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STREAM-TUBE ANALYSIS USED TO CALCULATE ELECTRON CONCENTRATION IN THE PRESENCE OF ACCELERATING AND EVAPORATING WATER DROPLETS

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16. Abstract

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SUMMARY

An analysis is presented for use in the determination of the electron concentration in a flowing plasma in the presence of accelerating and evaporating water droplets. For given input gas-flow properties and gas composition, the resulting computer program is used to calculate gas density, gas and droplet velocity, temperature of the gas, enthalpy, fraction of droplet evaporated, Mach number, and gas composition as a function of distance along a stream tube. Representative calculations for the injection of water into a stream tube flowing over a reentry vehicle traveling at a velocity of 5.4 km/sec (17 717 ft/sec) are given.

INTRODUCTION

When a vehicle enters the atmosphere at high velocity, blackout of radio signals to or from the vehicle will occur due to free electrons in the plasma surrounding the vehicle (refs. 1 and 2). Many investigations in the past have dealt with methods of reducing the electron concentration in a plasma by means of material injection (refs. 3 to 13). One of the more promising ways of reducing the electron concentration is by the recombination of electrons and ions after the addition of water droplets into a plasma, as discussed in references 3, 5, 6, 8, and 12. This method works well in cool overionized plasmas where the concentration of free electrons is larger than it would be if there were equilibrium at the local gas temperature.

The processes by which water droplets are placed in a flow field have been passed over because no way to include them in the analysis has been found. However, some understanding of these processes is necessary for practical application of water injection to relieve radio blackout. For instance, at the altitudes where blackout occurs, useful penetration distances into a supersonic flow can be achieved only by injection in the form of a high-velocity liquid jet, which is broken up into droplets by aerodynamic forces and/or boiling. Spatial distribution of the resultant droplets and the distribution of droplet sizes in a given stream tube are known to influence the effectiveness of water injection as an electron suppressant but are not available. However, experimental studies (ref. 14) of penetration and spreading permit the determination of average mass flux of water downstream of the injection site. Measured values of mean droplet size (ref. 15) are available as a substitute for knowledge of droplet size distribution.

A computer program has been written by Barbara L. Weigel of the Langley Research Center to implement a method for calculating the properties of a one-dimensional stream-tube flow of a mixture of air and water droplets. (See the appendix.) The program takes into consideration acceleration and evaporation of the droplets along with a chemical kinetic reaction system based on 15 chemical species and 40 homogeneous chemical reactions. In addition, five heterogeneous reactions are included to account for the recombination of electrons and ions at droplet surfaces. The program is used to compute gas density, velocity, temperature, composition, percent evaporation of water, and the velocity of droplets as a function of distance from the injection site. A derivation of the necessary equations is included. A program listing with a table of the necessary inputs is also given. Some typical results are presented.

SYMBOLS

A stream-tube area, cm^2

$\bar{A}$ constant in drag-coefficient expression (eq. (51))

B_1 mass fraction of oxygen, $\dfrac{16\left(\gamma_1 + 2\gamma_2 + \gamma_5 + \gamma_6 + \gamma_8 + \gamma_{10} + \gamma_{13}\right)_2 + \frac{16}{18}\,fw^*}{1 + fw^*}$

B_2 mass fraction of nitrogen, $\dfrac{14\left(2\gamma_3 + \gamma_5 + \gamma_7 + \gamma_{10} + 2\gamma_{11} + \gamma_{12}\right)_2}{1 + fw^*}$

B_3 mass fraction of hydrogen, $\dfrac{\frac{2}{18}\,fw^*}{1 + fw^*}$

B_{ij} term representing contribution of jth reaction to disappearance of ith species, mol^2/g^2

C_D droplet drag coefficient

$C_{D,C}$ continuum droplet drag coefficient

$C_{D,FM}$ free molecular droplet drag coefficient

$(C_D)_{M=0}$	droplet drag coefficient for $M = 0$
C_p	heat capacity at constant pressure, ergs/mol-^{o}K
c_p	specific heat at constant pressure, ergs/g-^{o}K
$\bar{c}_p$	specific heat of mixture at constant pressure, ergs/g-^{o}K
D	reaction energy (divided by RT_0), dimensionless
d_N	reference length, given as nose diameter, cm
$E_1, \ldots, E_6$	correction factors applied at end of each integration step to preserve correct mass fraction of total oxygen, nitrogen, and hydrogen
F	force on droplet, dynes
F_e	efficiency factor for capture of electrons by water droplet
F_i	free energy of ith species, ergs/mol
f	mass fraction of water evaporated, $1 - \hat{r}^3$
f_r	free molecular recovery factor
$f_{r,0}$	droplet recovery factor for zero mass transfer
G_{ij}	term representing contribution of jth reaction to production of ith species, mol^2/g^2
g	plasma-sheath thickness transition function, $g_b + \dfrac{g_a - g_b}{1 + \left(\dfrac{r\hat{r}}{\lambda_D}\right)^2}$

$$g_a = 3.8738 + 0.03432U + 0.19754U^2 - 0.10445U^3 + 0.013263U^4$$

$$g_b = 5.46466 - 0.09100U - 0.33579U^2 + 0.11571U^3 - 0.012074U^4$$

H_i	enthalpy of ith species, ergs/mol

h	specific enthalpy, ergs/g
h^*	total specific enthalpy of shocked gas, ergs/g
i	species identification number
j	reaction identification number
K	equilibrium constant, mol/cm^3 or dimensionless
k	specific reaction rate constant, cm^3/mol-sec; also, thermal conductivity, ergs/cm-sec-^{o}K
L	latent heat of water, ergs/g
M	Mach number of gas relative to droplet; also, third body in chemical reactions
$\overline{M}$	mean molecular weight of ions, g/mol
$(MW)_i$	molecular weight of species i, g/mol
$\dot{m}$	mass-flow rate, g/sec
N_A	Avogadro constant, 6.02486×10^{23} particles/mol
N_e	electron concentration, electrons/cm^3
N_{Nu}	Nusselt number for heat transfer to droplet
$N_{Nu,C}$	continuum Nusselt number
$N_{Nu,FM}$	free molecular Nusselt number
N_{Re}	effective Reynolds number, $\frac{\rho(u - v)2r}{\mu f}$; listed as RES in computer program
N_{St}	free molecular Stanton number; listed as ST in computer program
n	constant in drag-coefficient expression (eq. (51))
p	pressure, dynes/cm^2

q	heat-transfer rate to droplet, $ergs/cm^2$-sec
R	universal gas constant, 8.31696×10^7 ergs/mol-^{o}K or $82.1023 \frac{atm\text{-}cm^3}{^{o}K}$
r	droplet radius, cm
$\hat{r}$	droplet radius divided by r_2
S	speed ratio, $\dfrac{u - v}{\sqrt{2RT \sum_{i=1}^{15} \gamma_i}}$
s	distance along stream tube from bow shock on vehicle, cm
T	temperature, ^{o}K
t	time, sec
U	normalized relative velocity between gas and droplet
u	gas velocity, cm/sec
V	velocity, cm/sec
v	droplet velocity, cm/sec
W_i	net rate of production or disappearance of species i, mol/cm^3-sec
w^*	initial ratio of water mass flow to gas mass flow
X	mole fraction
x	distance along streamline path from injection site divided by d_N, $\dfrac{s - s_2}{d_N}$
Z	compressibility factor
α_{ij}	factor which selects nonzero contributions to W_i
Γ_i	specific-heat ratio of ith species, $\dfrac{(C_p/R)_i}{\left[(C_p/R)_i - 1\right]}$

γ_i specific concentration of ith species, mol/g

λ_D Debye length, $6.90\sqrt{\frac{T}{N_e}}$, cm

μ reduced mass of colliding species, g/mol; also, water viscosity, dynes-sec/cm^2

ρ density, g/cm^3

σ reaction rate cross section, cm^2

Ω collision integral for viscosity

Subscripts:

av average

aw zero heat transfer at droplet surface

f evaluated at mean temperature of droplet film

l water

m gas mixture after injection

rel relative

s saturated vapor

v vapor

w droplet surface

∞ free-stream condition

2 value at injection site

0 zero mass transfer; also, standard temperature

Dot over symbol denotes derivative with respect to time.

Arrow over symbol denotes vector.

METHOD OF CALCULATION

The equations derived herein have been programed in FORTRAN IV language and a description of the program is given in the appendix. As the program is presently written, the following limitations should be considered when it is being used:

(1) Although the liquid specified for injection is water, any suitable liquid could be used as long as the liquid droplet properties are known and the necessary changes are made in the finite-rate chemistry system.

(2) The program cannot be used with injection of liquids at the stagnation point in the flow.

(3) The finite-rate chemistry system does not take into account negative ions, such as H^-, OH^-, O^-, O_2^-, NO^-, and NO_2^-, but is otherwise believed to be valid up to speeds of about 9.14 km/sec (30 000 ft/sec).

(4) The use of a stream-tube analysis limits application to inviscid flows.

Thus, the growth of the boundary layer as altitude increases must be taken into account.

Conservation Equations

By passing over the difficult and complex questions which surround the actual injection of water into the flow field, the problem is reduced to the properties along a stream tube in which, at some initial station, water droplets have been deposited by an atomizing liquid jet. Due to the complicated two-phase nature of the problem, it is necessary to make several idealizations, among which are

(1) The flow is steady, one-dimensional, and inviscid.

(2) The droplet size, velocity, and distribution at any streamwise station are uniform.

(3) Nusselt number and drag coefficient for the droplets are the same as for an isolated sphere.

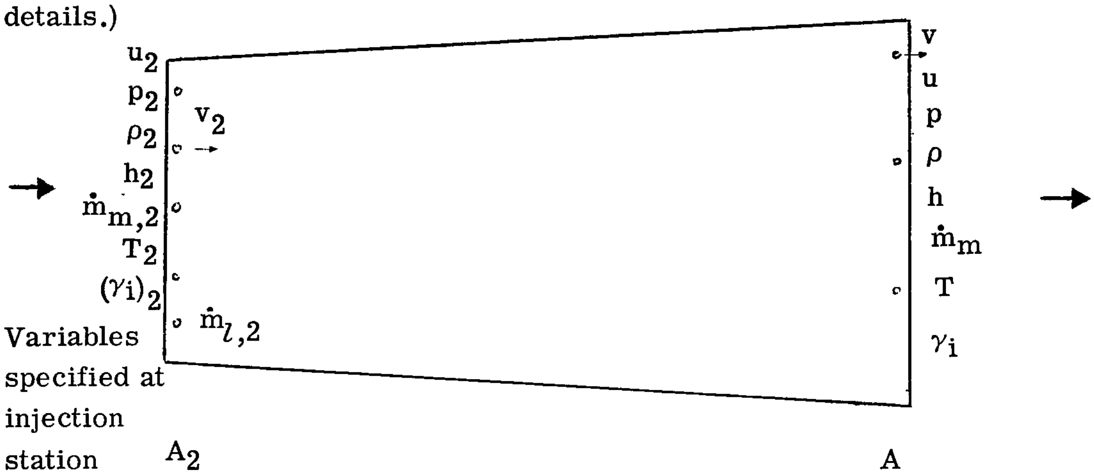
(4) The ratio of mass flow of water (liquid and vapor) to mass flow of air in the stream tube is constant; that is, downstream of the initial station no droplets enter or leave the stream tube.

(5) The gas phase is a uniform mixture of ideal gases.

(6) The pressure distribution along the stream tube is assumed to be known (see, for example, fig. 1).

Analysis of the stream-tube flow begins at the point where water droplets are suddenly assumed to be present. If injection-induced perturbations to the properties of a flow field are to be included, they must appear in the influence they have on the initial conditions specified at the injection station.

A control volume approach is used in which the integral form of the conservation laws are applied to a one-dimensional stream-tube flow of a mixture of liquid droplets and gas. (See sketch a). (Information concerning derivations similar to those that follow is available in refs. 5, 16, and 17, and these references should be consulted for complete details.)



Sketch a

<u>Conservation of mass.</u>- The conservation of mass for steady flow can be defined as

$$\int \rho \vec{V} \cdot d\vec{A} = 0$$

or

$$\dot{m}_{l,2} + \dot{m}_{m,2} = \dot{m}_m + \dot{m}_l \tag{1}$$

Inasmuch as droplets are assumed to be of a uniform size,

$$\left(\frac{r}{r_2}\right)^3 = 1 - f = \frac{\dot{m}_l}{\dot{m}_{l,2}} \tag{2}$$

By defining

$$w^* \equiv \frac{\dot{m}_{l,2}}{\dot{m}_{m,2}}$$

equation (1) becomes

$$1 + w^* = \frac{\dot{m}_m}{\dot{m}_{m,2}} + (1 - f)w^*$$

or

$$\frac{\dot{m}_m}{\dot{m}_{m,2}} = 1 + fw^* \tag{3}$$

and, therefore,

$$\frac{A}{A_2} = \frac{\rho_2 u_2}{\rho u}(1 + fw^*) \tag{4}$$

where the volume of the droplets is negligible as compared with the volume of the air-water mixture.

Conservation of momentum.- The conservation of momentum for steady flow can be expressed in the form

$$F = \int V\rho\vec{V} \cdot d\vec{A}$$

or

$$\dot{m}_{m,2}u_2 + \dot{m}_{l,2}v_2 + p_2A_2 + \left(\frac{p_2 + p}{2}\right)\left(A - A_2\right) = pA + \dot{m}_m u + (1 - f)\dot{m}_{l,2}v \tag{5}$$

In equation (5) the option of specifying pressure or area is given. For the present work the pressure distribution is specified. Dividing equation (5) by $\dot{m}_{m,2} = \rho_2 u_2 A_2$ and using equation (4) yield

$$u = \frac{p_2 - p}{2\rho u} + \frac{1}{1 + fw^*}\left\{\frac{p_2 - p}{2\rho_2 u_2} + u_2 + \left[v_2 - (1 - f)v\right]w^*\right\} \tag{6}$$

where $p = p(x)$ is assumed to be known.

Conservation of energy.- The conservation of energy for steady flow can be defined as

$$\int\left(\frac{V^2}{2} + h\right)\rho\vec{V} \cdot d\vec{A} = 0$$

or

$$\dot{m}_{l,2}\left(\frac{v_2{}^2}{2} + h_{l,2}\right) + \dot{m}_{m,2}\left(\frac{u_2{}^2}{2} + h_2\right) = \dot{m}_m\left(\frac{u^2}{2} + h\right) + (1 - f)\left(\frac{v^2}{2} + h_{l,2}\right)\dot{m}_{l,2} \tag{7}$$

It has been assumed in equation (7) that the average temperature of the liquid droplet does not change appreciably; that is, $h_l = h_{l,2}$. Also, it has been assumed that all the heat input to the droplet goes into evaporation. By solving equation (7) for h, using equation (3), and assuming that v_2 is small enough to be neglected, one obtains

$$h = \frac{h^* + h_l fw^* - \left(\frac{1 - f}{2}\right)v^2w^*}{1 + fw^*} - \frac{u^2}{2} \tag{8}$$

where

$$h_l = h_{v,s} - L \tag{9}$$

Initially the droplet velocity is computed from the following relationship:

$$v_2 = \frac{600\rho_2 u_2 w^*}{\pi(\hat{r})^3 \rho_l} + 1 \tag{10}$$

Chemical Relationships

The properties of the gas mixture after water injection are given by the equations that follow.

For a mixture of perfect gases, the equation of state is

$$\rho = \frac{p}{RT \sum_{i=1}^{15} \gamma_i} \tag{11}$$

The enthalpy of a mixture of ideal gases is defined as

$$h = RT\left[\sum_{i=1}^{15} \gamma_i \left(\frac{H_i}{RT}\right)\right] \tag{12}$$

where H_i/RT is obtained by fitting the data of references 18 and 19 to a set of fourth-order polynomial equations for enthalpy, entropy, heat capacity, and free energy as described in reference 20.

The rate equations governing the change in chemical composition have the form

$$\frac{d\gamma_i}{dx} = \frac{d_N}{\rho u} W_i \tag{13}$$

where

$$W_i = \sum_j W_{ij} \tag{14}$$

and

$$W_{ij} = \alpha_{ij} \rho^2 k_j \left(B_{ij} - G_{ij}\right) \tag{15}$$

The factor α_{ij} is equal to 1 if reaction j involves species i $(\alpha_{ij}$ is equal to 2 for atoms produced in dissociation of O_2, N_2, and $H_2)$; otherwise, α_{ij} is equal to 0. The species are listed in table I. The specific reaction rate constants k_j are obtained from data presented in table II. Reactions written in this table are given as forward rates in the endothermic direction. The constant k_j for the first reaction given in table II can be expressed in the form (ref. 21).

$$k_j = N_A\sigma_j\left(\frac{8RT}{\pi\mu_j}\right)^{1/2}\left[\frac{e^{-3/2}}{2}\left(\frac{D_jT_0}{T}+1\right)^2\right]\exp\left(-\frac{D_jT_0}{T}\right) \tag{16}$$

and for reactions 2 through 6 in the form (ref. 21)

$$k_j = N_A\sigma_j\left(\frac{8RT}{\pi\mu_j}\right)^{1/2}\left[\frac{4e^{-1}}{3\pi^{1/2}}\left(\frac{D_jT_0}{T}+\frac{1}{2}\right)^{3/2}\right]\exp\left(-\frac{D_jT_0}{T}\right) \tag{17}$$

On the basis of a simple collision model, the following form (ref. 22) holds for reactions 7 through 40:

$$k_j = N_A\sigma_j\left(\frac{8RT}{\pi\mu_j}\right)^{1/2}\exp\left(-\frac{D_jT_0}{T}\right) \tag{18}$$

The σ_j values for the preceding reactions represent the best available values based on information in references 21 and 22 and were adjusted for experimental data if any were available. The D_j values were obtained from reference 23. In addition to information in references 21 and 22 some helpful summaries and discussions on reaction rates can be found in references 24 to 26. The set of reactions in table II is for an air-water mixture flowing over a nonablating body.

For the dissociation and recombination of O_2, the B_{ij} and G_{ij} terms in equation (15) have the following form:

$$B_{2\,2} = -B_{8\,2} = \frac{\rho\gamma_8^{\,2}\sum\gamma_i}{K_2} \tag{19}$$

$$G_{2\,2} = -G_{8\,2} = \gamma_2\sum\gamma_i \tag{20}$$

For the formation and disappearance of electrons by reaction 16, they have the form

$$B_{7\,16} = -B_{15\,16} = \frac{\gamma_{11}\gamma_{15}}{K_{16}} \tag{21}$$

$$G_{7\,16} = -G_{15\,16} = \gamma_7\gamma_7 \tag{22}$$

The equilibrium constants for the reactions in table II are computed from the free energy of the species as defined by the previously mentioned polynomials and have the form similar to the following example:

$$K_2 = \exp\left(-\frac{F_8}{RT}-\frac{F_8}{RT}+\frac{F_2}{RT}\right)\left(\frac{1}{82.1023T}\right) \tag{23}$$

In addition to the 40 homogeneous gas reactions, the recombination of ions with electrons on the surfaces of water droplets can be included in the reaction system by defining net rates in the form

$$W_{ij} = \rho^2 k_j \gamma_i \tag{24}$$

where j refers to the five catalytic reactions and i refers to the ions NO^+, N_2^+, N^+, O^+, and H^+. The rate constants for reactions 41 to 45 can be expressed in the form

$$k_j = \frac{3u\hat{r}^2 w^*}{4r_2 \rho_l v(1 + fw^*)}\left(6.22 \times 10^5 \sqrt{T} F_e\right) \tag{25}$$

where F_e (refs. 3 and 6) can either be a constant or can be computed as follows:

$$F_e = e^{-g}$$

where

$$g = g_b + \frac{g_a - g_b}{1 + \left(\frac{r\hat{r}}{\lambda_D}\right)^2} \tag{26}$$

The exponent g is proportional to the electric potential attained by a droplet in the plasma. This potential has different limiting values (represented by g_a and g_b) depending upon the ratio of plasma-sheath thickness to drop radius (ref. 6), and the expression for g provides a convenient (but arbitrary) transition between the two limits. The limits g_a and g_b are themselves functions of the velocity of the droplets relative to the gas. Therefore, g_a and g_b are fitted with fourth-order polynomials as follows:

$$g_a = 3.8738 + 0.03432U + 0.19754U^2 - 0.10445U^3 + 0.013263U^4 \qquad (0 \leqq U \leqq 3) \tag{27}$$

$$g_b = 5.46466 - 0.091000U - 0.33579U^2 + 0.11571U^3 - 0.012074U^4 \qquad (0 \leqq U \leqq 3) \tag{28}$$

where

$$U = \frac{u - v}{\left(\frac{5.486 \times 10^{-4}}{\overline{M}}\right)^{1/2}\left(6.22 \times 10^5 \sqrt{T}\right)} \tag{29}$$

$$\lambda_D = 6.90\sqrt{\frac{T}{N_e}} \tag{30}$$

$$\overline{M} = \frac{\sum_{i=10}^{14} \gamma_i (MW)_i}{\sum_{i=10}^{14} \gamma_i} \tag{31}$$

In order to ensure that the correct mass fractions of total oxygen, nitrogen, and hydrogen were maintained in the mixture, γ_i values were replaced at the end of each computational step with

$$E_1\gamma_i = \left[\frac{B_1}{16(\gamma_1 + 2\gamma_2 + \gamma_5 + \gamma_6 + \gamma_8 + \gamma_{10} + \gamma_{13})}\right]\gamma_i \qquad (i = 2, 8, 13) \tag{32}$$

$$E_2\gamma_i = \left[\frac{B_2}{14(2\gamma_3 + \gamma_5 + \gamma_7 + \gamma_{10} + 2\gamma_{11} + \gamma_{12})}\right]\gamma_i \qquad (i = 3, 7, 11, 12) \tag{33}$$

$$E_3\gamma_i = \left[\frac{B_3}{2\gamma_1 + 2\gamma_4 + \gamma_6 + \gamma_9 + \gamma_{14}}\right]\gamma_i \qquad (i = 4, 9, 14) \tag{34}$$

$$E_4\gamma_i = \left[\frac{2E_3 + 16E_1}{18}\right]\gamma_i \qquad (i = 1) \tag{35}$$

$$E_5\gamma_i = \left[\frac{14E_2 + 16E_1}{30}\right]\gamma_i \qquad (i = 5, 10) \tag{36}$$

$$E_6\gamma_i = \left[\frac{E_3 + 16E_1}{17}\right]\gamma_i \qquad (i = 6) \tag{37}$$

When these corrections are made,

$$\sum_{i=1}^{15} \gamma_i (MW)_i = 1$$

is satisfied.

