) The following table presents assigned values given to input quantities when these quantities are omitted from INP:

Input quantity omitted (program symbol)	Assigned value
TØLPT	0.001
TØLQT	0.005
TWE	300
RN	0.01
TMAX1	8 000
TMAX2	16 000
TMIN1	0
TMIN2	0

The 26 species and five components considered are as follows:

Species:

e^-	O	C
Ar	O^+	C^+
Ar^+	O^{++}	C^{++}
Ar^{++}	O^-	C^-
N	O_2	CO
N^+	O_2^+	CO^+
N^{++}	O_2^-	CN
N_2	NO	CO_2
N_2^+	NO^+	

Components:

e^-

Ar

N

O

C

The thermodynamic data for these species, which are tabulated in reference 2, are read into the computer program from cards. A listing of these cards for all 26 species is as follows:

```
 E-     1     0      0    54847000-03    00000000+00    00000000+00
20000000+01    00000000+00
 A     30     0      0    39944000+02    00000000+00    00000000+00
10000000+01    00000000+00    50000000+01    93144000+05    30000000+01
93751000+05    10000000+01    94554000+05    30000000+01    95400000+05
30000000+01    10410200+06    12000000+02    10550000+06    80000000+01
10615000+06    10000000+01    10705400+06    80000000+01    10722000+06
40000000+01    10800000+06    40000000+01    11128000+06    16000000+02
11175000+06    80000000+01    11290000+06    20000000+02    11355000+06
16000000+02    11475000+06    80000000+01    11500000+06    30000000+01
11666000+06    12000000+02    11696000+06    80000000+01    11717000+06
10000000+01    11756300+06    16000000+02    11853000+06    36000000+02
11930000+06    56000000+02    12025000+06    20000000+02    12070000+06
32000000+02    12175000+06    36000000+02    12220000+06    56000000+02
12270000+06    20000000+02    12350000+06    28000000+02    12413600+06
 A+    30     0      0    39943000+02    15202350+14    00000000+00
60000000+01    00000000+00    20000000+01    10872300+06    20000000+02
13240000+06    12000000+02    13480000+06    60000000+01    13860000+06
28000000+02    14270000+06    60000000+01    14520000+06    12000000+02
14765000+06    10000000+02    14875000+06    10000000+02    15000000+06
12000000+02    15516000+06    30000000+02    15830000+06    12000000+02
16100000+06    20000000+01    16730900+06    14000000+02    17060000+06
26000000+02    17300000+06    38000000+02    17480000+06    60000000+01
17970000+06    40000000+02    18300000+06    60000000+02    18600000+06
62000000+02    19020000+06    34000000+02    19220000+06    12000000+03
19400000+06    84000000+02    19600000+06    48000000+02    20000000+06
18000000+02    20500000+06    60000000+01    20859300+06    22000000+03
21000000+06    50000000+02    21500000+06    70000000+02    22000000+06
A++    30     0      0    39943000+02    41851700+14    00000000+00
50000000+01    00000000+00    30000000+01    11120000+04    10000000+01
15700000+04    50000000+01    14010000+05    10000000+01    33267000+05
90000000+01    11440000+06    10000000+02    12800000+06    28000000+02
14465000+06    15000000+02    15695000+06    50000000+01    17437500+06
15000000+02    18200000+06    75000000+02    18950000+06    15000000+02
19660000+06    50000000+01    20000000+06    18000000+02    20470000+06
21000000+02    20830000+06    27000000+02    21080000+06    33000000+02
21450000+06    46000000+02    22450000+06    90000000+01    23150000+06
50000000+01    23500000+06    26000000+02    24000000+06    50000000+02
24603600+06    91000000+02    25100000+06    24000000+02    25800000+06
12700000+03    27000000+06    12100000+03    27850000+06    11600000+03
28200000+06    11100000+03    28600000+06    52400000+03    30200000+06
 N     30     0      0    14008000+02    47072900+13    00000000+00
40000000+01    00000000+00    10000000+02    19225000+05    60000000+01
28840000+05    12000000+02    83330000+05    60000000+01    86180000+05
```

```
 12000000+02   88140000+05   20000000+01   93582000+05   20000000+02
 94800000+05   12000000+02   95500000+05   40000000+01   96752000+05
 10000000+02   96810000+05   60000000+01   97800000+05   10000000+02
 99660000+05   18000000+02   10400000+06   34000000+02   10470000+06
 56000000+02   10500000+06   22000000+02   10660000+06   16000000+02
 10720000+06   16000000+02   10760000+06   54000000+02   10960000+06