The preceding equations apply for a mixture of air, water vapor, and the products of reactions involving both. They are used in the program to calculate the changes which occur in the gaseous mixture during a forward step. However, dilution of the mixture by evaporation during a step is accounted for only at the end of each step. At the end of a step a new value of f is computed from equation (2). This f value leads to new values of

B_1, B_2, and B_3 and also to an increase in the concentration variable for water vapor γ_1 given by

$$(\gamma_1)_{new} = (\gamma_1)_{old} + \frac{w^*}{18}(f_{new} - f_{old}) \tag{38}$$

Because of the revised values of B_1, B_2, B_3, and γ_1, it is necessary to recompute the correction factors which ensure conservation of total oxygen, nitrogen, and hydrogen. After these calculations are made, the program proceeds with computations for the next step.

Conversion of specific concentration to mole fraction can be achieved by using

$$X = \frac{\gamma_i}{\sum_{i=1}^{15} \gamma_i} \tag{39}$$

and electron number density can be obtained from

$$N_e = N_A \rho \gamma_{15} \tag{40}$$

The compressibility factor for the air and water mixture can be computed by the following relationship:

$$Z = \left[\frac{\sum_{i=1}^{15} \gamma_i}{(\gamma_2)_\infty + (\gamma_3)_\infty + \frac{fw^*}{18}}\right]\left(1 + fw^*\right) \tag{41}$$

where $(\gamma_2)_\infty + (\gamma_3)_\infty = 0.034674063$.

Auxiliary Relationships

Droplet acceleration.- The equation of motion for a mean droplet (based on ref. 5) assumed to be spherical in shape is (for an isolated spherical droplet)

$$F = \frac{1}{2} \rho V_{rel}^2 \pi r^2 C_D = \frac{4\pi r^3 \rho_l v}{3d_N} \frac{dv}{dx}$$

or

$$\frac{dv}{dx} = \frac{3(u - v)^2 \rho C_D d_N}{8\rho_l vr} \qquad (v \neq 0) \tag{42}$$

with $r = r_2\hat{r}$. The drag coefficient (ref. 5) was taken for $M < 0.5$ as

$$C_D = \frac{(C_D)_{M=0} + \frac{51.1M}{N_{Re}}}{1 + 0.256M\left[(C_D)_{M=0} + \frac{51.1M}{N_{Re}}\right]} \tag{43}$$

with

$$\left(C_D\right)_{M=0} = \frac{24}{N_{Re}} + 0.4 + 1.6 \exp\left[-0.028\left(N_{Re}\right)^{0.82}\right] \tag{44}$$

$$N_{Re} = \frac{\rho(u - v)2r}{\mu_f} \tag{45}$$

$$M = \frac{u - v}{\sqrt{RT \sum_{i=1}^{15} \gamma_i \Gamma_i}} \tag{46}$$

$$\Gamma_i = \frac{\left(\frac{C_p}{R}\right)_i}{\left[\left(\frac{C_p}{R}\right)_i - 1\right]} \tag{47}$$

and

$$\mu_f = \frac{26.693 \times 10^{-6}\sqrt{18T_{av}}}{(2.641)^2\Omega} \tag{48}$$

In order to use equation (48), one needs

$$\Omega = \Omega\left(\frac{T_{av}}{809.1}\right)$$

(obtained from ref. 27) and

$$T_{av} = \frac{1}{2}\left[\frac{(u - v)^2}{2\bar{c}_p} + T + T_w\right] \tag{49}$$

The specific heat of the mixture is

$$\bar{c}_p = R \sum_{i=1}^{15} \gamma_i\left(\frac{C_p}{R}\right)_i \tag{50}$$

For $M \geqq 0.5$ the drag coefficient (ref. 5) is given by

$$C_D = C_{D,C} + \left(C_{D,FM} - C_{D,C}\right)\exp\left(-\bar{A}N_{Re}^{n}\right) \tag{51}$$

where $C_{D,C}$, $C_{D,FM}$, $\bar{A}$, and n are given as a function of M in table III.

Heat transfer to droplets.- In accordance with the discussion of the global energy equation, it is assumed that all the heat transferred to the droplet goes into evaporation and, thus,

$$q\left(4\pi r^2\right) = -\frac{4}{3}\pi\rho_l L\frac{dr^3}{dt}$$

or

$$\frac{dr^2}{dx} = \frac{2qrd_N}{\rho_l Lv} \tag{52}$$

By defining an average droplet Nusselt number as

$$N_{Nu} \equiv \frac{2qr\bar{c}_p}{k_f\left(h_{aw} - h_w\right)} \tag{53}$$

the following equation can be used:

$$\frac{dr^2}{dx} = -\frac{N_{Nu}k_f d_N\left(h_{aw} - h_w\right)}{L\rho_l\bar{c}_p v} \tag{54}$$

In the present case,

$$h_{aw} - h_w = f_{r,0}\frac{(u - v)^2}{2} + \bar{c}_p T - \bar{c}_p T_w \tag{55}$$

which is the enthalpy available for droplet evaporation. By assuming that the Prandtl number is unity, the following relation can be utilized:

$$k_f = \mu_f c_{p,f} \tag{56}$$

where

$$c_{p,f} = \frac{R}{18}\left[\left(\frac{C_p}{R}\right)_{H_2O}\right]_{T=T_{av}} \tag{57}$$

The expression used for N_{Nu} is (ref. 5)

$$N_{Nu} = \frac{N_{Nu,C}\left(q/q_o\right)}{1 + \dfrac{N_{Nu,C}\left(q/q_o\right)}{N_{Nu,FM}}} \tag{58}$$

where

$$N_{Nu,C} = 2 + 0.6\sqrt{N_{Re}} \tag{59}$$

$$\frac{q}{q_o} = \frac{L}{c_{p,f}\,\Delta T} \ln\left(1 + \frac{c_{p,f}\,\Delta T}{L}\right) \tag{60}$$

$$\Delta T = \frac{f_{r,o}(u - v)^2}{2\bar{c}_p} + T - T_w \tag{61}$$

and

$$N_{Nu,FM} = \left[\frac{\sum_{i=1}^{15} \gamma_i \Gamma_i + \sum_{i=1}^{15} \gamma_i}{\sum_{i=1}^{15} \gamma_i \Gamma_i}\right]\left[\frac{\rho(u - v) 2r c_{p,v,w} N_{St}}{k_f}\right]\left[\frac{\frac{f_r(u - v)^2}{2} + \bar{c}_p(T - T_w)}{\frac{f_{r,o}(u - v)^2}{2} + \bar{c}_p(T - T_w)}\right] \tag{62}$$

with

$$f_r = \left[\frac{\sum_{i=1}^{15} \gamma_i \Gamma_i}{\sum_{i=1}^{15} \gamma_i \Gamma_i + \sum_{i=1}^{15} \gamma_i}\right]\left[2 + 0.7 \exp(-0.7075)\right] \tag{63}$$

$$N_{St} = \frac{0.1041}{S^{1.14}} + 0.125\left[1 - \exp\left(-1.166 S^{0.406}\right)\right] \tag{64}$$

$$S = \frac{u - v}{\sqrt{2RT \sum_{i=1}^{15} \gamma_i}} \tag{65}$$

TYPICAL EXAMPLE

Sample calculations were made for water injection into a stream tube flowing over a reentry vehicle at an altitude of 47.55 km (156 000 ft) with an entry velocity of 5.4 km/sec (17 717 ft/sec). The example given herein is intended to illustrate the use of the computer program. Necessary inputs for the program are listed in the appendix. Each printed output includes the inputs used.

Figure 1(a) shows the pressure distribution used in the present example (based on ref. 28). With one exception, this pressure distribution was used for all the examples in the figures. In order to investigate the effect of a change in this pressure distribution, one calculation was made by using the variation illustrated by curve B in figure 1(b) which was obtained from data of references 17 and 29. It should be noted that when curve B was used, the only input quantities changed were pressure and density, and momentum was not conserved between a station just upstream of injection and one just downstream of injection.

The four test cases with assumed conditions are as follows:

(1) Water and air mixture with finite rate chemistry

(2) Air with finite rate chemistry ($w^* = 0$)

(3) Water and air mixture without any neutral-gas chemical reactions (frozen)

(4) Water and air mixture with full gas chemistry but with $F_e = 0$ (no recombination of ions and electrons on droplet surfaces).

The mixture temperature, density, and velocity along the body streamline are shown as a function of distance from the injection site in figures 2 to 4, respectively. Results for the first three test cases are shown for each parameter (case 4 curves are identical to case 1 curves) along with results obtained by using curve B of figure 1(b) (only the water plus air finite-rate curves are used to illustrate this effect). Figure 5 shows the fraction of water evaporated for both frozen and finite-rate conditions (case 4 curve is identical to case 1 curve).

Figure 6 shows the reduction in electron concentration along the body streamline. Results for all four test cases are shown as well as the results obtained by using curve B of figure 1(b). The results indicate that the recombination of electrons and ions on the surface of water droplets is effective (for the conditions cited) in reducing electron concentration in the plasma sheath surrounding a reentry vehicle. The finite-rate curve obtained with the curve B pressure in figure 1(b) shows a larger reduction in N_e than that obtained with the curve A pressure of figure 1(b).

The variation of the neutral species with and without water addition is presented in figure 7. The curves represent the result of finite-rate calculation which does not include the effects of injection-induced compression. After water injection the N and O atom concentrations rapidly decrease. The importance of the removal of these atoms is that a condition of dynamic balance under local conditions for reaction 15 ($N + O \rightleftharpoons NO^+ + e^-$) is destroyed. (See ref. 30.) It should be noted that the group of reactions (7, 8, 9, 12, 13, 14) responsible for the increased speed of removal of the O and N atoms all contain hydrogen, which was introduced by the water injection.

CONCLUDING REMARKS

An analysis is presented for use in the determination of the electron concentration in a flowing plasma in the presence of accelerating and evaporating water droplets. For given input gas-flow properties and gas composition, the resulting computer program is used to calculate gas density, gas temperature, gas and droplet velocity, enthalpy, fraction of droplet evaporated, Mach number, and gas composition. Sample calculations indicate that a reduction in electron concentration can be achieved by injecting water into the plasma sheath surrounding a reentry vehicle.

Langley Research Center,
National Aeronautics and Space Administration,
Hampton, Va., July 10, 1970.

APPENDIX

DIGITAL COMPUTER PROGRAM FOR CALCULATING ELECTRON CONCENTRATION IN PRESENCE OF ACCELERATING AND EVAPORATING WATER DROPLETS

By Barbara L. Weigel

This appendix describes the digital computer program (D2331) developed in support of a stream-tube analysis used to calculate electron concentration in the presence of accelerating and evaporating water droplets. The program was written in FORTRAN IV language for the Control Data 6600 computer system with the SCOPE 3 operating system and library tape.

Input

The data input consists of one card for case identification, FORMAT (8A10), followed by the numeric input using FORTRAN IV NAMELIST. The NAMELIST input symbols are as follows:

FORTRAN symbol	Symbol in text	Description
$NAM1		
RHOL	ρ_l	Water density, g/cm^3
HL	h_l	Specific enthalpy of water, ergs/g
DN	d_N	Reference length given as nose diameter, cm
EL	L	Latent heat of water, ergs/g
ENTHAL	h_2	Initial specific enthalpy, ergs/g
TW	T_w	Droplet surface temperature, $^{\circ}$K
FRO	$f_{r,0}$	Droplet recovery factor for zero mass transfer

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FORTRAN symbol	Symbol in text	Description
CPVW	$c_{p,v,w}$	Specific heat of vapor at droplet surface, ergs/g-^{o}K
WASK	w^*	Initial ratio of water mass flow to gas mass flow
R	r_2	Initial droplet radius, cm
HASK	h^*	Total specific enthalpy of shocked gas, ergs/g
U2	u_2	Initial gas velocity, cm/sec
P2	p_2	Initial gas pressure, dynes/cm^2
RHO2	ρ_2	Initial gas density, g/cm^3
T	T_2	Initial gas temperature, ^{o}K
VAR(1)	x	Distance along streamline path from injection site divided by d_N, $(s - s_2)/d_N$; therefore, = 0 initially
VAR(2)	$\hat{r}^2$	$(\text{Droplet radius divided by } r_2)^2$
VAR(3)	v	Droplet velocity, cm/sec
VAR(4)	γ_1	Specific concentration of H_2O, mol/g; $\gamma_1 = 0$ at injection site
VAR(5)	γ_2	Specific concentration of O_2, mol/g
VAR(6)	γ_3	Specific concentration of N_2, mol/g
		Etc. for γ_i where i = 4 to 14; $\gamma_4,\gamma_6,\gamma_9,\gamma_{14} = 0$ at injection site
DER(1)	$\dot{\hat{r}}^2$	Derivative of $\hat{r}^2$

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FORTRAN symbol	Symbol in text	Description
DER(2)	$\dot{v}$	Derivative of droplet velocity
DER(3)	$\dot{\gamma}_1$	Derivative of specific concentration of H_2O Etc. for $\dot{\gamma}_i$ where $i = 2$ to 14
FE	F_e	Efficiency factor for capture of electrons by water droplet or catalytic efficiency
NTLUP		Number of points in VARIX and VARDP arrays, ≦40
VARIX		Array of x values
VARDP		Array of pressure ratios p/p_2 at each x of VARIX array
PRDEL		Print answers every PRDEL increment in x; PRDEL = 0.1 unless input otherwise
XTERM		Value of x at which run is to be terminated
HEPS		Percent by which enthalpy will be allowed to vary in two successive steps when -500000.0 < Enthalpy < 50000.0; HEPS = 0.1 unless input otherwise
CI		Initial computing interval 0.0001220703125 unless input otherwise
CIMAX		Maximum computing interval 0.1 unless input otherwise
ELE1		An array of 16 values used by the integration scheme to control the size of the computing interval, 0.0 < ELE1 ≦ 64.0; initially 0.5 unless input otherwise

FORTRAN symbol	Symbol in text	Description
ELE2		An array of 16 values used by the integration scheme to control the size of the computing interval, ELE2 < ELE1; initially 0.1 unless input otherwise
IBUG		An array of 20 integers which must be input as 1 to trigger debug printouts at critical points (see Program Listing)

The input subroutines are as follows:

1. ITR1 — A Newton-Raphson iteration method (see ref. 31, p. 192)

2. CALINT — A modified Runge-Kutta numerical integration scheme designed for chemistry problems by Charles E. Treanor (ref. 32)

3. BASIC — Evaluates derivatives: $\dot{r}^2$, $\dot{v}$, $\dot{\gamma}_1$ through $\dot{\gamma}_{14}$

4. CHECK — Controls the size of the computing interval

5. FOFX — A function subroutine to evaluate T

6. ERROR — Checks input to CALINT

7. FTLUP — A table lookup (see ref. 33, pp. 87-91)

Output

The output consists of the NAMELIST input, case identification, injection parameters w^*, r_2, d_N, and F_e, initial values for p, ρ, h, T, u, and v, and a list of the species 1 to 15. A typical output is presented as a function of distance from the water injection site.

APPENDIX

```
$NAM1

RHOL    =  0.1E+01,

HL      = -0.1515E+12,

DN      =  0.2032E+02,

EL      =  0.245E+11,

ENTHAL  =  0.80280264E+11,

TW      =  0.261E+03,

FRO     =  0.85E+00,

CPVW    =  0.186E+08,

WASK    =  0.35E+01,

R       =  0.78E-03,

HASK    =  0.12624843E+12,

IBUG    =  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,
           0,  0,  0,

U2      =  0.30321E+06,

P2      =  0.17326E+05,

RHO2    =  0.17008E-05,

T       =  0.287E+04,

PRDEL   =  0.1E+00,

VAR     =  0.0,  0.1D+01,  0.0,  0.0,  0.9783516D-05,  0.26255921D-01,  0.0,
           0.5861998D-04,  0.0,  0.2017667D-02,  0.14339319D-01,  0.0,
           0.10164856D-05,  0.4929865D-13,  0.25899178D-12,  0.15938891D-10,
           0.0,  0.10168052D-05,  0.0,  0.0,

DER     =  0.0,  0.0,  0.0,  0.0,  0.0,  0.0,  0.0,  0.0,  0.0,  0.0,  0.0,
           0.0,  0.0,  0.0,  0.0,  0.0,  0.0,  0.0,  0.0,  0.0,

ELE1    =  0.5E+00,  0.5E+00,  0.5E+00,  0.5E+00,  0.5E+00,  0.5E+00,  0.5E+00,
           0.5E+00,  0.5E+00,  0.5E+00,  0.5E+00,  0.5E+00,  0.5E+00,  0.5E+00,
           0.5E+00,  0.5E+00,  0.5E+00,  0.5E+00,  0.5E+00,  0.5E+00,

ELE2    =  0.1E+00,  0.1E+00,  0.1E+00,  0.1E+00,  0.1E+00,  0.1E+00,  0.1E+00,
```

```
          0.1E+00,  0.1E+00,  0.1E+00,  0.1E+00,  0.1E+00,  0.1E+00,  0.1E+00,
          0.1E+00,  0.1E+00,  0.1E+00,  0.1E+00,  0.1E+00,  0.1E+00,

CI      = 0.1220703125E-03,

CIMAX   = 0.1E+00,

XTERM   = 0.45E+01,

HEPS    = 0.1E+00,

FE      = 0.3E-01,

NTLUP   = 27,

VARIX   = 0.0,  0.1018E+00,  0.2011E+00,  0.3026E+00,  0.4003E+00,
          0.5058E+00,  0.6112E+00,  0.703E+00,  0.8046E+00,  0.9062E+00,
          0.10058E+01,  0.11034E+01,  0.13066E+01,  0.15097E+01,  0.17128E+01,
          0.19003E+01,  0.21034E+01,  0.23065E+01,  0.25097E+01,  0.27128E+01,
          0.29003E+01,  0.31034E+01,  0.33065E+01,  0.35097E+01,  0.37128E+01,
          0.39003E+01,  0.40878E+01, I, I, I, I, I, I, I, I, I, I, I, I, I,

VARDP   = 0.1E+01,  0.923E+00,  0.858E+00,  0.8E+00,  0.75E+00,  0.705E+00,
          0.667E+00,  0.639E+00,  0.612E+00,  0.591E+00,  0.573E+00,
          0.558E+00,  0.536E+00,  0.522E+00,  0.512E+00,  0.505E+00,
          0.498E+00,  0.489E+00,  0.478E+00,  0.465E+00,  0.451E+00,
          0.436E+00,  0.42E+00,  0.408E+00,  0.401E+00,  0.401E+00,
          0.401E+00, I, I, I, I, I, I, I, I, I, I, I, I, I,

$END
D2331 - STREAMTUBE//REPORT// PROGRAM

        TEST CASE FOR REPORT

   INJECTION PARAMETERS--
             W STAR= 3.50000000E+00     R= 7.80000000E-04          DN= 2.03200000E+01
   INITIAL VALUES--P= 1.73260000E+04   RHO= 1.70080000E-06  ENTHALPY= 8.02802640E+10
                  T= 2.87000000E+03    U2= 3.03210000E+05          V2= 3.45719769E+02
                 FE= 3.00000000E-02
 H2O          1
 O2           2
 N2           3
 H2           4
 NO           5
 OH           6
 N            7
 O            8
 H            9
 NO+         10
 N2+         11
 N+          12
```

```
O+              13
H+              14
E-              15

   X=DISTANCE ALONG STREAMLINE FROM INJECTION SITE/NOSE DIAMETER
   RHO=GAS DENSITY,G/CM**3
   R HAT=DROPLET RADIUS DIVIDED BY INITIAL DROPLET RADIUS
   LAMBDA SUB D=DEBYE LENGTH,CHARACTERISTIC DISTANCE OF FIELD BEYOND WHICH THE EFFECT OF A CHARGE IS NOT FELT,CM

   TEMPERATURE=GAS TEMPERATURE,DEG.K                               U=GAS VELOCITY,CM/SEC
   Z=COMPRESSIBILITY FACTOR                                        M BAR=MEAN MOLECULAR WEIGHT FOR IONS,G/MOLE
   S=DISTANCE ALONG STREAMLINE FROM INJECTION SITE,CM              TIME=ELAPSED TIME AFTER WATER INJECTION,SEC

   V=DROPLET VELOCITY,CM/SEC                                       ENTHALPY=SPECIFIC ENTHALPY OF GAS,ERG/G
   A SUM=SUM OF MASS FRACTIONS OF SPECIES                          W SUM=SUM OF ALL THE GROSS REACTION RATES,MOLE/CM**3-SEC,=0.0
   PRESSURE=GAS PRESSURE,DYNES/CM**2                               MACH NUMBER

   N SUB E=ELECTRON CONCENTRATION,ELECTRONS/CM**3
   FE=EFFICIENCY FACTOR FOR CAPTURE OF ELECTRONS BY WATER DROPLET OR CATALYTIC EFFICIENCY

   F=FRACTION OF WATER EVAPORATED
   CAPITAL U=NORMALIZED RELATIVE VELOCITY BETWEEN DROPLET AND GAS

   X            RHO              TEMPERATURE      U                V                ENTHALPY         N SUB E          F
                 R HAT           Z                M BAR            A SUM            W SUM            FE               CAPITAL U
                LAMBDA SUB D     S                TIME             PRESSURE         EM

 0.000000   1.69794503E-06   2.87442936E+03   3.03210000E+05   3.45719769E+02   8.02800688E+10   1.03986930E+12   0.
            1.00000000E+00   1.23098765E+00   2.99997763E+01   9.94944397E-01  -3.87771583E-18   3.00000000E-02   2.12379678E+00
            3.62773481E-04   0.               0.               1.73260000E+04   2.50752429E+00

        GAMMA,SPECIFIC CONCENTRATION OF SPECIES,MOLES/G,ON RETURN FROM INTEGRATION
         1 0.               9.78351600E-06   2.62559210E-02   0.               5.86199800E-05
         6 0.               2.01766700E-03   1.43393190E-02   0.               1.01648560E-06
        11 4.92986500E-14   2.58991780E-13   1.59388910E-11   0.               1.01650185E-06

        X,MOLE FRACTION OF SPECIE
           0.               2.29211566E-04   6.15132716E-01   0.               1.37336898E-03
           0.               4.72705940E-02   3.35946480E-01   0.               2.38145730E-05
           1.15498567E-12   6.06774818E-12   3.73421801E-10   0.               2.38149537E-05

        W,NET RATE OF PRODUCTION OR DISAPPEARANCE OF SPECIES,MOLE/CM**3-SEC
         1 0.              -4.10506688E-06   2.79522812E-06   0.               9.99898901E-06
         6 0.              -6.89624362E-06   6.88302419E-06   0.              -8.69321371E-06
        11 7.13939703E-12  -2.19758121E-12   2.13342736E-08   0.               0.

        LOWER CASE K SUB J,J=1,45,REACTION RATE CONSTANTS FOR A PARTICULAR REACTION,CM**3/MOLE-SEC
           8.12807257E+06   3.51012965E+06   6.84643620E-02   1.06394682E+08   1.96555567E+04   6.47714336E+07   2.40555199E+12
           2.35421897E+13   9.53710703E+09   5.76345143E+10   7.31421473E+07   8.47566225E+11   3.79601923E+12   8.72018000E+10
           4.30167004E+06   7.31101221E+01   8.45881519E-13   1.06378657E-01   5.63761105E-11   2.40840919E-09   2.50886332E-09
           1.96440443E+03   4.61927713E+12   1.03502394E+11   3.22759684E+11   1.61271557E+05   6.58923026E+06   2.25152743E+07
```

8.05219631E+12	2.18779306E+13	9.30829116E+14	6.10644081E+02	3.62297977E+10	3.73281198E+12	1.31103829E+09
1.01046708E+02	2.20441360E+10	4.46320053E+09	1.27294680E+07	9.24264027E+02	2.95285058E+12	2.95285058E+12
2.95285058E+12	2.95285058E+12	2.95285058E+12				

UPPER CASE K SUB J,J=1,40,EQUILIBRIUM CONSTANTS,MOLES/CM**3 OR DIMENSIONLESS

1.52911482E-08	2.20415997E-08	1.48666453E-16	4.63367423E-08	1.70046476E-11	2.83528181E-08	7.77404193E-01
1.63429054E+00	5.99751584E-04	7.71479739E-04	8.74269537E-06	5.39316698E-01	3.30000503E-01	1.81742627E-03
6.87764147E-10	9.07544680E-15	1.34921449E-30	1.16951869E-20	9.01794061E-29	7.65395155E-28	9.07321365E-28
1.15364936E-10	1.49614479E-02	1.76276853E-03	1.48703044E-03	7.71081357E-09	6.54453118E-08	7.75807493E-08
1.17820717E-01	9.93908108E-02	8.43576691E-01	5.94873644E-12	5.84348213E-04	7.48571339E-03	1.31955800E-05
4.62457265E-12	9.08962962E-05	5.96097962E-05	1.03007064E-06	1.40138352E-11		

CONTRIBUTION OF INDIVIDUAL REACTIONS TO GROSS REACTION,W,MOLE-CM**3/G**2-SEC

AA	AB	AC	AD	AE	AF	AG
AH	AI	AJ	AK	AL	AM	AN
AO	AP	AQ	AR	AS	AT	AU
AV	AW	AX	AY	AZ	BA	BB
BC	BD	BE	BF	BG	BH	BI
BJ	BK	BL	BM	BN	BO	BP
BQ	BR	BS	BT			

0.	2.37165123E+03	1.35872754E+02	0.	2.42364481E+03	0.	0.
0.	0.	1.42625033E+06	9.61966479E+05	0.	0.	0.
6.33813958E+03	1.06064516E-04	5.42254738E-14	1.62214013E-05	2.84062243E-13	8.79918532E-11	0.
-3.21929658E-06	-7.01037076E-04	-1.80800066E-03	0.	-1.32233259E-05	-1.97081906E-03	0.
-5.14449010E-03	0.	0.	2.51201831E-04	9.15684008E-04	-7.44705045E+03	-2.61861255E+00
0.	5.93911754E-04	0.	1.82291010E-04	0.	3.00153009E+06	1.45571547E-01
7.64764028E-01	4.70651636E+01	0.	0.			

GAMMA CORRECTED TO MAKE ASUM=1.0

0.	9.78351600E-06	2.62559210E-02	0.	5.86199800E-05
0.	2.01766700E-03	1.43393190E-02	0.	1.01648560E-06
4.92986500E-14	2.58991780E-13	1.59388910E-11	0.	1.01650185E-06

ASUM= 9.94944397E-01

FGAM(1)= 0.

GAMMA,COMPOSITION AFTER WATER ADDITION AND CORRECTION

0.	9.78351600E-06	2.62559210E-02	0.	5.86199800E-05
0.	2.01766700E-03	1.43393190E-02	0.	1.01648560E-06
4.92986500E-14	2.58991780E-13	1.59388910E-11	0.	1.01650185E-06

ASUM= 9.94944397E-01

X	RHO	TEMPERATURE	U	V	ENTHALPY	N SUB E	F
	R HAT	Z	M BAR	A SUM	W SUM	FE	CAPITAL U
	LAMBDA SUB D	S	TIME	PRESSURE	EM		
.101807	1.72137253E-06	2.40985322E+03	1.61103489E+05	1.81918868E+04	9.57785969E+09	2.78421466E+11	1.69424865E-01
	9.39128313E-01	1.09199131E+00	2.99999995E+01	9.96826338E-01	8.97240085E-17	3.00000000E-02	1.09449689E+00
	6.41937916E-04	2.06871094E+00	1.85793400E-04	1.59918227E+04	1.30061277E+00		

GAMMA,SPECIFIC CONCENTRATION OF SPECIES,MOLES/G,ON RETURN FROM INTEGRATION

```
 1 1.95926887E-02   4.87344039E-04   1.65312253E-02   1.69369741E-04   1.20311686E-03
 6 2.28948921E-03   1.53114292E-07   5.61645665E-03   4.61557202E-04   2.68460796E-07
11 9.83179955E-18   2.22850465E-20   8.04809249E-15   7.44084463E-16   2.68460805E-07

X,MOLE FRACTION OF SPECIE
   4.22694058E-01   1.05139949E-02   3.56645831E-01   3.65399483E-03   2.59561287E-02
   4.93936030E-02   3.30329861E-06   1.21169835E-01   9.95766789E-03   5.79179230E-06
   2.12111942E-16   4.80779177E-19   1.73630119E-13   1.60529311E-14   5.79179249E-06

W,NET RATE OF PRODUCTION OR DISAPPEARANCE OF SPECIES,MOLE/CM**3-SEC
 1-1.66511595E-04   1.00792367E-04   2.69013807E-09   2.95296302E-05   3.15594067E-08
 6 2.02680963E-04  -2.33020988E-08  -2.37772025E-04   7.12829662E-05  -1.36375840E-08
11-4.01122446E-18  -8.13721508E-21  -1.39217644E-15   1.04353378E-16   0.

LOWER CASE K SUB J,J=1,45,REACTION RATE CONSTANTS FOR A PARTICULAR REACTION,CM**3/MOLE-SEC
   1.95426066E+05   7.76513317E+04   4.09996994E-05   3.85676599E+06   1.49340249E+02   2.53768877E+06   1.23818433E+12
   1.99415828E+13   1.68996435E+09   1.81673860E+10   5.25419083E+06   4.39668816E+11   2.12856604E+12   2.52317334E+10
   4.56004330E+05   7.21639494E-01   4.19156160E-18   7.27298171E-05   6.27703175E-16   5.53027187E-14   5.80650034E-14
   1.30364309E+01   1.88248889E+12   2.04520052E+10   6.32836138E+10   2.40479731E+03   2.02634026E+05   6.97744814E+05
   3.57487553E+12   9.63765432E+12   8.45683716E+14   3.13449339E+00   5.84743117E+09   1.46317120E+12   1.10898205E+08
   2.91576460E-01   3.24057932E+09   3.83458590E+08   4.43395622E+05   4.35530839E+00   1.51149415E+10   1.51149415E+10
   1.51149415E+10   1.51149415E+10   1.51149415E+10

UPPER CASE K SUB J,J=1,40,EQUILIBRIUM CONSTANTS,MOLES/CM**3 OR DIMENSIONLESS
   2.79276784E-10   4.20429358E-10   7.53948473E-20   1.39064380E-09   1.08719305E-13   9.02462977E-10   4.65868816E-01
   1.54094277E+00   1.20469546E-04   2.58591135E-04   6.93481689E-07   3.09460655E-01   2.00825534E-01   5.99871658E-04
   6.03392297E-11   7.22874233E-17   5.45009925E-36   6.56003912E-24   8.39611722E-34   1.48248981E-32   1.75885134E-32
   8.30802857E-13   6.49121386E-03   3.67631481E-04   3.09866964E-04   1.27988828E-10   2.25987952E-09   2.68115983E-09
   5.66352441E-02   4.77363665E-02   8.42873855E-01   3.30967765E-14   1.06833899E-04   3.25874433E-03   1.19801701E-06
   1.54187561E-14   1.46453721E-05   5.75077841E-06   3.92755047E-08   7.67768707E-14

CONTRIBUTION OF INDIVIDUAL REACTIONS TO GROSS REACTION,W,MOLE-CM**3/G**2-SEC
        AA               AB               AC               AD               AE               AF               AG
        AH               AI               AJ               AK               AL               AM               AN
        AO               AP               AQ               AR               AS               AT               AU
        AV               AW               AX               AY               AZ               BA               BB
        BC               BD               BE               BF               BG               BH               BI
        BJ               BK               BL               BM               BN               BO               BP
        BQ               BR               BS               BT

  -1.18477613E+02   4.63107277E+02   9.85799910E-07   1.68632752E+01   8.59238878E-02   3.12315180E+02   3.38976000E+07
  -5.29427412E+06   3.97916640E+03  -1.17519236E+05   9.07872035E+02  -4.09345344E+07  -1.51389271E+07   1.21040810E+05
   5.44666487E+02   2.63494269E-08   9.38082629E-19   3.69252596E-07   2.06693117E-21   3.72464048E-15   3.04750336E-16
   1.27754582E-07  -2.56935892E-10   3.50948151E-07   1.48347306E-07   4.04915108E-10   5.62684883E-04   1.46514557E-04
   3.49517822E-09   9.78621642E-10   1.92826323E-04  -3.69762127E-09   1.14460316E-09  -4.06997830E-04   5.53109961E-07
   9.28710681E-10  -2.89747700E-08   3.05879576E-09   2.43693563E-10   2.45702614E-08   4.05776924E+03   1.48607075E-07
   3.36837174E-10   1.21646447E-04   1.12467932E-05   0.

GAMMA CORRECTED TO MAKE ASUM=1.0
   1.95778953E-02   4.88247455E-04   1.65323972E-02   1.65707045E-04   1.20434615E-03
   2.29057128E-03   1.53125145E-07   5.62686818E-03   4.51575824E-04   2.68735096E-07
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    9.83249648E-18   2.22866262E-20   8.06301167E-15   7.27993308E-16   2.68460805E-07
ASUM=   9.96826337E-01

FGAM(1)=   2.00250518E-02
GAMMA,COMPOSITION AFTER WATER ADDITION AND CORRECTION
    1.97973453E-02   4.84000003E-04   1.64487353E-02   1.60281028E-04   1.19591424E-03
    2.26740488E-03   1.52350259E-07   5.57791789E-03   4.36789138E-04   2.66853620E-07
    9.78273935E-18   2.21738452E-20   7.99286844E-15   7.04155432E-16   2.66853629E-07
ASUM=   9.96842292E-01

X           RHO              TEMPERATURE      U                V                ENTHALPY         N SUB E          F
            R HAT            Z                M BAR            A SUM            W SUM            FE               CAPITAL U
            LAMBDA SUB D     S                TIME             PRESSURE         EM

.201073     1.72547798E-06   2.22606350E+03   1.43560973E+05   2.32739587E+04  -3.70713870E+09   1.87574931E+11   2.14887789E-01
            9.22256962E-01   1.06640393E+00   2.99999999E+01   9.97114558E-01   4.01790934E-17   3.00000000E-02   9.58500428E-01
            7.51675626E-04   4.08581044E+00   2.82315746E-04   1.48660103E+04   1.14438113E+00

GAMMA,SPECIFIC CONCENTRATION OF SPECIES,MOLES/G,ON RETURN FROM INTEGRATION
  1 2.22828965E-02   1.10026245E-03   1.50313788E-02   1.64965814E-04   1.09305398E-03
  6 2.66234168E-03   4.67983605E-08   3.82319735E-03   3.76830759E-04   1.80434014E-07
 11 8.16984892E-19   9.42418774E-22   1.18530402E-15   1.29562171E-16   1.80434016E-07

X,MOLE FRACTION OF SPECIE
    4.78838210E-01   2.36435915E-02   3.23010005E-01   3.54495813E-03   2.34886883E-02
    5.72111854E-02   1.00565217E-06   8.21568673E-02   8.09773388E-03   3.87735501E-06
    1.75562267E-17   2.02516813E-20   2.54710537E-14   2.78416757E-15   3.87735504E-06

W,NET RATE OF PRODUCTION OR DISAPPEARANCE OF SPECIES,MOLE/CM**3-SEC
  1-7.80187245E-05   7.42042178E-05   8.67359525E-10   2.87519424E-05   7.88704862E-09
  6 5.30790753E-05  -4.06104548E-09  -1.23471113E-04   4.54544889E-05  -5.56072219E-09
 11-1.43269629E-19  -2.14307227E-22  -1.49570299E-16   1.23219133E-18   0.

LOWER CASE K SUB J,J=1,45,REACTION RATE CONSTANTS FOR A PARTICULAR REACTION,CM**3/MOLE-SEC
    2.86875975E+04   1.09713539E+04   9.16271548E-07   7.01351401E+05   1.22217840E+01   4.80174630E+05   8.86695751E+11
    1.84188940E+13   7.01932702E+08   1.01273200E+10   1.37598847E+06   3.16112995E+11   1.59247775E+12   1.34633227E+10
    1.45681828E+05   6.85636846E-02   8.21812254E-21   1.76678632E-06   1.86104170E-18   2.37318709E-16   2.50177146E-16
    1.01124739E+00   1.19651222E+12   8.98108419E+09   2.76796661E+10   2.82086437E+02   3.44032773E+04   1.18929913E+05
    2.37379145E+12   6.37419902E+12   8.09569402E+14   2.13247248E-01   2.31559622E+09   9.11689839E+11   3.15709573E+07
    1.47803385E-02   1.22347779E+09   1.10036415E+08   8.02262767E+04   2.83631413E-01   8.87205956E+09   8.87205956E+09
    8.87205956E+09   8.87205956E+09   8.87205956E+09

UPPER CASE K SUB J,J=1,40,EQUILIBRIUM CONSTANTS,MOLES/CM**3 OR DIMENSIONLESS
    3.59375628E-11   5.52524322E-11   1.55631902E-21   2.31104058E-10   8.19001552E-15   1.54591091E-10   3.57410197E-01
    1.49493776E+00   5.29785739E-05   1.48229050E-04   1.90026383E-07   2.32468525E-01   1.55503815E-01   3.40689866E-04
    1.77701694E-11   6.28101053E-18   9.77525617E-39   1.45537963E-25   2.29731047E-36   5.89288371E-35   6.99946088E-35
    6.71663664E-14   4.25508712E-03   1.65882387E-04   1.39657273E-04   1.57849568E-11   4.04903544E-10   4.80937119E-10
    3.89844867E-02   3.28212488E-02   8.41905372E-01   2.33978915E-15   4.46586350E-05   2.13077541E-03   3.53458112E-07
    8.36264502E-16   5.77863342E-06   1.73882295E-06   7.40808099E-09   5.37777482E-15

CONTRIBUTION OF INDIVIDUAL REACTIONS TO GROSS REACTION,W,MOLE-CM**3/G**2-SEC
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        AA                  AB                  AC                  AD                  AE                  AF                  AG
        AH                  AI                  AJ                  AK                  AL                  AM                  AN
        AO                  AP                  AQ                  AR                  AS                  AT                  AU
        AV                  AW                  AX                  AY                  AZ                  BA                  BB
        BC                  BD                  BE                  BF                  BG                  BH                  BI
        BJ                  BK                  BL                  BM                  BN                  BO                  BP
        BQ                  BR                  BS                  BT

      3.45581001E+01    2.32491161E+02    1.02892153E-07    2.92188523E+01    2.08170831E-02    2.99828655E+02    2.48845051E+07
      7.44175024E+05    1.36165816E+03   -3.88037382E+04    2.91326639E+02   -1.72918518E+07   -8.87415013E+06    3.87816483E+04
      2.66901244E+02    1.60915184E-09    3.85837771E-20    1.23047387E-07    4.28870913E-23    2.68151427E-16    2.60140224E-17
      1.07023351E-08   -6.19850588E-12    9.09621298E-09    7.11186044E-09    1.60268095E-11    8.63502549E-05    2.69341111E-05
      8.77174149E-11    3.03214270E-11    2.84901746E-05   -5.26020912E-11    4.61797504E-11   -7.51113626E-05    1.24055514E-08
      4.33404250E-11   -1.36560064E-09    1.43194251E-10    9.72631861E-12    1.09911765E-09    1.60082132E+03    7.24833862E-09
      8.36119549E-12    1.05160878E-05    1.14948330E-06    0.

 GAMMA CORRECTED TO MAKE ASUM=1.0
      2.22796429E-02    1.10076884E-03    1.50314954E-02    1.64141629E-04    1.09332624E-03
      2.66271250E-03    4.67987237E-08    3.82495695E-03    3.74948076E-04    1.80478958E-07
      8.16991231E-19    9.42426086E-22    1.18584955E-15    1.28914865E-16    1.80434016E-07
 ASUM=    9.97114558E-01

 FGAM(1)=    2.24117214E-02
 GAMMA,COMPOSITION AFTER WATER ADDITION AND CORRECTION
      2.23376245E-02    1.09783970E-03    1.50109999E-02    1.62751753E-04    1.09107891E-03
      2.65471755E-03    4.67349133E-08    3.81477875E-03    3.71773188E-04    1.80107983E-07
      8.15877258E-19    9.41141083E-22    1.18269400E-15    1.27823274E-16    1.80107984E-07
 ASUM=    9.97118468E-01

 X          RHO               TEMPERATURE        U                  V                  ENTHALPY           N SUB E            F
            R HAT             Z                  M BAR              A SUM              W SUM              FE                 CAPITAL U
            LAMBDA SUB D      S                  TIME               PRESSURE           EM

.302636   1.66198967E-06    2.14402118E+03    1.35374842E+05    2.67903644E+04   -1.14768154E+10    1.33692994E+11    2.44398108E-01
          9.10419934E-01    1.05570381E+00    2.99999999E+01    9.97275186E-01    7.84977468E-18    3.00000000E-02    8.81648663E-01
          8.73794489E-04    6.14956044E+00    3.64366823E-04    1.38604821E+04    1.05424749E+00

 GAMMA,SPECIFIC CONCENTRATION OF SPECIES,MOLES/G,ON RETURN FROM INTEGRATION
  1 2.40430942E-02    1.48674132E-03    1.42049716E-02    2.65708441E-04    1.01077811E-03
  6 2.62483527E-03    2.26066794E-08    2.70472592E-03    4.27666964E-04    1.33516017E-07
 11 2.18522759E-19    1.48628809E-22    3.60464867E-16    6.17403821E-17    1.33516017E-07

 X,MOLE FRACTION OF SPECIE
    5.14083926E-01    3.17891618E-02    3.03727444E-01    5.68131694E-03    2.16122258E-02
    5.61236258E-02    4.83370835E-07    5.78318293E-02    9.14427694E-03    2.85480885E-06
    4.67240351E-18    3.17794712E-21    7.70737712E-15    1.32011869E-15    2.85480886E-06

 W,NET RATE OF PRODUCTION OR DISAPPEARANCE OF SPECIES,MOLE/CM**3-SEC
  1-4.25930438E-05    4.58174821E-05    3.72633668E-10    2.19186816E-05    3.04573077E-09
  6 1.74502734E-05   -9.51025472E-10   -6.64923996E-05    2.38984510E-05   -2.83997263E-09
 11-2.45082712E-20   -9.08483583E-24   -2.30311294E-17    6.28855450E-19    0.
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LOWER CASE K SUB J,J=1,45,REACTICN RATE CONSTANTS FOR A PARTICULAR REACTION,CM**3/MOLE-SEC
   1.09213026E+04   4.10122674E+03   1.35776724E-07   2.97569119E+05   3.47366234E+00   2.07829410E+05   7.50768476E+11
   1.77192155E+13   4.52199069E+08   7.56211154E+09   7.03308804E+05   2.68188677E+11   1.37827627E+12   9.83488526E+09
   8.22717132E+04   2.10713274E-02   3.60371212E-22   2.73905215E-07   1.00426544E-19   1.54168477E-17   1.62850135E-17
   2.80714198E-01   9.54236712E+11   5.94966453E+09   1.83003717E+10   9.63616226E+01   1.41479302E+04   4.90050326E+04
   1.93514294E+12   5.18596309E+12   7.92926916E+14   5.54242679E-02   1.45646774E+09   7.19871050E+11   1.68270977E+07
   3.31425981E-03   7.51339005E+C8   5.88831817E+07   3.40625144E+04   7.21186369E-02   6.56398738E+09   6.56398738E+09
   6.56398738E+09   6.56398738E+C9   6.56398738E+09

UPPER CASE K SUB J,J=1,40,EQUILIBRIUM CONSTANTS,MOLES/CM**3 OR DIMENSIONLESS
   1.28320452E-11   1.99333935E-11   2.21878201E-22   9.38571703E-11   2.23558762E-15   6.37492052E-11   3.12684581E-01
   1.47228769E+00   3.50684783E-05   1.12152887E-04   9.92482690E-08   2.01289493E-01   1.36718859E-01   2.56500666E-04
   9.66438565E-12   1.85321588E-18   4.11188205E-40   2.16055809E-26   1.19355725E-37   3.69198614E-36   4.38857690E-36
   1.90315737E-14   3.44506479E-03   1.11373171E-04   9.36951123E-05   5.52430067E-12   1.70881133E-10   2.03122375E-10
   3.23283242E-02   2.71969087E-02   8.41271836E-01   6.19566266E-16   2.88088251E-05   1.72175429E-03   1.91757236E-07
   1.93728818E-16   3.62571488E-06   9.53754202E-07   3.20853022E-09   1.41698680E-15

CONTRIBUTION OF INDIVIDUAL REACTIONS TO GROSS REACTION,W,MOLE-CM**3/G**2-SEC
      AA               AB               AC               AD               AE               AF               AG
      AH               AI               AJ               AK               AL               AM               AN
      AO               AP               AQ               AR               AS               AT               AU
      AV               AW               AX               AY               AZ               BA               BB
      BC               BD               BE               BF               BG               BH               BI
      BJ               BK               BL               BM               BN               BO               BP
      BQ               BR               BS               BT

   6.19820965E+01   1.16708864E+02   2.42188975E-C8   4.13751478E+01   7.22062154E-03   2.67607042E+02   1.65687328E+07
   7.75889034E+05   5.69683802E+02  -1.84076543E+04   1.34904162E+02  -8.26071103E+06  -7.14106883E+06   1.81991129E+04
   1.51755001E+02   3.31738528E-10   5.67415476E-21   5.01490581E-08   3.70512889E-24   4.45957552E-17   6.78779601E-18
   2.72553317E-09  -6.46315259E-13   1.10954004E-09   2.20366770E-09   2.32965535E-12   2.50568285E-05   1.22577399E-05
   8.29403891E-12   4.88216327E-12   1.28884380E-05  -2.47597875E-13   6.73427469E-12  -3.19725253E-05   1.07522540E-09
   6.48492615E-12  -2.27959306E-10   2.04110787E-11   1.42047163E-12   1.79317356E-10   8.76397451E+02   1.43438063E-09
   9.75597629E-13   2.36608684E-06   4.05263089E-07   0.

GAMMA CORRECTED TO MAKE ASUM=1.0
   2.40373549E-02   1.48794069E-03   1.42054515E-02   2.63422797E-04   1.01122894E-03
   2.62550002E-03   2.26074433E-08   2.70690785E-03   4.23988142E-04   1.33575567E-07
   2.18530142E-19   1.48633831E-22   3.60755659E-16   6.12092868E-17   1.33516017E-07
ASUM=   9.97275185E-C1

FGAM(1)=   2.42293046E-02
GAMMA,COMPOSITION AFTER WATER ADDITION AND CORRECTION
   2.41137262E-02   1.48245061E-03   1.41788466E-02   2.59889254E-04   1.00835517E-03
   2.61431084E-03   2.25651026E-C8   2.69692013E-03   4.18300782E-04   1.33195965E-07
   2.18120865E-19   1.48355460E-22   3.59424572E-16   6.03882279E-17   1.33195965E-C7
ASUM=   9.97280250E-01
```