 12000000+02   10986000+06   10600000+03   11035000+06   13200000+03
 11160000+06   13600000+03   11220000+06   60000000+01   11231000+06
 68000000+02   11282000+06   30000000+02   11291000+06   20000000+01
 11360000+06   10000000+02   11390000+06   14000000+02   11700000+06
  N+     30     0     0    14007000+02    18726070+14    00000000+00
 90000000+01   00000000+00   50000000+01   15316000+05   10000000+01
 32687000+05   50000000+01   47168000+05   15000000+02   92245000+05
 90000000+01   10922000+06   50000000+01   14418900+06   12000000+02
 14900000+06   30000000+01   15513000+06   30000000+01   16461200+06
 18000000+02   16665000+06   30000000+01   16889300+06   90000000+01
 17062000+06   50000000+01   17421200+06   10000000+01   17827400+06
 41000000+02   18709000+06   16000000+02   18910000+06   30000000+01
 19012100+06   12000000+02   19720000+06   30000000+02   20300000+06
 21000000+02   20570000+06   15300000+03   21050000+06   12000000+02
 21482800+06   12000000+02   21800000+06   54600000+03   22050000+06
 37000000+02   22300000+06   15000000+02   22600000+06   15000000+02
 22800000+06   14000000+02   23030000+06   50000000+01   23425000+06
 N++     30     0     0    14007000+02    47288300+14    00000000+00
 60000000+01   00000000+00   12000000+02   57280000+05   10000000+02
 10102600+06   20000000+01   13104400+06   60000000+01   14592000+06
 40000000+01   18680200+06   10000000+02   20307800+06   20000000+01
 22130200+06   60000000+01   23040700+06   60000000+01   24569000+06
 10000000+02   26724200+06   12000000+02   28765000+06   60000000+01
 29721000+06   20000000+01   30108800+06   32000000+02   31050000+06
 40000000+01   31422400+06   22000000+02   31755000+06   14000000+02
 32028800+06   10000000+02   32104000+06   30000000+02   32900000+06
 22000000+02   33330000+06   22000000+02   33629000+06   20000000+02
 33955000+06   48000000+02   34300000+06   24000000+02   34800000+06
 32000000+02   36400000+06   12000000+02   36862000+06   22000000+02
 37400000+06   52000000+02   37900000+06   20000000+01   38070000+06
  N2      6     1     0    28016000+02    00000000+00    20000000+01
 10000000+01   00000000+00   30000000+01   49757000+05   60000000+01
 59314000+05   20000000+01   68953000+05   10000000+01   70700000+05
 60000000+01   87984000+05
 19980000+01   17000000-01   23580700+04   14190000+02   33
 14400000+01   13000000-01   14603700+04   13890000+02   26
 16380000+01   18400000-01   17341100+04   14470000+02   29
 16182000+01   18300000-01   16937000+04   13830000+02   30
```

```
14800000+01   16400000-01   15300000+04   12000000+02   31
18258000+01   19700000-01   20351000+04   17080000+02   29
N2+    4    1    0    28015000+02   15033360+14   20000000+01
20000000+01   00000000+00   40000000+01   90200000+04   20000000+01
25570000+05   20000000+01   64550000+05
19322000+01   20200000-01   22072300+04   16220000+02   32
17220000+01   18000000-01   19028400+04   14910000+02   31
20830000+01   19500000-01   24198400+04   23190000+02   25
16500000+01   50000000-01   20500000+04   14920000+02   30
 O    28    0    0    16000000+02   24674100+13   00000000+00
50000000+01   00000000+00   30000000+01   15900000+03   10000000+01
22700000+03   50000000+01   15868000+05   10000000+01   33792000+05
50000000+01   73768000+05   30000000+01   76795000+05   15000000+02
86630000+05   90000000+01   88630000+05   50000000+01   95476000+05
30000000+01   96226000+05   36000000+02   97420000+05   15000000+02
97488000+05   15000000+02   99094000+05   90000000+01   99680000+05
90000000+01   10000000+06   15000000+02   10114000+06   50000000+01
10211600+06   30000000+01   10241200+06   50000000+01   10266200+06
25000000+02   10286500+06   15000000+02   10290800+06   90000000+01
10386900+06   15000000+02   10400000+06   25000000+02   10538500+06
15000000+02   10540800+06   56000000+02   10600000+06   56000000+02
10700000+06
 O+   30    0    0    15999000+02   15603890+14   00000000+00
40000000+01   00000000+00   10000000+02   26820000+05   60000000+01
40465000+05   12000000+02   12000000+06   10000000+02   16599000+06
12000000+02   18540000+06   60000000+01   18900000+06   20000000+01
19571000+06   20000000+01   20394200+06   42000000+02   20760000+06
26000000+02   21280000+06   20000000+01   22685100+06   24000000+02
23000000+06   80000000+02   23270000+06   16000000+02   23390000+06
18000000+02   23960000+06   40000000+02   24550000+06   20000000+02
24800000+06   60000000+01   25030000+06   32000000+02   25190000+06
44000000+02   25400000+06   84000000+02   25550000+06   11600000+03
25600000+06   18000000+02   25810000+06   10000000+02   25930000+06
72000000+02   26150000+06   16600000+03   26550000+06   13400000+03
27000000+06   14200000+03   27650000+06   24000000+02   28300000+06
O++   30    0    0    15999000+02   49479960+14   00000000+00
90000000+01   00000000+00   50000000+01   20271000+05   10000000+01
43184000+05   50000000+01   60312000+05   15000000+02   12005000+06
90000000+01   14238300+06   50000000+01   18704900+06   30000000+01
19708700+06   30000000+01   21045900+06   12000000+02   27000000+06
90000000+01   28390000+06   26000000+02   29400000+06   14000000+02
30300000+06   10000000+01   31380100+06   50000000+02   32700000+06
10000000+02   33200000+06   15000000+02   33870000+06   10000000+01
34330300+06   90000000+01   35020000+06   12000000+02   35750000+06
```

```
46000000+02   36500000+06   48000000+02   37050000+06   15800000+03
38000000+06   62000000+02   39400000+06   90000000+02   39800000+06
55800000+03   40340000+06   72000000+02   42500000+06   31100000+03
43000000+06   48000000+02   43800000+06   15000000+02   44271000+06
 0-    1    0    0   16001000+02   10541000+13   00000000+00
60000000+01   00000000+00
 02    6    1    0   32000000+02   00000000+00   20000000+01
30000000+01   00000000+00   20000000+01   78824000+04   10000000+01
13120900+05   30000000+01   35713000+05   10000000+01   36212700+05
30000000+01   49363100+05
14457000+01   15800000-01   15803600+04   12070000+02   26
14264000+01   17100000-01   15093000+04   12900000+02   29
14004000+01   18200000-01   14326900+04   13950000+02   25
10500000+01   35700000-01   81900000+03   22500000+02    8
82600000+00   20500000-01   65040000+03   17030000+02    9
81900000+00   11000000-01   70036000+03   80000000+01   21
02+    4    1    0   31999000+02   11628080+14   20000000+01
40000000+01   00000000+00   80000000+01   31500000+05   40000000+01
38300000+05   40000000+01   48100000+05
16722000+01   19800000-01   18764000+04   16530000+02   28
11047000+01   15800000-01   10356900+04   10390000+02   24
10617000+01   19100000-01   90000000+03   13400000+02   16
12873000+01   22100000-01   11967700+04   17090000+02   17
02-    3    1    0   32001000+02  -96232000+12   20000000+01
40000000+01   00000000+00   40000000+01   13400000+05   40000000+01
24200000+05
12000000+01   16000000-01   13000000+04   14000000+02   29
97000000+00   17000000-01   99000000+03   15000000+02   16
92000000+00   27000000-01   56000000+03   13000000+02   10
 NO    8    1    0   30008000+02   89860000+12   10000000+01
20000000+01   00000000+00   20000000+01   12090000+03   20000000+01
44200000+05   40000000+01   45440000+05   20000000+01   53290000+05
40000000+01   52376000+05   20000000+01   60860000+05   40000000+01
60020000+05
17046000+01   17800000-01   19040300+04   13970000+02   27
17046000+01   17800000-01   19036800+04   13970000+02   33
19972000+01   19300000-01   23748000+04   16460000+02   35
11260000+01   15200000-01   10376800+04   76030000+01   33
20026000+01   21800000-01   23239000+04   22885000+02   25
20020000+01   30000000-01   23950000+04   15000000+02   39
19863000+01   18200000-01   23736000+04   15850000+02   37
13300000+01   19000000-01   12166000+04   15880000+02   18
NO+    5    1    0   30007000+02   98240300+13   10000000+01
10000000+01   00000000+00   60000000+01   39982000+05   30000000+01
```

```
58523000+05   60000000+01   72384000+05   20000000+01   73083800+05
20020000+01   20200000-01   23771000+04   16350000+02   36
16800000+01   19000000-01   17400000+04   14500000+02   29
13300000+01   16000000-01   12200000+04   95000000+01   31
12600000+01   17000000-01   11400000+04   76000000+01   37
15870000+01   24000000-01   16089000+04   23300000+02   17
 C    30    0    0    12011000+02    71123800+13    00000000+00
90000000+01   00000000+00   50000000+01   10194000+05   10000000+01