APPENDIX

The definitions of the output symbols are given as follows:

FORTRAN symbol	Symbol in text	Description
X	x	Distance along streamline from injection site divided by nose diameter
RHO	ρ	Gas density, g/cm^3
RHAT	$\hat{r}$	Droplet radius divided by initial droplet radius
LAMBDASUBD	λ_D	Debye length, cm
TEMPERATURE	T	Gas temperature, ^{o}K
Z	Z	Compressibility factor
S	s	Distance from injection site, cm
U	u	Gas velocity, cm/sec
MBAR	$\overline{M}$	Mean molecular weight of ions, g/mol
TIME	t	Elapsed time after water injection, sec; $t_n = t_{n-1} + \frac{d_N}{v}\left(x_n - x_{n-1}\right)$ where n refers to values at end of forward integration step
V	v	Droplet velocity, cm/sec
ASUM	$\sum \gamma_i(MW)_i$	Sum of mass fraction of species i, where $\gamma_{15} = \sum_{i=10}^{14} \gamma_i$
PRESSURE	p	Gas pressure, $dynes/cm^2$
ENTHALPY	h	Specific enthalpy of mixture, ergs/g

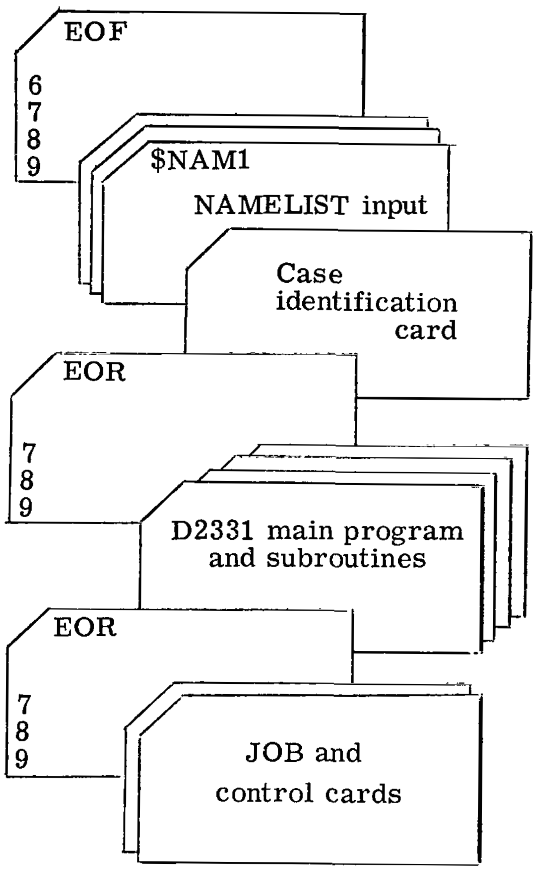
APPENDIX

FORTRAN symbol	Symbol in text	Description
WSUM	$\sum W_i$	Sum of all gross reaction rates for all species i where i = 1 to 15, ≈ 0, mol/cm^3-sec
EM	M	Mach number
NSUBE	N_e	Electron number density, electrons/cm^3
FE	F_e	Efficiency factor for capture of electrons by water droplet
F	f	Mass fraction of water evaporated
CAPITALU	U	Normalized relative velocity between droplet and gas
GAMMA	γ_i	Specific concentration of species i after integration where i = 1 to 15, mol/g
X	X_i	Mole fraction of species i where i = 1 to 15
W	W_i	Net rate of production or disappearance of species i where i = 1 to 15, mol/cm^3-sec
LOWERCASE KSUBJ	k_j	Reaction rate constant for reaction j where j = 1 to 45, cm/mol-sec
UPPERCASE KSUBJ	K_j	Equilibrium constant in mol/cm^3 for reaction j = 1 to 6 and j = 17 to 21 and dimensionless for all other j (j = 1 to 40)
AA,AB,AC etc., to BT	$k_j\left(B_{ij} - G_{ij}\right)$	Contribution of individual reactions to gross reaction W, mol-cm^3/g^2-sec

After each integration step, the concentrations are examined. If a concentration is negative, it is set equal to 0.0 and a comment "NEGATIVE GAMMAS" is printed. The concentrations are corrected to make the sum of the mass fractions of the species (ASUM) equal to 1.0. The corrected concentrations are printed when answers are printed. After the addition of water and a second correction to make the sum of the mass fractions of the species equal to 1.0, the concentrations are again printed when answers are printed.

Program Operation

The following sketch shows the deck setup:



The program stops are given in the following table:

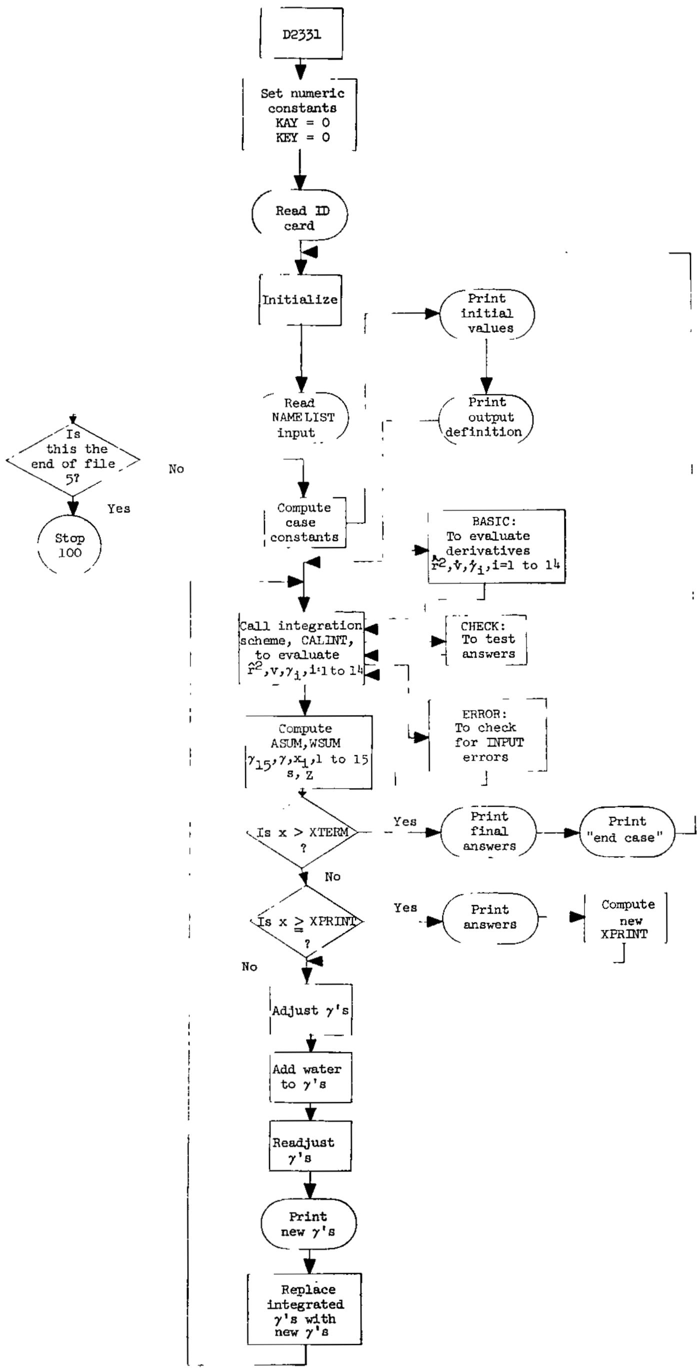
Stop	Subroutine	Reason	Action
11	BASIC	Iteration failed to converge	Reexamine input data
12	CHECK	Computing interval less than 10E-20	Vary ELE1 and ELE2
13	ERROR	Input data in error	Vary other parameters
			(HEPS, CI, CIMAX)
100	MAIN	EOF,5	Normal stop

APPENDIX

Flow Charts

The flow charts for the D2331 main program and for the BASIC, CHECK, and ERROR subroutines are as follows:

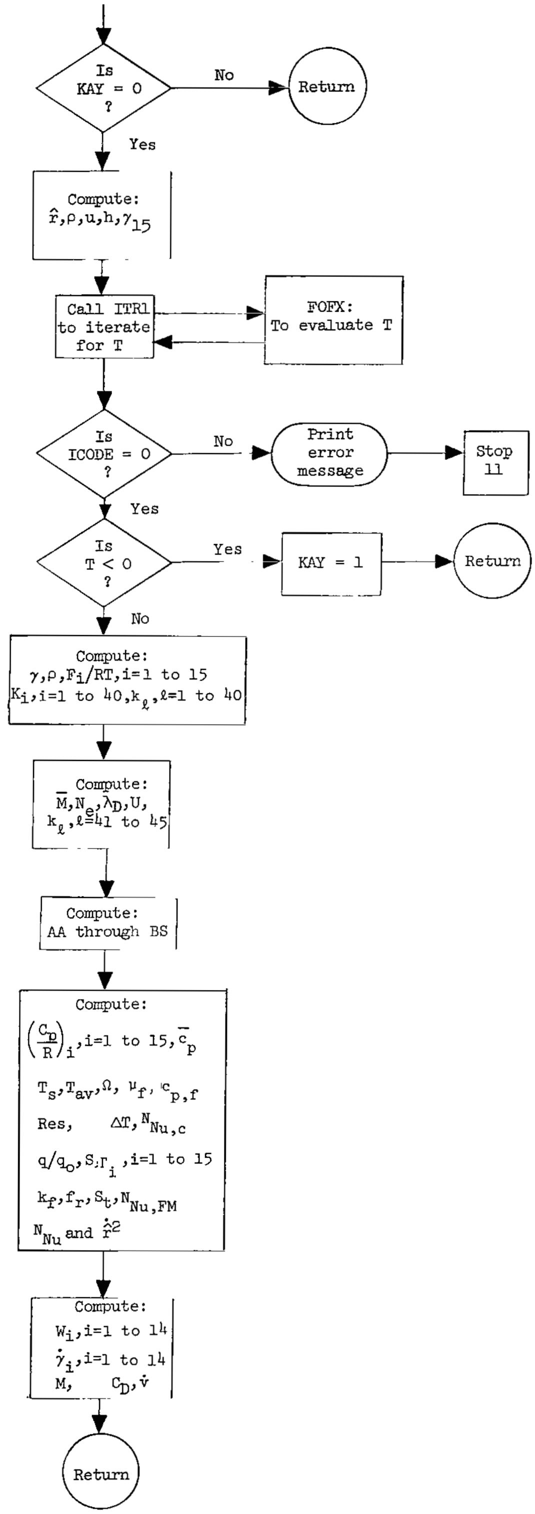
D2331 Main Program



APPENDIX

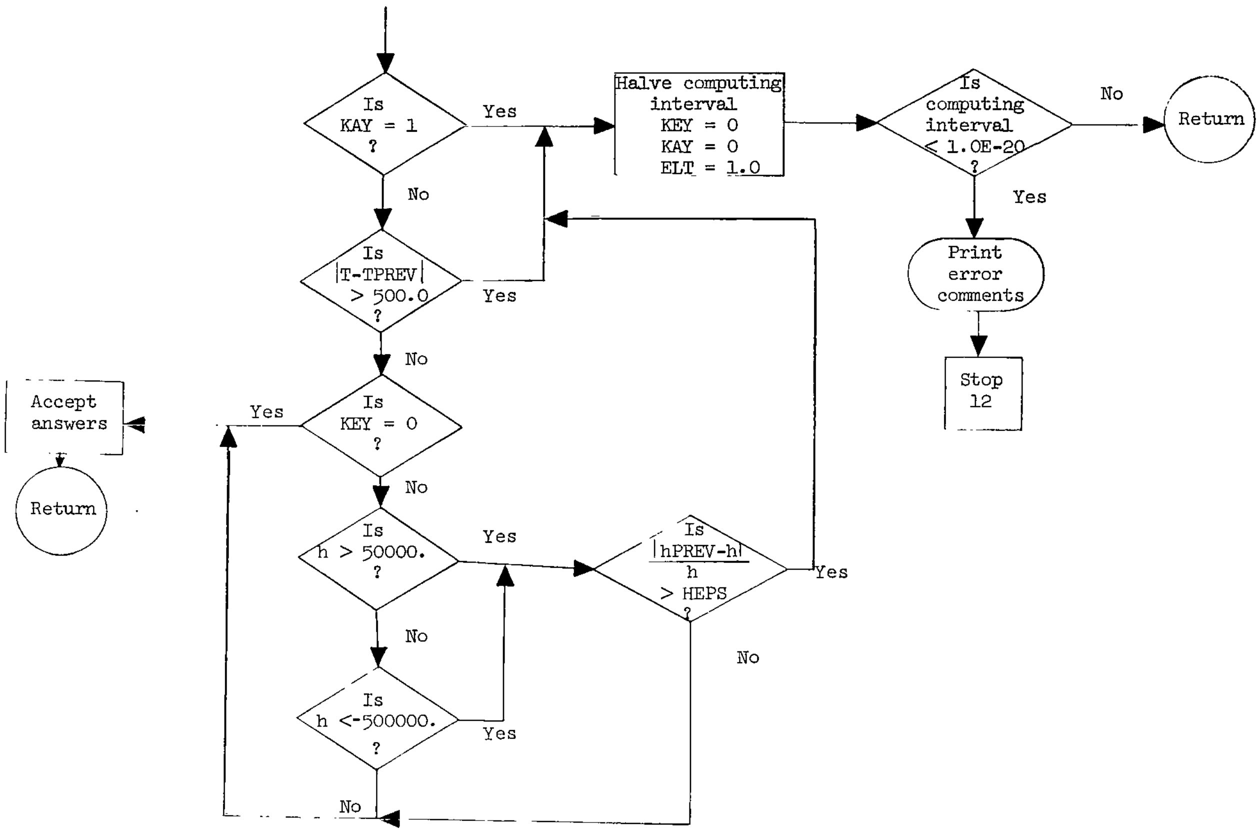
Subroutine BASIC

Used by CALINT to evaluate derivatives $\dot{\hat{r}}^2$, $\dot{v}$, $\dot{\gamma}_i$, i = 1 to 14



APPENDIX

Subroutine CHECK



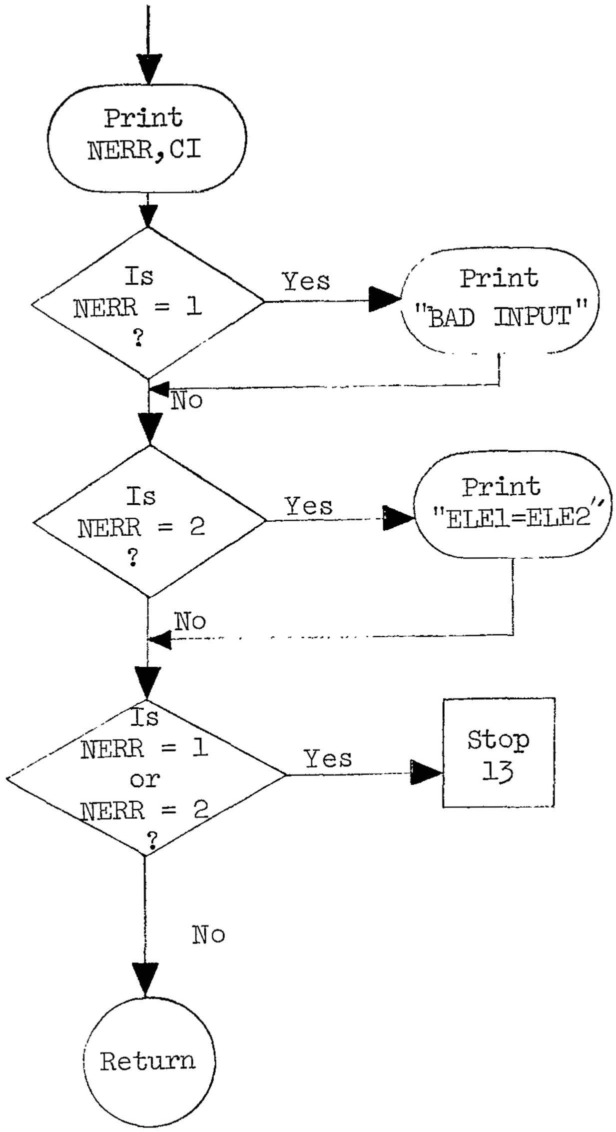
Subroutine FOFX

$$T = T_{estimate} + 0.1\left(T_{estimate}\, R \sum_{i=1}^{15} \gamma_i \left(\frac{H_i}{RT}\right) - h\right)$$