21648000+05   50000000+01   33735000+05   90000000+01   60360000+05
30000000+01   61982000+05   15000000+02   64090000+05   30000000+01
68858000+05   15000000+02   69700000+05   30000000+01   70744000+05
90000000+01   71365000+05   50000000+01   72611000+05   10000000+01
73976000+05   90000000+01   75256000+05   50000000+01   77681000+05
90000000+01   78130000+05   21000000+02   78230000+05   18000000+02
78320000+05   10000000+02   78600000+05   90000000+01   79318000+05
18000000+02   80400000+05   12000000+02   81200000+05   50000000+01
81770000+05   10000000+01   82252000+05   53000000+02   83800000+05
10300000+03   84000000+05   30000000+02   84940000+05   60000000+01
85400000+05   50300000+03   86400000+05   19000000+02   86500000+05
 C+   30    0    0    12010000+02    17971820+14    00000000+00
60000000+01   00000000+00   12000000+02   43030000+05   10000000+02
74931000+05   20000000+01   96494000+05   60000000+01   10180000+06
60000000+01   11065000+06   20000000+01   11490000+06   20000000+01
11653800+06   14000000+02   11940000+06   60000000+01   13173100+06
12000000+02   13580000+06   20000000+02   13600000+06   40000000+01
14202400+06   10000000+02   14555100+06   10000000+02   15046500+06
20000000+01   15723400+06   60000000+01   16252200+06   12000000+02
16700000+06   10000000+02   16812400+06   20000000+02   16890000+06
20000000+01   17334800+06   60000000+01   17529300+06   16000000+02
17835000+06   32000000+02   17900000+06   26000000+02   18200000+06
40000000+01   18468900+06   12000000+02   18645000+06   10000000+02
18860000+06   30000000+02   19550000+06   20000000+02   19657200+06
C++   30    0    0    12010000+02    41492250+14    00000000+00
10000000+01   00000000+00   90000000+01   52360000+05   30000000+01
10235100+06   90000000+01   13742000+06   50000000+01   14587500+06
10000000+01   18252000+06   30000000+01   23816100+06   10000000+01
24717000+06   30000000+01   25893100+06   90000000+01   25966200+06
15000000+02   26996000+06   50000000+01   27684300+06   15000000+02
30910000+06   10000000+01   31172100+06   12000000+02   31870000+06
61000000+02   32255000+06   50000000+01   32421200+06   12000000+02
32800000+06   31000000+02   33300000+06   15000000+02   33762600+06
13000000+02   34000000+06   70000000+01   34136800+06   30000000+01
34325600+06   30000000+02   34500000+06   60000000+02   34660000+06
70000000+01   34800000+06   12000000+02   37660000+06   18000000+02
```

```
38150000+06    13000000+02    38434500+06    34000000+02    38600000+06
 C-     1     0     0    12012000+02    58994400+13    00000000+00
60000000+01    00000000+00
 CO     7     1     0    28011000+02   -11381300+13    10000000+01
10000000+01    00000000+00    60000000+01    48473900+05    30000000+01
55380000+05    60000000+01    61784600+05    20000000+01    64746500+05
30000000+01    83831000+05    10000000+01    86917800+05
19313000+01    17480000-01    21702100+04    13461000+02    41
16810000+01    19300000-01    17392500+04    14470000+02    29
13310000+01    16000000-01    12180000+04    95000000+01    31
12615000+01    17000000-01    11377900+04    76240000+01    37
16116000+01    22290000-01    15156100+04    17250500+02    21
20750000+01    33000000-01    21980000+04    13476000+02    40
19610000+01    27000000-01    20820700+04    12092000+02    42
 CO+    3     1     0    28010000+02    12383670+14    10000000+01
20000000+01    00000000+00    40000000+01    20407500+05    20000000+01
45633500+05
19772000+01    18960000-01    22142400+04    15164000+02    30
15894000+01    19420000-01    15620600+04    13530000+02    28
17999000+01    30250000-01    17341800+04    27927000+02    15
 CN     3     1     0    26019000+02    45605600+13    10000000+01
20000000+01    00000000+00    40000000+01    91145900+04    20000000+01
25797850+05
18996000+01    17350000-01    20687050+04    13144000+02    29
17165000+01    17460000-01    18144300+04    12883000+02    34
19701000+01    22150000-01    21641300+04    20250000+02    26
 CO2    1     2     0    44011000+02   -39314600+13    20000000+01
10000000+01    00000000+00
39060000+00    22000000-02
66733000+03    00000000+00    66733000+03    00000000+00    13428600+04
00000000+00    23493000+04    00000000+00
```

Cases may arise in which the user of this program may be interested in a gas or gas mixture involving fewer than 26 species. If so, only the species cards for the species being considered need be included. The number of species (NUMSP) and number of components (JINDX) are basic inputs and must be adjusted accordingly. The inputs IAR, IN2, IØ2, and ICØ2, which designate the position of Ar, N_2, O_2, and CO_2, respectively, in the species array, must also be adjusted to provide meaningful initial estimates for the species concentrations as required by ROGO. Finally, the number of atoms of a particular component per particle of a species A(I,J) must be designated. For electrons, a charge constraint is used instead of a mass constraint.

The modifications required when the number of species is varied is best illustrated by example. First, consider a CO_2-N_2-O_2-Ar mixture in which double ionization is included (that is, all 26 species are included). A suggested aid to this case is first to construct a table of A(I,J) as follows:

	Component (J) / Species (I)	1 e^-	2 Ar	3 N	4 O	5 C
1	e^-	1	0	0	0	0
2	Ar	0	1	0	0	0
3	Ar^+	-1	1	0	0	0
4	Ar^{++}	-2	1	0	0	0
5	N	0	0	1	0	0
6	N^+	-1	0	1	0	0
7	N^{++}	-2	0	1	0	0
8	N_2	0	0	2	0	0
9	N_2^+	-1	0	2	0	0
10	O	0	0	0	1	0
11	O^+	-1	0	0	1	0
12	O^{++}	-2	0	0	1	0
13	O^-	1	0	0	1	0
14	O_2	0	0	0	2	0
15	O_2^+	-1	0	0	2	0
16	O_2^-	1	0	0	2	0
17	NO	0	0	1	1	0
18	NO^+	-1	0	1	1	0
19	C	0	0	0	0	1
20	C^+	-1	0	0	0	1
21	C^{++}	-2	0	0	0	1
22	C^-	1	0	0	0	1
23	CO	0	0	0	1	1
24	CO^+	-1	0	0	1	1
25	CN	0	0	1	0	1
26	CO_2	0	0	0	2	1

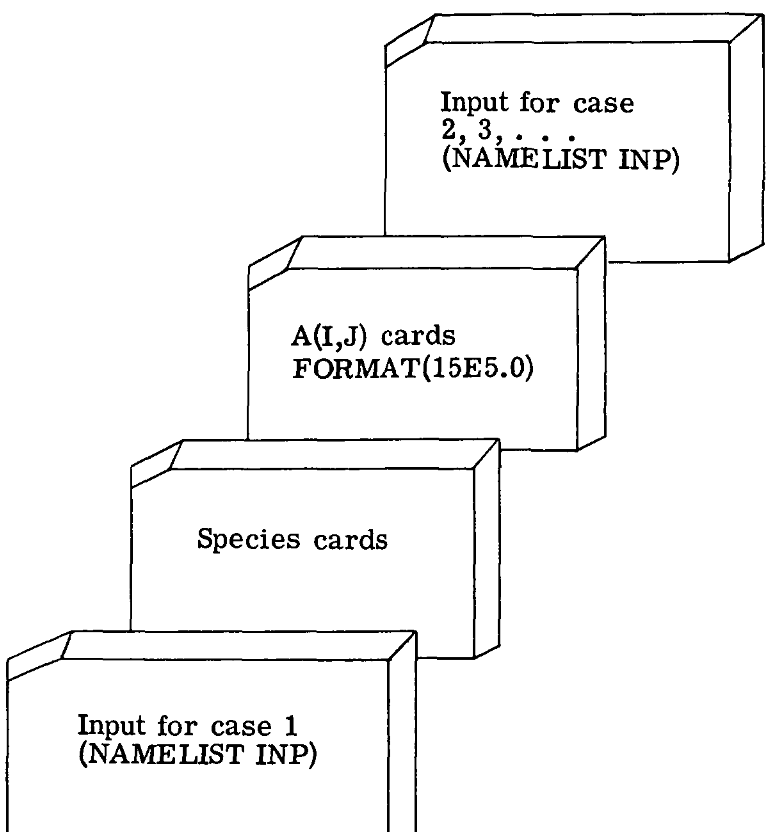
The sequence 0, 1, 0, 0, 0 for species Ar denotes that the only component contained in this species is Ar. (A zero denotes that a particular component does not appear in the species being considered.) In the sequence -1, 1, 0, 0, 0 for Ar^+, the -1 denotes that Ar^+ is a positive ion, and so forth.