Return

APPENDIX

Subroutine ERROR



Complete Program

The complete program including comments is reproduced in the following pages.

```
      PROGRAM D2331(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
C     ------------------------------------------------------------------
C               STREAMTUBE // REPORT // PROGRAM         12-14-67
C     ------------------------------------------------------------------
C
C     STREAMTUBE ANALYSIS TO CALCULATE ELECTRON CONCENTRATION IN THE
C     PRESENCE OF ACCELERATING AND EVAPORATING WATER DROPLETS
C
C     ///// INPUT /////
C
C     IN = ONE CARD - 80 COLS - FOR IDENTIFICATION
C
C$NAM1
C     RHOL   = WATER DENSITY,G/CM**3
C     HL     = SPECIFIC ENTHALPY OF WATER,ERGS/G
C     DN     = REFERENCE LENGTH GIVEN AS NOSE DIAMETER,CM
C     EL     = LATENT HEAT OF WATER,ERGS/G
C     ENTHAL = INITIAL SPECIFIC ENTHALPY,ERGS/G
C     TW     = DROPLET SURFACE TEMPERATURE,DEG.K
C     FRO    = DROPLET RECOVERY FACTOR FOR ZERO MASS TRANSFER
C     CPVW   = HEAT CAPACITY OF VAPOR AT DROPLET SURFACE,ERGS/G-DEG.K
C     WASK   = INITIAL MASS FLOW RATIO,WATER TO GAS
C     R      = INITIAL DROPLET RADIUS,CM
C     HASK   = TOTAL SPECIFIC ENTHALPY OF SHOCKED GAS,ERGS/G
C     U2     = INITIAL GAS VELOCITY AT INJECTION SITE,CM/SEC
C     P2     = INITIAL GAS PRESSURE AT INJECTION SITE,DYNES/CM**2
C     RHO2   = INITIAL GAS DENSITY AT INJECTION SITE,G/CM**3
C     T      = INITIAL TEMPERATURE OF MIXTURE,DEG.K
C     PRDEL  = PRINT ANSWERS EVERY PRDEL X. =0.1 UNLESS INPUT OTHERWISE
C
C     VAR(1) = X
C     VAR(2) = R HAT SQUARED,(DROPLET RADIUS/INITIAL DROPLET RADIUS)**2
C     VAR(3) = V, DROPLET VELOCITY,CM/SEC
C     VAR(4) = GAMMA FOR I=1  SPECIFIC CONCENTRATION OF H2O,MOLE/G
C     VAR(5) =           I=2                           O2
C     VAR(6) =           I=3                           N2
C
C     ETC FOR 14 GAMMAS                                ETC
C
C     DER(1) = DERIVATIVE OF R HAT SQUARED
C     DER(2)=  V DOT
C     DER(3)=  GAMMA(1) DOT
```

```
       C      DER(4)=  GAMMA(2) DOT
       C      ETC FOR 14 GAMMAS
       C
       C      ELE1  = AN ARRAY OF 16 VALUES USED BY THE INTEGRATION  SCHEME TO
       C              CONTROL THE SIZE OF THE COMPUTING INTERVAL
       C              0.0.LT.ELE1.LE.65.0
       C              INITIALLY 0.5 UNLESS INPUT OTHERWISE
       C      ELE2  = AN ARRAY OF 16 VALUES USED BY THE INTEGRATICN SCHEME TO
       C               CONTROL THE SIZE OF THE COMPUTING INTERVAL.
       C               ELE2.LT.ELE1
       C              INITIALLY 0.1 UNLESS INPUT OTHERWISE
       C      CI     =  INITIAL COMPUTING INTERVAL,=.0001220703125 UNLESS INPUT
       C      CIMAX  =  MAXIMUM COMPUTING INTERVAL , = .1 UNLESS INPUT OTHERWISE
       C      XTERM  =  TERMINAL VALUE OF X
       C      HEPS   =  PERCENT BY WHICH ENTHALPY ALLOWED TO VARY IN TWO
       C               SUCCESSIVE STEPS WHEN ENTHALPY.GT.50000..OR.ENTHALPY
       C               .LT.-500000.      TEST IN SUBROUTINE CHECK
       C               0.1 UNLESS INPUT OTHERWISE
       C      FE     = EFFICIENCY FACTOR FOR CAPTURE OF ELECTRONS BY WATER
       C                    DROPLET OR --- CATALYTIC EFFICIENCY
       C      NTLUP  = NUMBER OF POINTS IN VARIX AND VARDP TABLES
       C      VARIX  = TABLE OF X VALUES FOR  P/P2
       C      VARDP  = TABLE OF P/P2 VALUES CORRESPONDING TO VARIX
       C      IBUG   = 0 NO DEBUG PRINT OUT, 0 UNLESS INPUT
       C             = 1 FOR DEBUG PRINT OUT AT DESIRED PLACES
       C              ARRAY OF 20
       C$
       C
       C                  STOPS
       C         STOP 11  IN BASIC AT ITR1
       C         STOP 12  IN CHECK WHEN CI.LT.1.0E-20
       C         STOP 13  IN ERROR WHEN SOME INPUT IN ERROR
       C      STOP 100  EOF,5    NORMAL STOP
       C
000003        COMMON VAR(20),DER(20),ELE1(20),ELE2(20),CI,SPEC,NDE,ELT,NERR
000003        COMMON RHOL,HL,DN,EL,    TW,CDC,CDFM,FRO,CPVW,WASK,R,HASK
000003        COMMON   T
000003        COMMON  E1,E2,P2,U2,RHO2,V2
000003        COMMON  F,NE,Z,XI(15),FAC1,FAC2,U,RHOU,RHO2U2,RHO
000003        COMMON KLC(45),KUC(40),MBAR,FE,CAPU,LAMD,P
C00003        COMMON AA,AB,AC,AD,AE,AF,AG,AH,AI,AJ,AKK,AL,AM,AN,AO,AP,AQ,AR,
             1 AS,AT,AU,AV,AW,AX,AY,AZ,BA,BB,BC,BD,BE,BF,BG,BH,BI,BJ,BKK,
             2 BL,BM,BN,BO,BP,BQ,BR,BS,BT
```

```
000003          COMMON  NTLUP,VARIX(40),VARDP(40)
000003          EQUIVALENCE (AA,ALPDUM(1))
000003          DIMENSION ALPDUM(46)
           C
           C             LAB1 IN MAIN,BASIC,FOFX  CHECK
000003          COMMON/LAB1/IBUG,CUVAR,A1,A2,A3,A4,A5,A6,TLIM1,TLIM2,TLIM3
           C            LAB2 IN MAIN,BASIC,CHECK,FOFX
000003          COMMON/LAB2/ENTHAL
           C              LAB3 IN MAIN ,BASIC AND CHECK
000003          COMMON /LAB3/ TPREV,KEY,HEPS,KAY
           C            LAB4  IN MAIN AND BASIC
000003          COMMON /LAB4/ MW(15),W(15),GAMMA,HCITR,B,DELTX,EM
           C
000003          DIMENSION A1(15,4),A2(15,4),A3(15,4),A4(15,4),A5(15,4),A6(15,4)
000003          DIMENSION CUVAR(20),IBUG(20)
000003          DIMENSION SPECIE (15), FGAM(15)
000003          DIMENSION  IN(8)
           C
000003          REAL INITX,MW
000003          REAL LH,NE
           C
000003          DOUBLE PRECISION VAR
           C
           C               MOLECULAR WEIGHT OF SPECIES
000003          DATA (MW (I),I=1,15) / 18.,32.,28.,2.,30.,17.,14.,16.,1.,30.,28.,
               1 14.,16.,1., 5.486E-4/
           C               THE 15 SPECIES
000003          DATA (SPECIE(I),I=1,15) / 3HH2O,2HO2,2HN2,2HH2,2HNO,2HOH,1HN,1HO,
               1 1HH,3HNO+,3HN2+,2HN+,2HO+,2HH+,2HE-/
000003          DATA (A1(I),I=1,60)/ 4.20307985,3.81416055,3.69148176,3.45380035,
               1 3.87682186,3.44021610, 2.5  ,3.04980070,2.50020545,3.68482747,
               2 3.76510471,2.80887381,2.50047586, 2.5,  2.5,
               3 3.48589794,3.85044317,3.34031165,2.97106943,3.71537602,
               4 3.01845824,2.75947630,2.58926700,2.94053868,3.26815342,
               5 3.09030675,2.55758547,2.54621952,2.5       ,2.5       , 30*0./
000003          DATA (A2(I),I=1,60) / -2.14625506E-3,-3.24091983E-3,
               1 -1.33248199E-3, 4.21222704E-4,-3.14787008E-3, 5.67061081E-4, 0.,
               2 -2.38674835E-3,-1.36545791E-6,-1.27472750E-3,-1.98295059E-3,
               3 -1.48986257E-3,-2.87279601E-6, 0.,0.,
               4  1.81720121E-3, 3.89989763E-4, 7.71936051E-4, 7.60556499E-4,
               5  4.81403278E-4, 7.91617340E-4,-3.58661047E-4,-1.11816431E-4,
               6 -6.70062044E-4, 8.74276324E-4, 1.03070158E-3,-7.92952860E-5,
               7 -5.12662872E-5, 0., 0., 30*0./
```

```
000003          DATA (A3(I),I=1,60) /  6.72040236E-6, 1.04955352E-5,
               1  2.64950496E-6,-1.10268215E-6, 8.40430066E-6,-1.79909482E-6, 0.,
               2  4.31872217E-6, 3.01173718E-9, 2.48461737E-6, 4.53722826E-6,
               3  2.87577760E-6, 5.66990999E-9, 0., 0.,
               4 -3.41338632E-7,-2.89418093E-8,-1.75622629E-7,-1.16571433E-7,
               5 -9.72194239E-8,-1.39046762E-7, 1.23219036E-7, 4.36058822E-8,
               6  2.93518521E-7,-2.18467818E-7,-1.55910644E-7, 3.11152083E-8,
               7  6.71501704E-9, 0., 0., 30*0./
000003          DATA (A4(I),I=1,60) / -5.56262948E-09,-1.03969441E-08,
               1 -9.78420615E-10, 1.22466555E-9,-7.20675049E-09, 2.32091070E-09,0,
               2 -3.61567602E-09,-2.74516450E-12,-8.11027164E-10,-2.91306271E-09,
               3 -2.51218974E-09,-5.16787546E-12, 0., 0.,
               4  2.68468828E-11, 1.16076839E-12, 1.61416590E-11, 8.39248279E-12,
               5  9.43591661E-12, 1.12282753E-11,-1.08890156E-11,-4.77729929E-12,
               6 -4.67055452E-11, 2.27116436E-11, 9.92335507E-12,-2.92816335E-12,
               7  1.65349937E-12, 0., 0., 30*0./
000003          DATA (A5(I),I=1,60) / 1.74338938E-12, 3.52280537E-12,
               1 -9.81789775E-14,-3.64412032E-13, 2.15362612E-12,-8.49441471E-13,
               20,1.14963730E-12, 8.94961997E-16,-1.55190996E-13, 5.75631866E-13,
               3  8.22728827E-13, 1.87850329E-15, 0., 0.,
               4 -7.46344776E-16,-3.23099982E-17,-4.45648938E-16,-2.12101689E-16,
               5 -3.02796533E-16,-3.17987057E-16, 3.06742425E-16, 1.68389768E-16,
               6  2.41598190E-15,-7.03854576E-16,-2.28531083E-16, 8.69691886E-17,
               7 -1.04213024E-16, 0., 0., 30* 0./
000003          DATA (A6(I),I=1,60) / -2.87498491E4,-2.19318605E1,-1.90713653E1,
               1  4.18216914   , 1.07744359E4,4.68483226E3,5.66215000E4,
               2  2.96493580E4, 2.59754478E4,1.18655571E5,1.80779386E5,
               3  2.25281087E5, 1.87666445E5,1.83755000E5, 0.,
               4 -2.87104401E4,-2.61240243E2,-4.75889275E1, 2.20188265E2,
               5  1.05804742E4, 4.84850446E3, 5.64949247E4, 2.97246231E4,
               6  2.57823978E4, 1.18658935E5, 1.80896602E5, 2.25312369E5,
               7  1.87643224E5, 1.83755000E5, 0.,  30*0./
          C
          C     INPUT
000003          NAME LIST /NAM1/ RHOL,HL,DN,EL,ENTHAL,TW,FRO,CPVW,
               1 WASK,R,HASK,      IBUG,           U2,   P2,RHO2,T ,
               2 PRDEL,          VAR,DER,ELE1,ELE2,CI,CIMAX,XTERM,    HEPS ,
               3 FE,NTLUP,VARIX,VARDP
          C
          C        ***** SET NUMERICAL CONSTANTS *****
          C
          C     TLIM1=1000. DEG.K
C00003          TLIM1=1000.
```

```
                C      TLIM2=15000. DEG K
      C00005           TLIM2=15000.
                C        TLIM3=1000000.
      000006           TLIM3=1000000.
      000010           SAVECI=.0001220703125
      000011           PRDEL=.1
      000013           CIMAX=.1
      000014           FAC1=  4./(3.*2.7182818284 * 3.1415926536**.5 )
      000022           FAC2=  1./(2.*2.7182818284**1.5)
                C       *** READ IDENTIFICATION CARD
      000027           READ(5,2) (IN(I),I=1,8)
      000040         2 FORMAT( 8A10)
                C       KEY SET = 1 IN CHECK TO ALLOW TESTING OF ENTHALPY AFTER FIRST INTERVAL
                C       KAY SET = 1 IN BASIC WHEN T.LT.0.
                C                    BEGIN NEW CASE  AT EFN 1
                C       *** INITIALIZE
      000040         1 CONTINUE
      000040           HEPS=0.1
      000042           KEY=0
      000043           CI=SAVECI
      000044           KAY=0
      000045           DO 4 I=1,46
      000046           ALPDUM(I)=0.
      000047           IF(I.GT.20) GO TO 4
      000053           VAR(I)=0.
      000055           DER(I)=0.
      000056           CUVAR(I)=0
      000057           IBUG(I)=0.
      000060           ELE1(I)= .5
      000061           ELE2(I)= .1
      000063           IF(I.GT.15) GO TO 4
      000066           W(I)=0.
      000067         4 CONTINUE
                C
                C       *** READ NAMELIST  INPUT
      000071           READ(5,NAM1)
                C
      000074           IF(EOF,5) 7,9
      000077         7 PRINT 8
      000103         8 FORMAT(// 18H  EOF,5 - NAMELIST//)
      000103           STOP 100
      000105         9 CONTINUE
                C
```

```
000105         WRITE(6,NAM1)
         C                                                                    0012
         C         ***** CCMPUTE CASE CONSTANTS FROM INPUT
         C
000110         INITX=VAR(1)
000112         TIME=0.
         C                     EQUATION (10)
000113         VAR(3)=( (600.*RHO2*U2*WASK)/3.141592653589793)/
              1 (RHOL*VAR(2)*SQRT(VAR(2))) +1.
000151         V2=VAR(3)
000153         U=U2
000154         RHO2U2=RHO2*U2
000155         RHOU= RHO2U2
         C         *** PRINT INITIAL VALUES ***
000156         PRINT 5
000162       5 FORMAT(1X,*D2331 - STREAMTUBE//REPORT// PROGRAM*/)
000162         PRINT 3, (IN(I),I=1,8)
000174       3 FORMAT( 8A10/ )
000174         PRINT 6, WASK,R,DN,P2,RHO2,ENTHAL,T,U2,V2,FE
000224       6 FORMAT(26H     INJECTION PARAMETERS--/ 15X 7HW STAR=E15.8,6X
              1 2HR=E15.8, 10X 3HDN=E15.8/
              2                22H    INITIAL VALUES--P=E15.8,8H    RHO=E15.8,
              213H    ENTHALPY=E15.8/22H                        T=E15.8,8H     U2=
              3E15.8,13H            V2=E15.8/ 19X 3HFE=E15.8)
000224         DO 10 I=1,15
000226      10 PRINT 11,SPECIE(I),I
000237      11 FORMAT(2X,A10,I5)
000237         F=0.
000240         XPREV=VAR(1)
000242         TPREV=T
000244         DO 42 I=1,14
000245      42 FGAM(I)=VAR(I+3)
000252         D1GI2= 16.*(FGAM(1)+2.*FGAM(2)+FGAM(5)+FGAM(6)+FGAM(8)+FGAM(10)
              1 +FGAM(13))
000263         D2GI2= 14.*(2.*FGAM(3)+FGAM(5)+FGAM(7)+FGAM(10)+2.*FGAM(11)
              1  +FGAM(12))
000273         DO 40 I=1,17
000274      40 CUVAR(I)=VAR(I)
000301         NDE=16
000302         PHMAX=65.
000303         XPRINT=VAR(1)
000305         IFIN=0
000306         IWAY=1
```

```
             C      *** DEFINE OUTPUT
000307              PRINT 45
000313           45 FORMAT(/5X,61HX=DISTANCE ALONG STREAMLINE FROM INJECTION SITE/NOSE
                   1 DIAMETER/5X,23HRHO=GAS DENSITY,G/CM**3/5X,54HR HAT=DROPLET RADIUS
                   2 DIVIDED BY INITIAL DROPLET RADIUS/5X,109HLAMBDA SUB D=DEBYE LENGT
                   3H,CHARACTERISTIC DISTANCE OF FIELD BEYOND WHICH THE EFFECT OF A CH
                   4ARGE IS NOT FELT,CM//
                   45X,33HTEMPERATURE=GAS TEMPERATURE,DEG.K,27X,21HU=GAS VELOCITY,CM/S
                   5EC/5X,24HZ=COMPRESSIBILITY FACTOR,36X,43HM BAR=MEAN MOLECULAR WEIG
                   6HT FOR IONS,G/MOLE/5X,50HS=DISTANCE ALONG STREAMLINE FROM INJECTIO
                   7N SITE,CM,10X,43HTIME=ELAPSED TIME AFTER WATER INJECTION,SEC//
                   85X,25HV=DROPLET VELOCITY,CM/SEC,35X,39HENTHALPY=SPECIFIC ENTHALPY
                   9OF GAS,ERG/G/5X,38HA SUM=SUM OF MASS FRACTIONS OF SPECIES,22X,
                   A61HW SUM=SUM OF ALL THE GROSS REACTION RATES,MOLE/CM**3-SEC,=0.0/
                   B5X,33HPRESSURE=GAS PRESSURE,DYNES/CM**2,27X,11HMACH NUMBER//
                   C5X,46HN SUB E=ELECTRON CONCENTRATION,ELECTRONS/CM**3/
                   D5X,86HFE=EFFICIENCY FACTOR FOR CAPTURE OF ELECTRONS BY WATER DROPL
                   EET OR CATALYTIC EFFICIENCY//
                   F5X,30HF=FRACTION OF WATER EVAPORATED/
                   G5X,62HCAPITAL U=NORMALIZED RELATIVE VELOCITY BETWEEN DROPLET AND G
                   HAS/)
             C
             C                    REINITIALIZE EACH COMPUTING INTERVAL SINCE GAMMAS ARE
             C                    ALTERED
000313          101 CONTINUE
000313              ELT= 0
000314              SPEC=0
000315          102 CONTINUE
             C
             C         ***** CALINT EVALUATES DERIVATIVES IN SUBROUTINE BASIC
             C               SEE SUBROUTINE BASIC FOR DETAILS OF CALCULATION PROCEDURE
             C               FOR R HAT SQUARED DOT, V DOT AND GAMMA 1 DOT THRU GAMMA
             C               14 DOT  AND THUS THE EVALUATION OF THE BULK OF THE
             C               EQUATIONS AND AUXILIARY RELATIONSHIPS
             C
000315              CALL CALINT(VAR,DER,ELE1,ELE2,CI,SPEC,NDE,CUVAR,ELT,CIMAX,NERR,
                   1 PHMAX)
000331              IWAY=-1*IWAY
             C             GO TO 51 TO PRINT INITIA3 CONDITIONS
000334              IF(INITX.EQ.VAR(1)) GO TO 51
000336              IF(IWAY.EQ.-1.AND.VAR(1).NE.INITX) GO TO 102
             C
             C      5/13/67   TREAT THE PRODUCT RHO*U AS CONSTANT OVER AN INTERVAL
```

```
000346          IF(WASK.EQ.0.) VAR(3)=U
000351          RHOU= RHO*U
000353       51 CONTINUE
          C
000353          DO 59 I=1,14
000355       59 FGAM(I)=VAR(I+3)
000362       57 CONTINUE
          C       *** COMPUTE  ASUM,WSUM,GAMMA(15),X,S,Z,TIME
          C                ASUM SHOULD BE = 1.0
000362          ASUM= 18.* FGAM(1)+32.*FGAM(2)+28.*(FGAM(3)+FGAM(11)) + 2.*FGAM(4)
               1 +30.*(FGAM(5)+FGAM(10)) + 17.*FGAM(6) + 14.*(FGAM(7)+FGAM(12))
               2 +16.*(FGAM(8)+FGAM(13)) + FGAM(9) + FGAM(14)
          C
          C                WSUM SHOULD BE = 0.0    I=1,14
000414       63 CONTINUE
000414          WSUM=0.
000415          DO  65 I=1,14
000417       65 WSUM= WSUM + MW(I)* W(I)
000424          FWASK= F*WASK
000426          FGAM(15)=0.
000427          DO 68 I= 10,14
000430       68 FGAM(15)= FGAM(15)+FGAM(I)
000434          GAMMA=0.
000435          DO 67 I=1,15
000436       67 GAMMA=GAMMA+FGAM(I)
000442          DO 66 I=1,15
          C                EQUATION (39)
000443       66 XI(I)= FGAM(I)/GAMMA
000447          S= VAR(1)*DN
          C                EQUATION (41)
000455          Z =   GAMMA*(1.0+ FWASK)/(.034674063 + FWASK/18.)
000462          IF(VAR(3).EQ.0.) TIME =0.
000464          IF(VAR(3).EQ.0.) GO TO 69
000465          TIME=TIME+DN*(VAR(1)-XPREV)/VAR(3)
000513       69 XPREV= VAR(1)
          C               TPREV USED IN CHECK
000515          TPREV=T
          C        *** TERMINATION TEST
000517          IF(VAR(1).LT.XTERM) GO TO 52
000521          IF(IFIN.NE.0) GO TO 82
000522          XPRINT=VAR(1)
000524          IFIN=1
000525          GO TO 54
```

```
000526        52 CONTINUE
         C        *** TEST  PRINT FREQUENCY
000526           IF(XPRINT-VAR(1).GT.0.0) GO TO 81
         C             PRINT ANSWERS EVERY PRDEL IN X
000532           XPRINT=XPRINT+PRDEL
000533        54 CONTINUE
000533           IKY=0
         C        *** PRINT ANSWERS
000534           PRINT 70
000540        70 FORMAT(5X 1HX 10X 3HRHO 14X 11HTEMPERATURE 6X 1HU 16X 1HV 16X
                1 8HENTHALPY 9X 7HN SUB E 10X 1HF/
                1 16X 5HR HAT 12X 1HZ 16X 5HM BAR 12X 5HA SUM 12X 5HW SUM 12X 2HFE
                215X 9HCAPITAL U/ 15X 12HLAMBDA SUB D 6X 1HS 16X 4HTIME
                3 13X 8HPRESSURE  9X 2HEM/)
         C
000540           FX=VAR(1)
000542           FV=VAR(3)
000544           FRHAT= SQRT(VAR(2))
000547           PRINT 71 ,FX     ,RHO,T,U,FV     ,ENTHAL,NE,F
000572        71 FORMAT(F11.6,7E17.8)
         C
000572           PRINT 72 , FRHAT ,Z,MBAR,ASUM,WSUM,FE,CAPU
000614        72 FORMAT(E28.8,6E17.8)
         C
000614           PRINT 73, LAMD,S,TIME,P,EM
000632        73 FORMAT(E28.8,4E17.8/)
         C
000632           PRINT 74, (FGAM(I),I=1,15)
000644        74 FORMAT(11X,74HGAMMA,SPECIFIC CONCENTRATION OF SPECIES,MOLES/G,ON R
                1ETURN FROM INTEGRATION/12X,1H1,E15.8,4E17.8/12X,1H6,E15.8,4E17.8/
                211X,2H11,E15.8,4E17.8/)
         C
000644           PRINT 75,  (XI(I),I=1,15)
000656        75 FORMAT(11X 25HX,MOLE FRACTION OF SPECIE/ 3(E28.8,4E17.8/))
         C
000656           PRINT 76, (W(I),I=1,15)
000670        76 FORMAT(11X,67HW,NET RATE OF PRODUCTION OR DISAPPEARANCE OF SPECIES
                1,MOLE/CM**3-SEC/12X,1H1,E15.8,4E17.8/12X,1H6,E15.8,4E17.8/11X,2H11
                2,E15.8,4E17.8 /)
         C
000670           PRINT 77, (KLC(I),I=1,45)
000702        77 FORMAT(11X,90HLOWER CASE K SUB J,J=1,45,REACTION RATE CONSTANTS FO
                1R A PARTICULAR REACTION,CM**3/MOLE-SEC/6(E28.8,6E17.8/)E28.8,2E17.
```