Now, for the mixture being considered, NUMSP = 26, JINDX = 5, IAR = 2, IN2 = 8, IØ2 = 14, and ICØ2 = 26. Naturally, all 26 species decks are included and are placed in the order that they appear in the preceding table of A(I,J). It now remains to read in the A(I,J) as illustrated by the following listing:

1	0	0	0	0	0	1	0	0	0	-1	1	0	0	0
-2	1	0	0	0	0	0	1	0	0	-1	0	1	0	0
-2	0	1	0	0	0	0	2	0	0	-1	0	2	0	0
0	0	0	1	0	-1	0	0	1	0	-2	0	0	1	0
1	0	0	1	0	0	0	0	2	0	-1	0	0	2	0
1	0	0	2	0	0	0	1	1	0	-1	0	1	1	0
0	0	0	0	1	-1	0	0	0	1	-2	0	0	0	1
1	0	0	0	1	0	0	0	1	1	-1	0	0	1	1
0	0	1	0	1	0	0	0	2	1					

Thus, the first card contains the A(I,J) for e^-, Ar, and Ar^+; the second, for Ar^{++}, N, and N^+; and so forth.

The sequence of cards following the main program and subroutines is as follows:



If the simplified air model used in the previously discussed computer time study is now considered, the table of A(I,J) takes the following form:

		1	2	3	4
	Component (J) / Species (I)	e^-	Ar	N	O
1	e^-	1	0	0	0
2	Ar	0	1	0	0
3	N	0	0	1	0
4	N^+	-1	0	1	0
5	N_2	0	0	2	0
6	O	0	0	0	1
7	O^+	-1	0	0	1
8	O_2	0	0	0	2
9	NO	0	0	1	1
10	NO^+	-1	0	1	1

Then, NUMSP = 10, JINDX = 4, IAR = 2, IN2 = 5, and IØ2 = 8. Only the decks for the 10 species considered are included, and these are placed in the order that they appear in the preceding table of A(I,J). The A(I,J) are read in as illustrated by the following listing:

```
1  0  0  0  0  1  0  0  0  0  1  0 -1  0  1
0  0  0  2  0  0  0  0  1 -1  0  0  1  0  0
0  2  0  0  1  1 -1  0  1  1
```

Since the format for reading in the A(I,J) is the same as for the 26-species case, the first card contains all the A(I,J) for e^-, Ar, N, and the first three A(I,J) for N^+; the second card contains the fourth A(I,J) for N^+, all the A(I,J) for N_2, O, and O^+, and the first two A(I,J) for O_2; and so forth.

APPENDIX C

SAMPLE DATA PRINTOUTS OF COMPUTER PROGRAM

Sample data printouts are given herein. These printouts are for a 26-species air model, a 10-species air model, a 95-percent CO_2, 5-percent N_2 Venus model, and an 85-percent CO_2, 1-percent N_2, 14-percent Ar Mars model, respectively. Procedure ITEST = 3 was used to obtain these printouts.

The headings for the various free-stream and postshock flow conditions of interest correspond to those in the section entitled "SYMBOLS." The units of these flow conditions are also given in this section. The sample computer printouts are as follows:

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GAS MIXTURE DATA REDUCTION PROGRAM OF MILLER
ALL PHYSICAL QUANTITIES IN MKS UNITS-NASA SP-7012

AIR MODEL(26 SPECIES)

MEASURED INPUTS

RUN	P1	U1	PT	QT	RHO1	WO	XCO2	XN2	XO2	XAR
1.000E+00	1.040E+03	6.100E+03	0.	0.	4.850E-03	2.897E+01	3.300E-04	7.808E-01	2.095E-01	9.370E-03

FREE-STREAM CONDITIONS

P	RHO	T	H	S/R	Z	GAME	A	U	M	VRE
1.040E+03	4.850E-03	7.472E+02	7.602E+05	3.178E+01	1.000E+00	1.359E+00	5.399E+02	6.100E+03	1.130E+01	8.453E+05

STATIC CONDITIONS BEHIND NORMAL SHOCK

P	RHO	T	H	S/R	Z	GAME	A	U	M
1.674E+05	6.229E-02	6.620E+03	1.925E+07	4.399E+01	1.415E+00	1.142E+00	1.752E+03	4.753E+02	2.713E-01

STAGNATION CONDITIONS BEHIND NORMAL SHOCK

P	RHO	T	H	S/R	Z	GAME	A	QTZO	HW	RN
1.746E+05	6.462E-02	6.644E+03	1.937E+07	4.399E+01	1.417E+00	1.142E+00	1.757E+03	2.742E+07	2.960E+05	1.270E-02

MOLE FRACTIONS AT STAGNATION CONDITIONS

SPECIE	MOLE FRACTION
E-	4.0696E-04
A	6.6130E-03
A+	1.4978E-07
A++	8.0850E-22
N	2.9828E-01
N+	2.1156E-05
N++	1.7142E-21
N2	3.9864E-01
N2+	6.1787E-06
O	2.8904E-01
O+	2.0531E-05
O++	3.8095E-25
O-	7.3659E-07
O2	1.3728E-04
O2+	2.8967E-07
O2-	4.5576E-10
NO	6.2398E-03
NO+	3.5917E-04
C	3.1329E-05
C+	1.9291E-07
C++	3.6281E-20
C-	5.2360E-11
CO	1.9868E-04
CO+	3.1563E-08
CN	2.6528E-06
CO2	2.3941E-08

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GAS MIXTURE DATA REDUCTION PROGRAM OF MILLER
ALL PHYSICAL QUANTITIES IN MKS UNITS-NASA SP-7012

AIR MODEL(10 SPECIES)

MEASURED INPUTS

RUN	P1	U1	PT	QT	RHO1	WO	XCO2	XN2	XO2	XAR
1.000E+00	1.040E+03	6.100E+03	0.	0.	4.850E-03	2.897E+01	0.	7.808E-01	2.095E-01	9.700E-03

FREE-STREAM CONDITIONS

P	RHO	T	H	S/R	Z	GAME	A	U	M	NRE
1.040E+03	4.850E-03	7.472E+02	7.646E+05	3.178E+01	1.000E+00	1.359E+00	5.399E+02	6.100E+03	1.130E+01	8.452E+05

STATIC CONDITIONS BEHIND NORMAL SHOCK

P	RHO	T	H	S/R	Z	GAME	A	U	M
1.674E+05	6.229E-02	6.621E+03	1.926E+07	4.398E+01	1.415E+00	1.142E+00	1.752E+03	4.754E+02	2.714E-01

STAGNATION CONDITIONS BEHIND NORMAL SHOCK

P	RHO	T	H	S/R	Z	GAME	A	QTZO	HW	RN
1.746E+05	6.461E-02	6.645E+03	1.937E+07	4.398E+01	1.417E+00	1.142E+00	1.757E+03	2.742E+07	3.005E+05	1.270E-02

MOLE FRACTIONS AT STAGNATION CONDITIONS

SPECIE	MOLE FRACTION
E-	4.0425E-04
A	6.8466E-03
N	2.9862E-01
N+	2.1411E-05
N2	3.9850E-01
O	2.8886E-01
O+	2.0736E-05
O2	1.3692E-04
NO	6.2318E-03
NO+	3.6210E-04

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GAS MIXTURE DATA REDUCTION PROGRAM OF MILLER
ALL PHYSICAL QUANTITIES IN MKS UNITS-NASA SP-7012

VENUS MODEL

MEASURED INPUTS

RUN	P1	U1	PT	QT	RHO1	WO	XCO2	XN2	XO2	XAR
1.000E+00	1.040E+03	6.100E+03	0.	0.	4.850E-03	4.321E+01	9.500E-01	5.000E-02	0.	0.