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                 28/)
              C
000702             PRINT 78,  (KUC(I),I=1,40)
000714          78 FORMAT(11X,76HUPPER CASE K SUB J,J=1,40,EQUILIBRIUM CONSTANTS,MOLE
                  1S/CM**3 OR DIMENSIONLESS/ 5(E28.8,6E17.8/),E28.8,4E17.8/)
              CCCCC
000714             PRINT 179
000720         179 FORMAT(11X,76HCONTR IBUTION CF INDIVIDUAL REACTIONS TO GROSS REACTI
                  1ON,W,MOLE-CM**3/G**2-SEC)
000720             PRINT 79
000724          79 FORMAT(16X 2HAA 15X 2HAB 15X 2HAC 15X 2HAD 15X2HAE15X2HAF15X2HAG/
                  116X 2HAH 15X 2HAI 15X 2HAJ 15X 2HAK 15X 2HAL 15X 2HAM 15X 2HAN/
                  216X 2HAO 15X 2HAP 15X 2HAQ 15X 2HAR 15X 2HAS 15X 2HAT 15X 2HAU/
                  316X 2HAV 15X 2HAW 15X 2HAX 15X 2HAY 15X 2HAZ 15X 2HBA 15X 2HBB/
                  416X 2HBC 15X 2HBD 15X 2HBE 15X 2HBF 15X 2HBG 15X 2HBH 15X 2HBI/
                  516X 2HBJ 15X 2HBK 15X 2HBL 15X 2HBM 15X 2HBN 15X 2HBO 15X 2HBP/
                  616X 2HBQ 15X 2HBR 15X 2HBS 15X 2HBT/)
              C
000724          80 FORMAT(6(E28.8,6E17.8/),E28.8,3E17.8/)
000724             PRINT 80, AA,AB,AC,AD,AE,AF,AG,    AH,AI,AJ,AKK,AL,AM,AN,
                  1          AO,AP,AQ,AR,AS,AT,AU,    AV,AW,AX,AY,AZ,BA,BB,
                  2          BC,BD,BE,BF,BG,BH,BI,    BJ,BKK,BL,BM,BN,BO,BP,
                  3          BQ,BR,BS,BT
              C
001064          81 CONTINUE
              C       *** TEST FOR NEGATIVE GAMMAS, IF NEGATIVE SET = 0.0
001064             DO 61 I=1,15
001066             IF(FGAM(I).GE.0.0) GO TO 61
001070             PRINT 37
001073          37 FORMAT(19H     NEGATIVE GAMMAS)
001073             VAR(I+3)=0.
001076             FGAM(I)=0.
001077          61 CONTINUE
              C
              C      REPLACE GAMMAS WITH ADJUSTED VALUES
              C
001101             IPATH= 1
001102          30 CONTINUE
001102             B1=(D1GI2 +(16./18.)* FWASK)/(1.0+FWASK)
001111             B2= D2GI2/(1.0+FWASK)
001113             B3= ((2./18.)*FWASK)/(1.0+FWASK)
001120             D1=  B1/(16.*(FGAM(1)+2.*FGAM(2)+FGAM(5)+FGAM(6)+FGAM(8)+FGAM(10)
                  1 +FGAM(13)))
```

```
001132          D2= B2/(14.*(2.*FGAM(3)+FGAM(5)+FGAM(7)+FGAM(10)+2.*FGAM(11)
               1 +FGAM(12)))
001143          D3= B3/(2.*FGAM(1)+2.*FGAM(4)+FGAM(6)+FGAM(9)+FGAM(14))
001152          IF(FGAM(1).EQ.0..AND.  FGAM(4).EQ.0. .AND.
               1   FGAM(6).EQ.0. .AND.   FGAM(9).EQ.0. .AND. FGAM(14).EQ.0.) D3=0.
001167          D4=  (2.*D3+16.*D1)/18.
001174          D5= (14.*D2+16.*D1)/30.
001177          D6= (D3+16.*D1)/17.
          C
          C                         EQUATION (32)
001202          FGAM(2)= FGAM(2)*D1
001203          FGAM(8)= FGAM(8)*D1
001204          FGAM(13)=FGAM(13)*D1
          C
          C                         EQUATION (33)
001205          FGAM(3)= FGAM(3) * D2
001207          FGAM(7)= FGAM(7) * D2
001210          FGAM(11)=FGAM(11)* D2
001211          FGAM(12)=FGAM(12)* D2
          C
          C                         EQUATION (34)
001212          FGAM(4 )=FGAM(4 ) *D3
001213          FGAM(9 )=FGAM(9 ) *D3
001214          FGAM(14)=FGAM(14) *D3
          C
          C                         EQUATION (35)
001215          FGAM(1)=FGAM(1)*D4
          C
          C                         EQUATION (36)
001217          FGAM(5 )=FGAM(5 )* D5
001220          FGAM(10)=FGAM(10)* D5
          C
          C                         EQUATION (37)
001221          FGAM(6)= FGAM(6) * D6
          C                         ASUM SHOULD BE = 1.0
001223          ASUM= 18.* FGAM(1)+32.*FGAM(2)+28.*(FGAM(3)+FGAM(11)) + 2.*FGAM(4)
               1 +30.*(FGAM(5)+FGAM(10)) + 17.*FGAM(6) + 14.*(FGAM(7)+FGAM(12))
               2 +16.*(FGAM(8)+FGAM(13)) + FGAM(9) + FGAM(14)
001254          IF(IPATH.EQ.2) GO TO 32
001256          IF(            IKY.EQ.0 ) PRINT 64, (FGAM(I),I=1,15),ASUM
001273       64 FORMAT(11X 32HGAMMA CORRECTED TO MAKE ASUM=1.0/ 3(E28.8,4E17.8/)
               1  11X  5HASUM=E17.8/)
          C
```

```
              C        *** ADD WATER
001273                FOLD= F
001275                RHAT=SQRT(VAR(2))
              C                          EQUATION ( 2)
001277                F=1.0 -RHAT**3
001301                FWASK= F*WASK
              C                          EQUATION (38)
001303                FGAM(1)=FGAM(1)+(WASK/18.)*(F-FOLD)
001307                IF(IKY.EQ.0) PRINT 35, FGAM(1)
001316             35 FORMAT(11X 8HFGAM(1)= E17.8)
001316                IPATH = 2
001317                GO TO 30
001320             32 CONTINUE
001320                FGAM(15)=0.
001321                DO 34 I=10,14
001323             34 FGAM(15)=FGAM(15)+FGAM(I)
              C        *** PRINT GAMMAS AFTER ADJUSTMENT AND WATER ADDITICN
001327                IF(IKY.EQ.0             ) PRINT 33, (FGAM(I),I=1,15),ASUM
001343             33 FORMAT(11X 53HGAMMA,COMPOSITION AFTER WATER ADDITION AND CORRECTIO
                     1N/  3(E28.8,4E17.8/) 11X 5HASUM=E17.8/)
              C                        PUT CORRECTED GAMMAS IN VAR
              C                        OR---REPLACE INTEGRATED GAMMAS WITH ADJUSTED, WATERED
              C                        DOWN GAMMAS----
001343                DO 38 I=1,15
001345                VAR(I+3)=0.
001347             38 VAR(I+3)=FGAM(I)
001354                IKY=1
              C        *** AT INITIAL CONDITIONS, CONTINUE INTEGRATION
001355                IF(VAR(1).EQ.INITX) GO TO 102
              C        *** IS THE CASE  FINISHED
001357                IF(VAR(1).LT. XTERM) GO TO 101
001361                IF(IFIN.NE.0) GO TO 82
              C           TO PRINT FINAL ANSWERS
001362                IPFK=IPF
001364                XPRINT=VAR(1)
001366                IFIN=1
001367                GO TO 57
              C
001367             82 CONTINUE
001367                PRINT 50
001373             50 FORMAT(10H  END CASE/)
001373                GO TO 1
001374                END
```

```
                SUBROUTINE BASIC
          C     SUBROUTINE BASIC EVALUATES DERIVATIVES OF  R HAT SQUARED, V, AND
          C                     GAMMA 1 THRU GAMMA 14
          C
          C     IBUG= 0, NO DEBUG PRINT OUTS
          C           NOT=0 TO GET DEBUG PRINT OUTS
          C      CUVAR(1) = X
          C     CUVAR(2)= RHATS               DER(1) = DRHATD    DERIV R HAT SQUARED
          C     CUVAR(3) = V                  DER(2) = VDOT
          C     CUVAR(4) = GAM(1)             DER(3) = GAMDOT(1)
          C
          C
000002          COMMON VAR(20),DER(20),ELE1(20),ELE2(20),CI,SPEC,NDE,ELT,NERR
000002          COMMON RHOL,HL,DN,EL,    TW,CDC,CDFM,FRO,CPVW,WASK,R,HASK
000002          COMMON   T
000002          COMMON   E1,E2,P2,U2,RHO2,V2
000002          COMMON   F,NE,Z,XI(15),FAC1,FAC2,U,RHOU,RHO2U2,RHO
000002          COMMON KLC(45),KUC(40),MBAR,FE,CAPU,LAMD,P
000002          COMMON AA,AB,AC,AD,AE,AF,AG,AH,AI,AJ,AKK,AL,AM,AN,AO,AP,AQ,AR,
               1 AS,AT,AU,AV,AW,AX,AY,AZ,BA,BB,BC,BD,BE,BF,BG,BH,BI,BJ,BKK,
               2 BL,BM,BN,BO,BP,BQ,BR,BS,BT
000002          COMMON  NTLUP,VARIX(40),VARCP(40)
000002          EQUIVALENCE (AA,ALPDUM(1))
000002          DIMENSION ALPDUM(46)
          C
          C             LAB1 IN MAIN,BASIC,FOFX
000002          COMMON/LAB1/IBUG,CUVAR,A1,A2,A3,A4,A5,A6,TLIM1,TLIM2,TLIM3
          C            LAB2 IN MAIN,BASIC,CHECK,FOFX
C00002          COMMON/LAB2/ENTHAL
          C              LAB3 IN MAIN ,BASIC AND CHECK
000002          COMMON /LAB3/ TPREV,KEY,HEPS,KAY
          C             LAB4 IN MAIN AND BASIC
000002          COMMON /LAB4/ MW(15),W(15),GAMMA,HCITR,B,DELTX,EM
          C
000002          DIMENSION MULT(40),DLT(40),SIGLT(40)
000002          DIMENSION  GAM(15), GAMDOT(15),FORT(15)
000002          DIMENSION         CPOR(15),G(15)
000002          DIMENSION  TKETAB(82),ZOMTAB(82)
000002          DIMENSION EMTAB(20),CDCTAB(20),CDFMTB(20),AYATAB(20),ENTAB(20)
000002          DIMENSION AK(3),BK(3),CK(3),DK(3),EK(3)
000002          DIMENSION A7(15,4)
000002          DIMENSION A1(15,4),A2(15,4),A3(15,4),A4(15,4),A5(15,4),A6(15,4)
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```
000002        DIMENSION CUVAR(20),IBUG(20)
           C
C00002        REAL NLT
000002        REAL MULT,KUC,KLC
C00002        REAL NU,NUFM,MUF,KF,NUC,NE,LAMD,MBAR,MW
           C
C00002        DOUBLE PRECISICN VAR
           C
000002        EQUIVALENCE   (CUVAR(1),X),(CUVAR(2),RHATS),
             1 (CUVAR(3),V),(CUVAR(4),GAM(1))
C00002        EQUIVALENCE (DER(1),DRHATD),(DER(2),VDOT),(DER(3),GAMDOT(1))
           C
000002        DATA (A7(I),I=1,60) / -.881789073,3.51339873,2.28796557,
             1 -4.06566271, 3.91170120, 2.42672054, 4.18000000,2.53040711,
             2 -.460878520, 3.10953628, 2.72216325, 3.53897944,4.37796250,
             3 -1.15390000,-11.7338,
             4  2.21116037, 2.308005C7, 3.66508552,-1.24873923, 3.78027312,
             5  4.84331426, 2.68820982, 4.65791645,-2.96581444, 4.87313762,
             6  5.88646745, 4.65578522, 4.10796742,-1.15390000,-11.7338,30*0./
           C
           C       CONSTANTS FOR USE IN REACTION RATE FORMULAS
000002        DATA (MULT(I),I=1,40) /10.957,14.933,14.0,1.867,14.483,10.578,
             1 .970,1.778, .968,10.435, 10.182, 8.471, .947, 1.875, 7.467,
             2 7.0, 5* 5.486E-4, 14.483, 9.333,10.182,0.966, 9.545, 10.435,
             3 0.968,7.467,0.933,0.941,10.435,10.182,9.545,9.545,C.968,10.435,
             4 0.968,10.182,1.875 /
000002        DATA (DLT(I),I=1,40) / 217.10, 217.34, 414.50,190.34,275.74,
             1 186.09, 31.440, 4.249,89.646, 58.206,138.93,31.015, 26.766,
             2 62.880, 117.69, 247.27, 661.94, 393.00, 617.75, 578.24,577.81,
             3 268.94, 44.186, 83.698, 84.122, 224.75, 185.24, 184.82, 39.512,
             4 39.937,  0.425, 282.96, 94.744, 46.310, 130.01, 314.40, 99.843,
             5 129.16, 178.44, 287.63 /
000002        DATA(SIGLT(I),I=1,40) / 6* 10.0E-16, 4*1.0E-16, 2.69E-16,
             1 3*1.0E-16, 0.C18E-16,0.066E-16, 5*0.879E-16, 19* 20.0E-16/
           C
000002        DATA (TKETAB(I),I=1,82)/.30,.35,.40,.45,.50,.55,.60,.65,.70,.75,
             1 .80,.85,.90,.95,1.00,1.05,1.10,1.15,1.20,1.25,1.30,1.35,1.40,
             2 1.45,1.50,1.55,1.60,1.65,1.70,1.75,1.80,1.85,1.90,1.95,2.00,
             3 2.10,2.20,2.30,2.4C,2.50,2.60,2.70,2.80,2.90,3.00,3.10,3.20,
             4 3.30,3.40,3.50,3.60,3.70,3.80,3.90,4.00,4.10,4.20,4.30,4.40,
             5 4.50,4.60,4.70,4.80,4.90,5.0C,6.00,7.00,8.00,9.00,10.0,20.0,
             6 30.0,40.0,50.0,60.0,70.0,80.0,90.0,100.,200.,300.,400./
000002        DATA (ZOMTAB(I),I=1,82)/
```

```
            1 2.785,2.628,2.492,2.368,2.257,2.156,2.065,1.982,1.908,1.841,
            2 1.780,1.725,1.675,1.629,1.587,1.549,1.514,1.482,1.452,1.424,
            3 1.399,1.375,1.353,1.333,1.314,1.296,1.279,1.264,1.248,1.234,
            4 1.221,1.209,1.197,1.186,1.175,1.156,1.138,1.122,1.107,1.093,
            5 1.081,1.069,1.058,1.048,1.039,1.030,1.022,1.014,1.007,.9999,
            6 .9932,.9870,.9811,.9755,.9700,.9649,.9600,.9553,.9507,.9464,
            7 .9422,.9382,.9343,.9305,.9269,.8963,.8727,.8538,.8379,.8242,
            8 .7432,.7005,.6718,.6504,.6335,.6194,.6076,.5973,.5882,.5320,
            9 .5016,.4811/
000002        DATA  (EMTAB(I),I=1,20)/ .5,.6,.7,.8,.9,1.0,1.2,1.4,1.6,1.8,2.0,
            1 2.4,2.8,3.2,4.0,5.0,6.0,8.0,10.0,12.0/
000002        DATA (CDCTAB(I),I=1,20)/ 0.520,.551,.586,.625,.666,.712,.801,
            1 .880,.929,.955,.971,.981,.969,.949,.919,.910,.910,.910,.910,.910/
000002        DATA (CDFMTB(I),I=1,20)/ 7.80,6.50,5.57,4.92,4.45,4.10,3.60,
            1 3.23,2.98,2.80,2.68,2.48,2.36,2.28,2.17,2.10,2.05,2.02,2.0,2.0/
000002        DATA (AYATAB(I),I=1,20)/ 0.315,.240,.182,.141,.110,.090,.065,
            1 .055,.049,.047,.046,.0455,.0455,.0453,.0452,.0451,.0449,.0448,
            2 .0447,.0447/
000002        DATA (ENTAB(I),I=1,20)/ 0.410,.460,.500,.545,.590,.620,.670,.690,
            1 .710,.715,.720,.725,.725,.730,.730,.735,.735,.740,.745,.745 /
000002        DATA PI,A,TZ,REMD/3.1415926536,6.02486E23,273.16,8.31696E7/
      C
000002        EXTERNAL FOFX
      C
      C        KAY SET = 1 IN BASIC WHEN T.LT.0.
000002        IF(KAY.NE.0) RETURN
000004        IF(WASK.EQ.0.) RHATS=0.
000006        RHAT= SQRT(RHATS)
000011        MTLUP=1
      C                KNOWN PRESSURE DISTRIBUTION
000012        CALL FTLUP(X,POP2,MTLUP,NTLUP,VARIX,VARDP)
000016        P= POP2 * P2
      C                   COMPUTE F IN MAIN PROGRAM
000020        TEM= 1.+F*WASK
      C       5/13/67   TREAT THE PRODUCT RHO*U AS CONSTANT OVER AN INTERVAL
      C                        EQUATION ( 6)
000023        U=(P2-P)/(2.*RHOU)+(1./TEM)*((P2-P)/(2.*RHO2U2)+U2+
            1     (V2-(1.-F)*V)*WASK)
000043        IF(WASK.EQ.0.) V=U
      C                        EQUATION ( 8)
000045        ENTHAL= (HASK+HL*F*WASK-(1.-F)/2.*V**2*WASK)/TEM - U**2/2.
000062        GAM(15)=0.
000063        DO 10 I= 10,14
```

```
000064         10 GAM(15)= GAM(15)+ GAM(I)
          C
          C       ITERATE FOR T            LFITR1  C5
          C
000071            DELTT=.001
000073            E1=.0000001
000074            E2=.0001
000076            MAXI=100
          C                FOFX VERY SENSITIVE TO SMALL CHANGES IN T
000077            CALL ITR1(T,DELTT,FOFX,E1,E2,MAXI,ICODE)
000105            IF(ICODE.EQ.0) GO TO 12
000106            PRINT 11,ICODE,T,DELTT,MAXI
000122         11 FORMAT(22H  IN BASIC-ITR1-ICODE=I2,4H  T=E17.8,8H  DELTT=E17.8,
                 1 7H  MAXI=I3/)
          C        ***                                              STOP 11
000122            STOP 11
          C
000124         12 CONTINUE
000124            IF(T.GT.0.) GO TO 13
000127            KAY=1
000130            RETURN
000131         13 CONTINUE
000131            SQRTT=SQRT(T)
000134            UMV=U-V
000136            TEM5=UMV*UMV
000137            GAMMA=0.
000140            DO 15 I=1,15
000141         15 GAMMA= GAMMA + GAM(I)
          C
          C       *****    COMPUTE RHO,(F SUB I)/(RT), CAPITAL K(I),I=1,40,
          C
          C                        EQUATION (11)
000145            RHO=P/(REMD*T*GAMMA)
          C
000151            IF(IBUG(1).EQ.0)GO TO 17
          C
          C
000152            PRINT 18,P,POP2,T
000163         18 FORMAT(* P,POP2,T = * 3E17.8)
000163            PRINT 16,F,TEM,U,ENTHAL,GAMMA,RHO,(GAM(I),I=1,15)
000211         16 FORMAT(26H  F,TEM,U,ENTHAL,GAMMA,RHO/6E17.8/6H  GAM=/3(5E20.8/))
          C
000211         17 CONTINUE
```