FREE-STREAM CONDITIONS

P	RHO	T	H	S/R	Z	GAME	A	U	M	NRE
1.040E+03	4.850E-03	1.114E+03	-7.528E+06	3.761E+01	1.000E+00	1.181E+00	5.033E+02	6.100E+03	1.212E+01	7.036E+05

STATIC CONDITIONS BEHIND NORMAL SHOCK

P	RHO	T	H	S/R	Z	GAME	A	U	M
1.701E+05	7.688E-02	5.845E+03	1.100E+07	6.251E+01	1.968E+00	1.231E+00	1.650E+03	3.848E+02	2.332E-01

STAGNATION CONDITIONS BEHIND NORMAL SHOCK

P	RHO	T	H	S/R	Z	GAME	A	QTZO	HW	RN
1.759E+05	7.900E-02	5.878E+03	1.108E+07	6.251E+01	1.969E+00	1.228E+00	1.653E+03	3.109E+07	-8.426E+06	1.270E-02

MOLE FRACTIONS AT STAGNATION CONDITIONS

SPECIE	MOLE FRACTION
E-	9.0688E-05
A	6.5844E-19
A+	1.3509E-24
A++	4.2397E-41
N	1.7813E-02
N+	1.5280E-07
N++	4.6683E-26
N2	1.4891E-02
N2+	2.0328E-08
O	4.8028E-01
O+	5.0564E-06
O++	1.0027E-28
O-	5.2561E-07
O2	1.2943E-03
O2+	5.9274E-07
O2-	1.6196E-09
NO	3.0313E-03
NO+	7.0221E-05
C	3.2367E-03
C+	5.1040E-06
C++	1.1922E-20
C-	2.2304E-09
CO	4.7885E-01
CO+	1.0071E-05
CN	9.6076E-05
CO2	3.3266E-04

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GAS MIXTURE DATA REDUCTION PROGRAM OF MILLER
ALL PHYSICAL QUANTITIES IN MKS UNITS-NASA SP-7012

MARS MODEL

MEASURED INPUTS

RUN	P1	U1	PT	QT	RHO1	WO	XCO2	XN2	XO2	XAR
1.000E+00	1.040E+03	6.100E+03	0.	0.	4.850E-03	4.328E+01	8.500E-01	1.000E-02	0.	1.400E-01

FREE-STREAM CONDITIONS

P	RHO	T	H	S/R	Z	GAME	A	U	M	VRF
1.040E+03	4.850E-03	1.116E+03	-6.674E+06	3.653E+01	1.000E+00	1.198E+00	5.069E+02	6.100E+03	1.203E+01	6.729E+05

STATIC CONDITIONS BEHIND NORMAL SHOCK

P	RHO	T	H	S/R	Z	GAME	A	U	M
1.692E+05	7.140E-02	6.474E+03	1.184E+07	6.013E+01	1.906E+00	1.161E+00	1.659E+03	4.144E+02	2.498E-01

STAGNATION CONDITIONS BEHIND NORMAL SHOCK

P	RHO	T	H	S/R	Z	GAME	A	QTZO	HW	RN
1.755E+05	7.365E-02	6.500E+03	1.193E+07	6.014E+01	1.908E+00	1.160E+00	1.662E+03	3.199E+07	-7.513E+06	1.270E-02

MOLE FRACTIONS AT STAGNATION CONDITIONS

SPECIE	MOLE FRACTION
E-	2.6168E-04
A	7.3373E-02
A+	1.3229E-06
A++	3.4724E-21
N	8.9053E-03
N+	5.2798E-07
N++	1.9083E-23
N2	5.3246E-04
N2+	6.5341E-09
C	4.7054E-01
O+	2.8932E-05
O++	1.9298E-25
O-	8.6768E-07
O2	4.5026E-04
O2+	8.7718E-07
O2-	1.0570E-09
NO	3.9920E-04
NO+	2.3569E-05
C	2.5815E-02
C+	1.5080E-04
C++	1.5628E-17
C-	3.1004E-08
CO	4.1927E-01
CO+	5.6546E-05
CN	8.8518E-05
CO2	1.0205E-04

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