```
000211          NLT =  ALOG(T)
000214          T2= T**2
000215          T3= T2*T
000216          T4= T3*T
        C                TLIM1=1000.
        C                TLIM2=15000.
        C                TLIM3=1000000.
000217          IF(T.LE.TLIM1) IT=1
000222          IF(T.GT.TLIM1.AND.T.LE.TLIM2) IT=2
000234          IF(T.GT.TLIM2.AND.T.LE.TLIM3) IT=3
000246          IF(T.GT.TLIM3) IT=4
000251          DO 20  I=1,15
        C
        C            (F SUB I)/RT  COEFFICIENTS FROM ZELEZNIK AND GORDON
        C                                              NASA TN D-1454
        C
000253       20 FORT(I)= A1(I,IT)*(1.-NLT)-A2(I,IT)/2.*T- A3(I,IT)/6.*T2-A4(I,IT)
               1 /12.*T3 -A5(I,IT)/20.*T4 +A6(I,IT)/T -A7(I,IT)
        C                FIND CAP K (KUC)
        C             R,UNIVERSAL GAS CONSTANT, 82.1023(ATM CM**3)/ DEG.K
        C             R,UNIVERSAL GAS CONSTANT, 8.31696E7  ERG/(MOLE-DEG.K)
000322          OORT=  1./(82.1023*T)
000325          KUC(1)= EXP(-FORT(6)-FORT(9)+FORT(1)) *OORT
        C                     EQUATION (23)
000334          KUC(2)= EXP(-FORT(8)-FORT(8)+FORT(2)) *OORT
000342          KUC(3)= EXP(-FORT(7)-FORT(7)+FORT(3)) *OORT
000350          KUC(4)= EXP(-FORT(9)-FORT(9)+FORT(4)) *OORT
000356          KUC(5)= EXP(-FORT(7)-FORT(8)+FORT(5)) *OORT
000365          KUC(6)= EXP(-FORT(8)-FORT(9)+FORT(6)) *OORT
        C
000374          KUC(17)=EXP(-FORT(11)-FORT(15)+ FORT(3 )) *OORT
000403          KUC(18)=EXP(-FORT(10)-FORT(15)+ FORT(5 )) *OORT
000412          KUC(19)=EXP(-FORT(12)-FORT(15)+ FORT(7 )) *OORT
000421          KUC(20)=EXP(-FORT(13)-FORT(15)+ FORT(8 )) *OORT
000430          KUC(21)=EXP(-FORT(14)-FORT(15)+ FORT(9 )) *OORT
        C
000437          KUC( 7)= EXP(-FORT(6 ) -FORT(8 ) +FORT(2 ) +FORT(9 ))
000446          KUC( 8)= EXP(-FORT(6 ) -FORT(9 ) +FORT(4 ) +FORT(8 ))
000455          KUC( 9)= EXP(-FORT(6 ) -FORT(7 ) +FORT(5 ) +FORT(9 ))
000464          KUC(10)= EXP(-FORT(2 ) -FORT(7 ) +FORT(5 ) +FORT(8 ))
000473          KUC(11)= EXP(-FORT(5 ) -FORT(7 ) +FORT(3 ) +FORT(8 ))
000502          KUC(12)= EXP(-FORT(6 ) -FORT(6 ) +FORT(1 ) +FORT(8 ))
000510          KUC(13)= EXP(-FORT(4 ) -FORT(6 ) +FORT(1 ) +FORT(9 ))
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000517          KUC(14)= EXP(-FORT(1 ) -FORT(7 ) +FORT(4 ) +FORT(5 ))
000526          KUC(15)= EXP(-FORT(10) -FORT(15) +FORT(7 ) +FORT(8 ))
000535          KUC(16)= EXP(-FORT(11) -FORT(15) +FORT(7 ) +FORT(7 ))
          C
000543          KUC(22)= EXP(-FORT(5 ) -FORT(11) +FORT(3 ) + FORT(10))
000552          KUC(23)= EXP(-FORT(7 ) -FORT(11) +FORT(3 ) + FORT(12))
000561          KUC(24)= EXP(-FORT(8 ) -FORT(11) +FORT(3 ) + FORT(13))
000570          KUC(25)= EXP(-FORT(9 ) -FORT(11) +FORT(3 ) + FORT(14))
000577          KUC(26)= EXP(-FORT(5 ) -FORT(12) +FORT(7 ) + FORT(10))
000606          KUC(27)= EXP(-FORT(5 ) -FORT(13) +FORT(8 ) + FORT(10))
000615          KUC(28)= EXP(-FORT(5 ) -FORT(14) +FORT(9 ) + FORT(10))
000624          KUC(29)= EXP(-FORT(8 ) -FORT(12) +FORT(7 ) + FORT(13))
000633          KUC(30)= EXP(-FORT(9 ) -FORT(12) +FORT(7 ) + FORT(14))
000642          KUC(31)= EXP(-FORT(9 ) -FORT(13) +FORT(8 ) + FORT(14))
000651          KUC(32)= EXP(-FORT(2 ) -FORT(12) +FORT(8 ) + FORT(10))
000660          KUC(33)= EXP(-FORT(5 ) -FORT(12) +FORT(8 ) + FORT(11))
000667          KUC(34)= EXP(-FORT(3 ) -FORT(13) +FORT(7 ) + FORT(10))
000676          KUC(35)= EXP(-FORT(8 ) -FORT(11) +FORT(7 ) + FORT(10))
000705          KUC(36)= EXP(-FORT(6 ) -FORT(12) +FORT(9 ) + FORT(10))
000714          KUC(37)= EXP(-FORT(2 ) -FORT(12) +FORT(5 ) + FORT(13))
000723          KUC(38)= EXP(-FORT(6 ) -FORT(12) +FORT(5 ) + FORT(14))
000732          KUC(39)= EXP(-FORT(5 ) -FORT(12) +FORT(3 ) + FORT(13))
000741          KUC(40)= EXP(-FORT(1 ) -FORT(12) +FORT(4 ) + FORT(10))
          C
000750          IF(IBUG(2).EQ.0)GO TO 22
000751          PRINT 21,OORT,NLT,T, (KUC(I),I=1,40),(FORT(I),I=1,15)
000776       21 FORMAT(13H  OORT,NLT,T=3E20.8/6H  KUC=/8(5E20.8/),7H  FORT=/
               1  3(5E20.8/))
          C
          C            FIND KLC, SPECIFIC REACTION RATE CONSTANTS
          C              A=AVOGADRO CONSTANT PARTICLES/MOLE
          C                   LOWER CASE K(L),L=1,40
000776       22 CONTINUE
000776          TZOT=TZ/T
001000          EREMDT=8.0*REMD*T/PI
001003          DO 30 I= 1,40
001005          FAC3=SQRT(EREMDT/MULT(I))
001012          DLTTZOT= DLT(I)*TZOT
001015          FAC4=EXP(-DLTTZOT)
001020          FAC34=FAC3*FAC4
          C                         EQUATION (18)
001021       32 KLC(I)=A*SIGLT(I)*FAC34
001026          IF(I.GT.1) GO TO 31
```

```
        C                   EQUATION (16)
001030        KLC(I)= KLC(I)*(FAC2*(DLTTZOT+1.0)**2)
001035        GO TO 34
001035     31 IF(I.GT.6) GO TO 34
        C                   EQUATION (17)
001041        KLC(I)= KLC(I)*(FAC1*(DLTTZOT+0.5)**1.5)
001050     34 IF(IBUG(3).EQ.0) GO TO 30
001051        PRINT 33, FAC1,FAC2,FAC3,FAC4,SIGLT(I),DLT(I),MULT(I)
001076     33 FORMAT(7E17.8)
001076     30 CONTINUE
        C
        C     *****    COMPUTE  M BAR, N SUB E, LAMBDA SUB D, CAP U,
        C              LJWER CASE K(L),L=41,45
        C
001100        MBAR=0
001101        DO 40 I =10,14
001103     40 MBAR=MBAR + GAM(I)* MW(I)
        C                   EQUATION (31)
001111        MBAR= MBAR/ GAM(15)
        C                   EQUATION (40)
001112        NE=A*RHO*GAM(15)
        C                   EQUATION (30)
001115        LAMD= 6.90*SQRT(T/NE)
        C                   EQUATION (29)
001122        CAPU= UMV/(SQRT(5.486E-4/MBAR)*6.22E5*SQRTT )
001131        IF(WASK.EQ.0.) VTEST=0.
001133        IF(WASK.EQ.0.) GO TO 35
001134        VTEST=(600.*RHO2U2*WASK)/(PI*RHAT**3*RHOL)
001142     35 CONTINUE
001142        IF(V.LE.VTEST) GO TO 43
001145        FIRST=(3.*U*RHATS)/(4.*R*RHOL*V*TEM)*WASK
        C                   EQUATION (25)
001153        FIRST=FIRST* 6.22E5*SQRTT*FE
001157        DO 45 I=41,45
001160     45 KLC(I)=FIRST
001164        GO TO 42
001165     43 DO 44 I=41,45
001167     44 KLC(I)=0.
        C
        C
001172     42 CONTINUE
001172        IF(IBUG(3).EQ.0)GO TO 47
001173        PRINT 46, (KLC(I),I=1,45),MBAR,NE,LAMD,CAPU,GA,GB,GL,FE,VTEST
```

```
001227      46 FORMAT(6H  KLC=/9(5E20.8/)/20H  MBAR,NE,LAMD,CAPU=4E20.8/19H  GA,G      80800000
              1B,G,FE,VTEST=5E18.8/)                                                  80900000
001227         PRINT 41,R,RHAT                                                        81000000
001237      41 FORMAT(2E17.8)                                                         81100000
         C                                                                            81200000
         C                                 AA  THRU BS                                81300000
001237      47 CONTINUE                                                               81400000
001237         AA= KLC(1)*(RHO*GAM(6)*GAM(9)*GAMMA/KUC(1) -GAM(1)*GAMMA)              81500000
         C                                                                            81600000
         C         AB=KLC(2)*(B2,2-G2,2)                                              81900001
         C         B2,2= EQUATION (19)                                                81900002
         C         G2,2= EQUATION (20)                                                81900003
001246         AB= KLC(2)*((RHO *GAM(8)*GAM(8)* GAMMA)/KUC(2) - GAM(2)*GAMMA)         82000000
001254         AC= KLC(3)*((RHO *GAM(7)*GAM(7)* GAMMA)/KUC(3) - GAM(3)*GAMMA)         82100000
001262         AD= KLC(4)*((RHO *GAM(9)*GAM(9)* GAMMA)/KUC(4) - GAM(4)*GAMMA)         82200000
001270         AE= KLC(5)*((RHO *GAM(7)*GAM(8)* GAMMA)/KUC(5) - GAM(5)*GAMMA)         82300000
001276         AF= KLC(6)*((RHO *GAM(8)*GAM(9)* GAMMA)/KUC(6) - GAM(6)*GAMMA)         82400000
001304         AG= KLC(7)* (( GAM(6 )* GAM(8 ))/KUC(7 ) - GAM(2 ) *GAM(9 ) )          82500000
001311         AH= KLC(8 )*(( GAM(6 )* GAM(9 ))/KUC(8 ) - GAM(4 ) *GAM(8 ) )          82600000
001316         AI= KLC(9 )*(( GAM(6 )* GAM(7 ))/KUC(9 ) - GAM(5 ) *GAM(9 ) )          82700000
001324         AJ= KLC(10)*(( GAM(2 )* GAM(7 ))/KUC(10) - GAM(5 ) *GAM(8 ) )          82800000
001331         AKK=KLC(11)*(( GAM(5 )* GAM(7 ))/KUC(11) - GAM(3 ) *GAM(8 ) )          82900000
001336         AL=  KLC(12)*((GAM(6 )*GAM(6 ))/KUC(12) - GAM(1 )* GAM(8 ) )           83000000
001343         AM=  KLC(13)*((GAM(4 )*GAM(6 ))/KUC(13) - GAM(1 )* GAM(9 ) )           83100000
001350         AN=  KLC(14)*((GAM(1 )*GAM(7 ))/KUC(14) - GAM(4 )* GAM(5 ) )           83200000
001355         AO=  KLC(15)*((GAM(10)*GAM(15))/KUC(15) - GAM(7 )* GAM(8 ) )           83300000
         C                                                                            83400000
         C         AP=KLC(16)*(B7,16-G7,16)                                           83700001
         C         B7,16= EQUATION (21)                                               83700002
         C         G7,16= EQUATION (22)                                               83700003
001363         AP=  KLC(16)*((GAM(11)*GAM(15))/KUC(16) - GAM(7 )* GAM(7 ) )           83800000
001370         AQ=KLC(17)*((RHO*GAM(11)*GAM(15)*GAM(15))/KUC(17)-GAM(3 )*GAM(15))     83900000
001376         AR=KLC(18)*((RHO*GAM(10)*GAM(15)*GAM(15))/KUC(18)-GAM(5 )*GAM(15))     84000000
001404         AS=KLC(19)*((RHO*GAM(12)*GAM(15)*GAM(15))/KUC(19)-GAM(7 )*GAM(15))     84100000
001412         AT=KLC(20)*((RHO*GAM(13)*GAM(15)*GAM(15))/KUC(20)-GAM(8 )*GAM(15))     84200000
001420         AU=KLC(21)*((RHO*GAM(14)*GAM(15)*GAM(15))/KUC(21)-GAM(9 )*GAM(15))     84300000
001426         AV=KLC(22)*((GAM(5 )*GAM(11))/KUC(22) - GAM(3 )*GAM(10) )              84400000
001433         AW=KLC(23)*((GAM(7 )*GAM(11))/KUC(23) - GAM(3 )*GAM(12) )              84500000
001441         AX=KLC(24)*((GAM(8 )*GAM(11))/KUC(24) - GAM(3 )*GAM(13) )              84600000
001446         AY=KLC(25)*((GAM(9 )*GAM(11))/KUC(25) - GAM(3 )*GAM(14) )              84700000
001454         AZ=KLC(26)*((GAM(5 )*GAM(12))/KUC(26) - GAM(7 )*GAM(10) )              84800000
001461         BA=KLC(27)*((GAM(5 )*GAM(13))/KUC(27) - GAM(8 )*GAM(10) )              84900000
001467         BB=KLC(28)*((GAM(5 )*GAM(14))/KUC(28) - GAM(9 )*GAM(10) )              85000000
```

```
001474         BC=KLC(29)*((GAM(8  )*GAM(12))/KUC(29) - GAM(7  )*GAM(13) )
001501         BD=KLC(30)*((GAM(9  )*GAM(12))/KUC(30) - GAM(7  )*GAM(14) )
001507         BE=KLC(31)*((GAM(9  )*GAM(13))/KUC(31) - GAM(8  )*GAM(14) )
001514         BF=KLC(32)*((GAM(2  )*GAM(12))/KUC(32) - GAM(8  )*GAM(10) )
001521         BG=KLC(33)*((GAM(5  )*GAM(12))/KUC(33) - GAM(8  )*GAM(11) )
001527         BH= KLC(34)*((GAM(3  )*GAM(13))/KUC(34)-GAM(7  )*GAM(10) )
001534         BI= KLC(35)*((GAM(8  )*GAM(11))/KUC(35)-GAM(7  )*GAM(10) )
001541         BJ= KLC(36)*((GAM(6  )*GAM(12))/KUC(36)-GAM(9  )*GAM(10) )
001546         BKK=KLC(37)*((GAM(2  )*GAM(12))/KUC(37)-GAM(5  )*GAM(13) )
001553         BL= KLC(38)*((GAM(6  )*GAM(12))/KUC(38)-GAM(5  )*GAM(14) )
001561         BM= KLC(39)*((GAM(5  )*GAM(12))/KUC(39)-GAM(3  )*GAM(13) )
001566         BN= KLC(40)*((GAM(1  )*GAM(12))/KUC(40)-GAM(4  )*GAM(10) )
001574         BO= KLC(41) * GAM(10)
001575         BP= KLC(42) * GAM(11)
001577         BQ= KLC(43) * GAM(12)
001601         BR= KLC(44) * GAM(13)
001603         BS= KLC(45) * GAM(14)
         C
001605         IF(IBUG(4).EQ.0)GO TO 49
001606         PRINT 48, AA,AB,AC,AD,AE,AF,AG,AH,AI,AJ,AKK,AL,AM,AN,AO,AP,AQ,AR,
              1 AS,AT,AU,AV,AW,AX,AY,AZ,BA,BB,BC,BD,BE,BF,BG,BH,BI,BJ,BKK,BL,BM,
              2 BN,BO,BP,BQ,BR,BS
001744      48 FORMAT(20H  AA,AB,AC,AD,AE,AF=/6E20.8/20H  AG,AH,AI,AJ,AK,AL=/
              1 6E20.8/20H  AM,AN,AO,AP,AQ,AR=/6E20.8/20H  AS,AT,AU,AV,AW,AX=/
              2 6E20.8/20H  AY,AZ,BA,BB,BC,BD=/6E20.8/20H  BE,BF,BG,BH,BI,BJ=/
              3 6E20.8/20H  BK,BL,BM,BN,BO,BP=/6E20.8/11H  BQ,BR,BS=/3E20.8/)
         C
         C                               BEGIN RHAT SQUARED DOT EVALUATION
         C                               COMPUTE  (CP/R) SUB I
         C     TLIM1=1000. DEG.K
         C     TLIM2=15000. DEG K
001744      49 CONTINUE
001744         IF(T.LE.TLIM1) IT=1
001750         IF(T.GT.TLIM1.AND.T.LE.TLIM2) IT=2
001762         IF(T.GT.TLIM2.AND.T.LE.TLIM3) IT=3
001774         IF(T.GT.TLIM3) IT=4
001777         DO 51 I=1,15
         C
         C         CP/R
         C
002001      51 CPOR(I)=A1(I,IT) +A2(I,IT)*T + A3(I,IT)*T2 +A4(I,IT)*T3
              1    + A5(I,IT)*T4
002031         CPBAR= 0.
```

```
002032          DO 50 I=1,15
002033       50 CPBAR= CPBAR+ GAM(I)* CPOR(I)
          C                      EQUATION (50)
002041          CPBAR= CPBAR *REMD
002042          TS= T+TEM5/(2.*CPBAR)
          C                      EQUATION (49)
002046          TAV=(TS+TW)/2.
002050          TAV809= TAV/809.1
002052          CALL FTLUP(TAV809,OMEGA,1,82,TKETAB,ZOMTAB)
          C               FIND OMEGA      2.641**2=6.974881
          C                      EQUATION (48)
002056          MUF = (26.693*SQRT(18.*TAV))/ (6.974881*OMEGA )*1.0E-6
          C                      EQUATION (45)
002067          RES=(RHO*UMV*(2.*R*RHAT))/MUF
          C                      EQUATION (59)
002074          NUC= 2.+ .6 * SQRT(RES)
          C                      EQUATION (61)
002101          DELT=(FRO*TEM5)/(2.*CPBAR)+T-TW
          C               FIND (CP/R) FOR H2O AT  T=TAV         R/18.=.46205333E7
002106          IF(TAV.LE.TLIM1) IT=1
002112          IF(TAV.GT.TLIM1.AND.TAV.LE.TLIM2) IT=2
002124          IF(TAV.GT.TLIM2.AND.TAV.LE.TLIM3) IT=3
002136          IF(TAV.GT.TLIM3) IT=4
002141          CPORSP=A1(1,IT)+A2(1,IT)*TAV+A3(1,IT)*TAV**2+A4(1,IT)*TAV**3
               1 +A5(1,IT)*TAV**4
          C                      EQUATION (57)
002163          CPF=.46205333E7*CPORSP
002164          TEM= 1.+ (CPF*DELT)/EL
002170          TEM1=  ALOG(TEM)
          C                      EQUATION (60)
002172          QOQZ=EL/(CPF*DELT)*TEM1
          C                                                 2*R=16.63392E7 ERG/MOLE-DEG
          C                      EQUATION (65)
002175          S=UMV/SQRT(16.63392E7*T*GAMMA)
002203          SUMGG=0.
002204          DO 55 I= 1,15
          C                      EQUATION (47)
002205          G(I)=  CPOR(I)/(CPOR(I)-1.)
002211       55 SUMGG= SUMGG + GAM(I)*G(I)
          C                      EQUATION (56)
002217          KF = CPF * MUF
002221          IF(S.NE.0.) GO TO 52
002222          FR=0.
```

```
002223          ST=0.                                                       93700000
002224          NUFM=0.                                                     93800000
002225          NU=0.                                                       93900000
002226          GO TO 53                                                    94000000
002226       52 CONTINUE                                                    94100000
002226          TEM2= EXP(-.707*S)                                          94200000
          C                    EQUATION (63)                                94300000
002233          FR= SUMGG/(SUMGG+GAMMA) * (2.+.7*TEM2)                      94400000
002240          TEM3= EXP(-1.166* S**.406)                                  94500000
          C                    EQUATION (64)                                94600000
002247          ST = .1041/S**1.14  +.125*(1.- TEM3)                        94700000
002257          ST1=S**.406                                                 94800000
002263          ST2=S**1.14                                                 94900000
          C                                                                 95000000
002267          TEM4= CPBAR*(T-TW)                                          95100000
002272          TEM6= ((FR*TEM5)/2. + TEM4) /( (FRO*TEM5)/2.+ TEM4)         95200000
002301          TEM7=(RHO*UMV*2.*R*RHAT*CPVW*ST)/KF                         95300000
          C                    EQUATION (62)                                95400000
002310          NUFM= (SUMGG+GAMMA)/SUMGG * TEM7 * TEM6                     95500000
          C                    EQUATION (58)                                95600000
002314          NU= (NUC *QOQZ)/( 1.+ NUC*QOQZ/NUFM)                        95700000
002322       53 CONTINUE                                                    95800000
002322          IF(WASK.EQ.0.) DRHATD=0.                                    95900000
002324          IF(WASK.EQ.0.) GO TO 58                                     96000000
002325          IF(V.LE.VTEST) DRHATD=0.                                    96100000
002331          IF(V.LE.VTEST) GO TO 58                                     96200000
002333          TEM8=(-NU*KF*DN)/(EL*R**2*RHOL*CPBAR*V)                     96300000
          C                    EQUATION (55)                                96300001
002343          TEM9=(FRO*TEM5)/2.+CPBAR*T-CPBAR*TW                         96400000
          C                                  (R HAT)**2 DOT = DER(1)        96500000
          C                    EQUATION (54)                                96600000
002351          DRHATD = TEM8* TEM9                                         96700000
002352       58 CONTINUE                                                    96800000
          C                                                                 96900000
002352          RHO2=RHO**2                                                 97000000
          C                                                                 97100000
002354          IF(IBUG(5).EQ.0)GO TO 57                                    97200000
002355          PRINT 56, (CPOR(I),I=1,15),CPBAR,TS,TAV,MUF,OMEGA,NUC,DELT,CPF,  97300000
               1 TEM,TEM1,QOQZ,S,SUMGG,TEM2,FR,KF,TEM3,ST,TEM4,TEM5,TEM6,TEM7,  97400000
               2 NUFM,NU,TEM8,TEM9,RHATDD,RHATD,DRHATD,BT,RHO2,RES          97500000
002466       56 FORMAT(7H  CPOR=/3(5E20.8/)/29H  CPBAR,TS,TAV,MUF,OMEGA,NUC=/   97600000
               1 6E20.8/27H  DELT,CPF,TEM,TEM1,QOQZ,S=/6E20.8/27H  SUMGG,TEM2,FR,K  97700000
               2F,TEM3,ST=/6E20.8/30H  TEM4,TEM5,TEM6,TEM7,NUFM,NU=/6E20.8/35H  TE  97800000
```

```
               3M8,TEM9,RHATDD,RHATD,DRHATD,BT=/6E20.8/7H  RHO2=E20.8,
               4 6H  RES=E18.8/)
          C
          C
          C
          C
          C                                       COMPUTE  W SUB I, I=1,14
002466       57 CONTINUE
          C                       EQUATION (14)
002466          W(1)= RHO2*(AA+AL+AM-AN-BN    )
002474          W(2)= RHO2*(AB+AG-AJ-BF-BKK)
002502          W(3)= RHO2*(AC+AKK+AQ+AV+AW+AX+AY-BH+BM+BP)
002515          W(4)= RHO2*(AD+AH-AM+AN+BN)
002523          W(5)= RHO2*(AE+AI+AJ-AKK+AN+AR-AV-AZ-BA-BB-BG+BKK+BL-BM+BO)
002543          W(6)= RHO2*(-AA+AF-AG-AH-AI-2.*AL-AM-BJ-BL)
002557          W(7)= RHO2*(-2.*AC-AE-AI-AJ-AKK-AN+AO+2.*AP+AS-AW+AZ+BC+BD+BH+BI
               1 +BQ)
002602          W(8)= RHO2*(-2.*AB-AE-AF-AG+AH+AJ+AKK+AL+AO+AT-AX+BA-BC+BE+BF+BG
               1 -BI+BR)
002626          W(9)= RHO2*(-AA-2.*AD-AF+AG-AH+AI+AM+AU-AY+BB-BD-BE+BJ+BS)
002646          W(10)= RHO2*(-AO-AR+AV+AZ+BA+BB+BF+BH+BI+BJ+BN-BO)
002663          W(11)= RHO2*(-AP-AQ-AV-AW-AX-AY+BG-BI-BP)
002675          W(12)= RHO2*(-AS+AW-AZ-BC-BD-BF-BG-BJ-BKK-BL-BM-BN-BQ)
002713          W(13)= RHO2*(-AT+AX-BA+BC-BE-BH+BKK+BM-BR)
002725          W(14)= RHO2*(-AU+AY-BB+BD+BE+BL-BS)
          C
          C                                            GAMDOT(I) =DER(4) - DER(18)
002735          DO 60  I=1,14
          C                       EQUATION (13)
002736       60 GAMDOT(I)= (DN* W(I)) /(RHO*U)
          C                       EQUATION (46)
002747          EM= UMV/SQRT(REMD*T*SUMGG)
002755          IF(WASK.NE.0.) GO TO 67
002756          CDZ=0.
002757          CD=0.
002760          GO TO 65
002760       67 CONTINUE
002760          TEM10= EXP(-.028*RES**.82)
          C                       EQUATION (44)
002767          CDZ = 0.4 + 24./RES +1.6*TEM10
          C
002774       68 CONTINUE
002774          IF( EM.GE..5)  GO TO 61
```

```
002777          FMORES=CDZ+51.1*(EM/RES)
003002          TEM11=1.0+0.256*EM*FMORES
         C                     EQUATION (43)
003006          CD= FMORES/TEM11
003007          GO  TO  65
003007       61 CALL FTLUP(EM,AYA ,1,20,EMTAB,AYATAB)
003013          CALL FTLUP(EM,EN  ,1,20,EMTAB,ENTAB )
003017          CALL FTLUP(EM,CDC ,1,20,EMTAB,CDCTAB)
003023          CALL FTLUP(EM,CDFM,1,20,EMTAB,CDFMTB)
003027          TEM11=EXP(-AYA*RES**EN)
         C                     EQUATION (51)
003037          CD = CDC + (CDFM -CDC)* TEM11
003043       65 CONTINUE
003043          IF(IBUG(6).EQ.0)GO TO 63
003044          PRINT 62,EM,AYA,EN,CDC,CDFM
003062       62 FORMAT(21H  EM,AYA,EN,CDC,CDFM=5E18.8/)
003062       63 CONTINUE
         C
         C               *** VDOT = DER(2) ***
003062          IF(WASK.EQ.0.) VDOT=0.
003064          IF(WASK.EQ.0.) GO TO 64
         C         DER(1) = DRHATD . DERIV R HAT SQ.
003065          IF(V.LE.VTEST) VDOT=0.
003071          IF(V.LE.VTEST) GO TO 64
         C                     EQUATION (42)
003073          VDOT= ( 3.*DN*RHO*TEM5 *CD)/(8.*R*RHOL*V*RHAT)
         C
003105       64 CONTINUE
003105          IF(IBUG(7).EQ.0)RETURN
003107          PRINT 66, (W(I),I=1,14),(GAMDOT(I),I=1,15),EM,TEM10,CDZ,TEM11,CD,
               1 VDOT
003143       66 FORMAT(4H  W=/2(6E20.8/),2E20.8,9H  GAMDOT=/3(5E20.8/)/29H  EM,TEM
               110,CDZ,TEM11,CD,VDOT=/6E20.8/11H  END BASIC/////)
003143          RETURN
         C
003144          END
         C
```

```
                   SUBROUTINE CHECK
            C       *** SUBROUTINE CHECK, USED BY CALINT TO CONTROL SIZE OF COMPUTING
            C       *** INTERVAL CI
            C      IN CHECK, CUVAR = UPDATED VALUES
            C                VAR = VALUES AT BEGINNING OF INTERVAL
            C                SPEC= COMPUTING INTERVAL USED ACROSS INTERVAL
            C                CI = COMPUTING INTERVAL FOR NEXT INTERVAL
            C      IF ANSWERS NOT ACCEPTABLE, MODIFY SPEC, SET ELT=1.AND RETURN
            C      IF ANSWERS     ACCEPTABLE,             SET  ELT=0 AND RETURN
            C
            C
            C
C00002             COMMON VAR(20),DER(20),ELE1(20),ELE2(20),CI,SPEC,NDE,ELT,NERR
000002             COMMON RHOL,HL,DN,EL,     TW,CDC,CDFM,FRO,CPVW,WASK,R,HASK
C00002             COMMON   T
            C              LAB1 IN MAIN,BASIC,FOFX   CHECK
000002             COMMON/LAB1/IBUG,CUVAR,A1,A2,A3,A4,A5,A6,TLIM1,TLIM2,TLIM3
000002             DIMENSION CUVAR(20),IBUG(20)
            C             LAB2 IN MAIN,BASIC,CHECK,FOFX
000002             COMMON/LAB2/ENTHAL
            C               LAB3 IN MAIN ,BASIC AND CHECK
000002             COMMON /LAB3/ TPREV,KEY,HEPS,KAY
            C
000002             DOUBLE PRECISION VAR
            C
            C         KEY SET =1 IN CHECK TO ALLOW TESTING OF ENTHALPY AFTER FIRST INTERVAL
            C        KAY SET = 1 IN BASIC WHEN T.LT.0.
            C
000002             IF(KAY.EQ.1) GO TO 10
000004             IF( ABS(T-TPREV).GT.500.)  GO TO 10
000012             IF(KEY.EQ.0) GO TO 20
            C                          CONTROL CHANGE IN ENTHAL
000013             IF(ENTHAL.GT.50000.) GO TO 21
000016             IF(ENTHAL.LT.-500000.) GO TO 21
000020             GO TO 20
000020          21 IF(ABS((HPREV-ENTHAL)/ENTHAL).GT.HEPS) GO TO 10
000026          20 CONTINUE
000026             TPREV=T
000027             ELT=0.
000030             HPREV=ENTHAL
000032             KEY=1
000033             RETURN
```

```
       C
000034    10 ELT=1.0
000035       IF(IBUG(10).EQ.0) GO TO 30
000037       PRINT 11, T,TPREV,SPEC,ENTHAL,KEY,CI,HPREV
000060    11 FORMAT(4H  T=E15.8, 8H  TPREV=E15.8, 7H  SPEC=E15.8, 9H  ENTHAL=
            1 E15.8, 6H  KEY=I1/ 32H   REDUCE COMPUTING INTERVAL CI=E15.8/
            2 8H  HPREV=E15.8/)
000060    30 CONTINUE
       C         SPEC = COMPUTING INTERVAL JUST USED
       C         CI = COMPUTING INTERVAL FOR NEXT STEP
000060       SPEC=SPEC/2.
000062       CI=SPEC/2.
000063    16 CONTINUE
000063       KEY=0
000064       KAY=0
000064       IF(CI.LT.1.0E-20) PRINT 12
000073    12 FORMAT(50H  SOMETHING MUST BE WRONG, CI.LT.1.0E-20,  STOP 12/
            1       17H  REEXAMINE INPUT)
       C      ***                                              STOP 12
000073       IF(CI.LT.1.0E-20) STOP 12
000100       RETURN
000101       END
```

```
                  FUNCTION   FOFX(TD)
            C     FUNCTION FOFX(TD), USED BY ITR1 TO EVALUATE T
            C
            C             LAB1 IN MAIN,BASIC,FOFX
000003            COMMON/LAB1/IBUG,CUVAR,A1,A2,A3,A4,A5,A6,TLIM1,TLIM2,TLIM3
            C            LAB2 IN MAIN,BASIC,CHECK,FOFX
000003            COMMON/LAB2/ ENTHAL
000003            DIMENSION A1(15,4),A2(15,4),A3(15,4),A4(15,4),A5(15,4),A6(15,4)
000003            DIMENSION CUVAR(20),IBUG(20)
000003            DIMENSION GAM(15)
000003            EQUIVALENCE (CUVAR(4),GAM(1))
000003            DATA REMD/8.31696E7/
            C
000003            TB=TD
000004            T2=TD**2
000005            T3= T2*TD
000006            T4= T3*TD
000007            SUM=0.
            C     TLIM1=1000. DEG.K
            C     TLIM2=15000. DEG K
            C       TLIM3=100000.
000010            DO  10  I=1,15
000011            IF(TD.LE.TLIM1) IT=1
000014            IF(TD.GT.TLIM1.AND.TD.LE.TLIM2) IT=2
000026            IF(TD.GT.TLIM2.AND.TD.LE.TLIM3) IT=3
000040            IF(TD.GT.TLIM3) IT=4
            C
            C        (H SUB I)/RT
            C
000043            HIORT   = A1(I,IT)+A2(I,IT)/2.*TD+A3(I,IT)/3.*T2+A4(I,IT)/4.*T3
                 1 +A5(I,IT)/5.*T4+A6(I,IT)/TD
000072            IF(IBUG(8).EQ.0) GO TO 10
            C
            C
000073            PRINT 20, IT,TD,HIORT,GAM(I),SUM
000113         10 SUM =SUM+ GAM(I)*HIORT
            C                                    R=8.31696E7  ERG/ MOLE-DEG
            C     TC  =ENTHAL/(8.31696E7*SUM)
            C     FOFX=TC
            C     BECAUSE SUM SO SENSITIVE, TAKE IT OUT OF DENOMINATOR AND REDUCE
            C      ITS EFFECT BY A FACTOR   9-8-67
            C                  EQUATION (12)
```

```
000122          TC=TD+.1*(TD*REMD*SUM-ENTHAL)                    116500000
000127          FOFX=TC                                          116600000
          C                                                      116700000
000130          IF(IBUG(9).EQ.0) RETURN                          116800000
          C                                                      116900000
          C                                                      117000000
000131          PRINT 20, TB,TC,SUM,ENTHAL                       117100000
000145       20 FORMAT(5E18.8)                                   117200000
          C                                                      117300000
000145          RETURN                                           117400000
000147          END                                              117500000
```

```
                  SUBROUTINE ERROR
         C         *** SUBROUTINE ERROR, USED BY CALINT IF INPUT IS BAD,BAD,BAD
000002            COMMON VAR(20),DER(20),ELE1(20),ELE2(20),CI,SPEC,NDE,ELT,NERR
         C
000002            DOUBLE PRECISICN VAR
         C
000002            PRINT 10, NERR,CI
000012         10 FORMAT(10H     NERR= I5,5H  CI=E17.8/)
000012            IF(NERR.EQ.1) PRINT 11
000020         11 FORMAT(25H    ***** BAD INPUT *****/)
000020            IF(NERR.EQ.2) PRINT 12
000026         12 FORMAT(25H    ***** ELE1=ELE2 *****/)
         C                                                    STOP 13
000026            IF(NERR.EQ.1.OR.NERR.EQ.2) STOP 13
000040            RETURN
000041            END
```

```
                SUBROUTINE CALINT(VAR,DER,ELE1,ELE2,CI,SPEC,N,CUVAR,ELT,         119200000
               1CIMAX,NERR,PHMAX)                                                 119300000
          C                                                                       119400000
          C     CALINT,INTEGRATION ROUTINE                                        119500000
          C     THE NUMERICAL INTEGRATION ALGORITHM USED IS FOUND IN - A METHOD   119600000
          C     FOR THE NUMERICAL INTEGRATION OF COUPLED FIRST ORDER DIFFERENTIAL 119700000
          C     EQUATIONS WITH GREATLY DIFFERENT TIME CONSTANTS - BY CHARLES E.   119800000
          C     TREANOR, CONTRACT NO.NASR-119, CAL REPORT NO.AG-1729-A-4, JANUARY 119900000
          C     1964. CORNELL AERONAUTICAL LABORATORY,INC.,CORNELL UNIVERSITY,    120000000
          C     BUFFALO,N.Y.                                                      120100000
          C                                                                       120200000
000017          DOUBLE PRECISION VAR                                              120300000
000017          DIMENSION VAR(42),DER(41),ELE1(41),ELE2(41),CUVAR(42),F1(41),     120400000
               1F2(41),F3(41),CAPF1(41),CAPF2(41),CAPF3(41),P(41),PH(41),         120500000
               2DELTY(41),Y3(41),Y4(41),F4(41),Y2(41)                             120600000
          C                                                                       120700000
          C     NERR=1           CI,N,OR,NT IS EQUAL TO ZERO                      120800000
          C                                                                       120900000
          C     NERR=2           ELE1 LESS THAN OR EQUAL TO ELE2                  121000000
          C                                                                       121100000
          C                                                                       121200000
          C        TEST INPUT                                                     121300000
          C                                                                       121400000
000017          FN=N                                                              121500000
000020          TEST=CI*FN                                                        121600000
000021          IF(TEST)998,997,998                                               121700000
000023      997 NERR=1                                                            121800000
000025          GO TO 100                                                         121900000
000025      998 IF(ELE1-ELE2)999,999,1000                                         122000000
000027      999 NERR=2                                                            122100000
000031          GO TO 100                                                         122200000
000031     1000 IF(SPEC)5,1,5                                                     122300000
          C                                                                       122400000
          C        SECTION FOR INITIALIZATICN COMPUTATION OF DERIVATIVES          122500000
          C                                                                       122600000
000032        1 SPEC=CI                                                           122700000
000033          ICONT=1                                                           122800000
000034        2 N1=N+1                                                            122900000
000037          DO 3 I=1,N1                                                       123000000
          C                                                                       123200000
000040        3 CUVAR(I)=VAR(I)                                                   123100000
000047          CALL BASIC                                                        123300000
```

```
       C
       C        RETURN WITH DERIVATIVES IN DER
       C
000050        DO 4 I=1,N
000055      4 F1(I)=DER(I)
       C
000062        RETURN
       C
       C        COMPUTE  Y2,X2
       C
000063      5 CUVAR(1)=VAR(1)+CI/2.
000101        DO 6 I=1,N
000102        I1=I+1
000103        Y2(I)=VAR(I1)+CI/2.*F1(I)
000127        IF(Y2(I))65,6,6
000132      6 CUVAR(I1)=Y2(I)
000141        GO TO 66
000141     65 SPEC=CI
000142        CI=CI/2.
000143        GO TO 5
       C
       C        CALL BASIC TO EVALUATE F2
       C
000144     66 CALL BASIC
       C
       C        RETURN
       C
000145        DO 7 I=1,N
000152        I1=I+1
000153        F2(I)=DER(I)
       C
       C        COMPUTE  Y3
       C
000156        Y3(I)=VAR(I1)+CI/2.*F2(I)
000202        IF(Y3(I))65,7,7
000205      7 CUVAR(I1)=Y3(I)
       C
       C        CALL BASIC TO EVALUATE F3
       C
000214        CALL BASIC
       C        RETURN
       C
000215        DO 10 I=1,N
```

```
000222          F3(I)=DER(I)
          C
          C        COMPUTE P,PH AND CAP F TERMS
          C
000225          IF(Y3(I)-Y2(I)) 9,8,9
000230        8 P(I)=0.
000232          GO TO 91
000233        9 P(I)=-((F3(I)-F2(I))/(Y3(I)-Y2(I)))
000245       91 PH(I)=P(I)*CI
000251          IF(PH(I))83,83,103
000253       83 PH(I)=0.
000255          P(I)=0.
000257          GO TO 84
000257      103 IF(ABS(Y3(I)-Y2(I))/((ABS(Y3(I))+ABS(Y2(I)))/2.)-.5E-4)83,83,84
000272       84 IF(PH(I)-.1)85,85,95
000276       85 CAPF1(I)=1.-PH(I)/2.+(PH(I)**2)/6.-(PH(I)**3)/24.
000310          CAPF2(I)=.5-PH(I)/6.+(PH(I)**2)/24.-(PH(I)**3)/120.
000323          CAPF3(I)=1./6.-PH(I)/24.+(PH(I)**2)/120.-(PH(I)**3)/720.
000341          GO TO 10
000342       95 CAPF1(I)=(EXP(-PH(I))-1.)/(-PH(I))
000352          CAPF2(I)=(CAPF1(I)-1.)/(-PH(I))
000361          CAPF3(I)=(CAPF2(I)-.5)/(-PH(I))
000371       10 CONTINUE
          C
          C        IS PH BETWEEN ELE2 AND ELE1
          C
000400          IF(ICONT-1)101,101,102
000402      102 ICONT=ICONT-1
000404          SPEC=CI
000405          GO TO 17
000405      101 DO 11 I=1,N
000407      104 IF(ABS(PH(I))-ELE1(I))11,11,13
000415       11 CONTINUE
          C
000420       12 SPEC=CI
000421          GO TO 15
          C
          C        HALVE INTERVAL AND DOUBLE PH RANGE
          C
000422       13 DO 96 I=1,N
000424          ELE1(I)=ELE1(I)*2.
000426          IF(ELE1(I)-PHMAX)94,94,955
000432       94 ELE2(I)=ELE2(I)*2.
```

```
000435           GO TO 96
000435       955 ELE1(I)=ELE1(I)/2.
000440        96 CONTINUE
000443           SPEC=CI
000443           CI=CI/2.
000444           ICONT=3
000446           GO TO 5
           C
           C     RETURN TO RECOMPUTE INTERVAL
           C
           C
           C        RETURN TO RECOMPUTE INTERVAL
           C
000446        15 DO 16 I=1,N
000450           IF(ABS(PH(I))-ELE2(I))16,17,17
000456        16 CONTINUE
           C
           C        DOUBLE INTERVAL
           C
000461           CI=2.*CI
000462           IF(CI-CIMAX)17,17,165
000465       165 CI=CIMAX
000467        17 CONTINUE
           C
           C        COMPUTE Y4,X4
           C
000467           DO 18 I=1,N
000471           I1=I+1
000472           CUVAR(I1)=VAR(I1)+SPEC*(F3(I)*(2.*CAPF2(I))+F1(I)*
                1(CAPF1(I)-2.*CAPF2(I))+F2(I)*PH(I)*CAPF2(I))
000531           IF(CUVAR(I1))175,18,18
000534       175 CI=SPEC
000535           CI=CI/2.
000537           GO TO 5
000537        18 Y4(I)=CUVAR(I1)
           C
000546           CUVAR(1)=VAR(1)+SPEC
           C
           C        CALL BASIC TO EVALUATE F4
           C
000553           CALL BASIC
           C        RETURN
           C
```

```
000554          DO 20 I=1,N
000561          I1=I+1
000562          F4(I)=DER(I)
          C
          C        COMPUTE DELTA Y
          C
000565          DELTY(I)=SPEC*(F1(I)*CAPF1(I)+(-3.*(F1(I)+P(I)*VAR(I1))
               1+2.*(F2(I)+P(I)*Y2(I))+2.*(F3(I)+P(I)*Y3(I))-F4(I)
               2-P(I)*Y4(I))*CAPF2(I)+4.*((F1(I)+P(I)*VAR(I1))-(F2(I)
               3+P(I)*Y2(I))-(F3(I)+P(I)*Y3(I))+(F4(I)+P(I)*Y4(I)))*
               4CAPF3(I))
          C
          C        COMPUTE Y+DELTA Y
          C
000742       20 CUVAR(I1)=VAR(I1)+DELTY(I)
          C
          C        CALL CHECK FOR DECISION TO ACCEPT OR RECOMPUTE
          C          INTERVAL
000757          CALL CHECK
000760          IF (ELT)21,21,23
          C
          C        UPDATE Y VALUES
          C
000766       21 N1=N+1
000771          DO 22 I=2,N1
000772          I1=I-1
000773       22 VAR(I)=VAR(I)+DELTY(I1)
001006          VAR(1)=VAR(1)+SPEC
          C
          C        RETURN TO COMPUTE DERIVATIVES AT Y+DELTA Y
          C
001014          GO TO 2
          C
          C        RETURN TO RECOMPUTE INTERVAL
          C
001014       23 GO TO 5
          C
001015      100 CALL ERROR
001016          RETURN
001017          END
```

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TABLE I.- CHEMICAL SPECIES

i	Species
1	H_2O
2	O_2
3	N_2
4	H_2
5	NO
6	OH
7	N
8	O
9	H
10	NO^+
11	N_2^+
12	N^+
13	O^+
14	H^+
15	e^-

TABLE II.- CONSTANTS FOR USE IN REACTION RATE FORMULAS

j	Reaction	μ_j, g/mol	D_j	σ_j, cm^2
1	$H_2O + M \rightleftarrows OH + H + M$	10.957	217.10	10.00×10^{-16}
2	$O_2 + M \rightleftarrows O + O + M$	14.933	217.34	10.00
3	$N_2 + M \rightleftarrows N + N + M$	14.000	414.50	10.00
4	$H_2 + M \rightleftarrows H + H + M$	1.867	190.34	10.00
5	$NO + M \rightleftarrows N + O + M$	14.483	275.74	10.00
6	$OH + M \rightleftarrows O + H + M$	10.578	186.09	10.00
7	$H + O_2 \rightleftarrows OH + O$	.970	31.44	1.00
8	$O + H_2 \rightleftarrows OH + H$	1.778	4.25	1.00
9	$H + NO \rightleftarrows OH + N$	.968	89.65	1.00
10	$O + NO \rightleftarrows O_2 + N$	10.435	58.21	1.00
11	$O + N_2 \rightleftarrows NO + N$	10.182	138.93	2.69
12	$O + H_2O \rightleftarrows OH + OH$	8.471	31.02	1.00
13	$H + H_2O \rightleftarrows OH + H_2$	.947	26.77	1.00
14	$NO + H_2 \rightleftarrows H_2O + N$	1.875	62.88	1.00
15	$N + O \rightleftarrows NO^+ + e^-$	7.467	117.69	.018
16	$N + N \rightleftarrows N_2^+ + e^-$	7.000	247.27	.066
17	$N_2 + e^- \rightleftarrows N_2^+ + e^- + e^-$	5.486×10^{-4}	661.94	.879
18	$NO + e^- \rightleftarrows NO^+ + e^- + e^-$	5.486×10^{-4}	393.00	.879
19	$N + e^- \rightleftarrows N^+ + e^- + e^-$	5.486×10^{-4}	617.75	.879
20	$O + e^- \rightleftarrows O^+ + e^- + e^-$	5.486×10^{-4}	578.24	.879
21	$H + e^- \rightleftarrows H^+ + e^- + e^-$	5.486×10^{-4}	577.81	.879

TABLE II.- CONSTANTS FOR USE IN REACTION

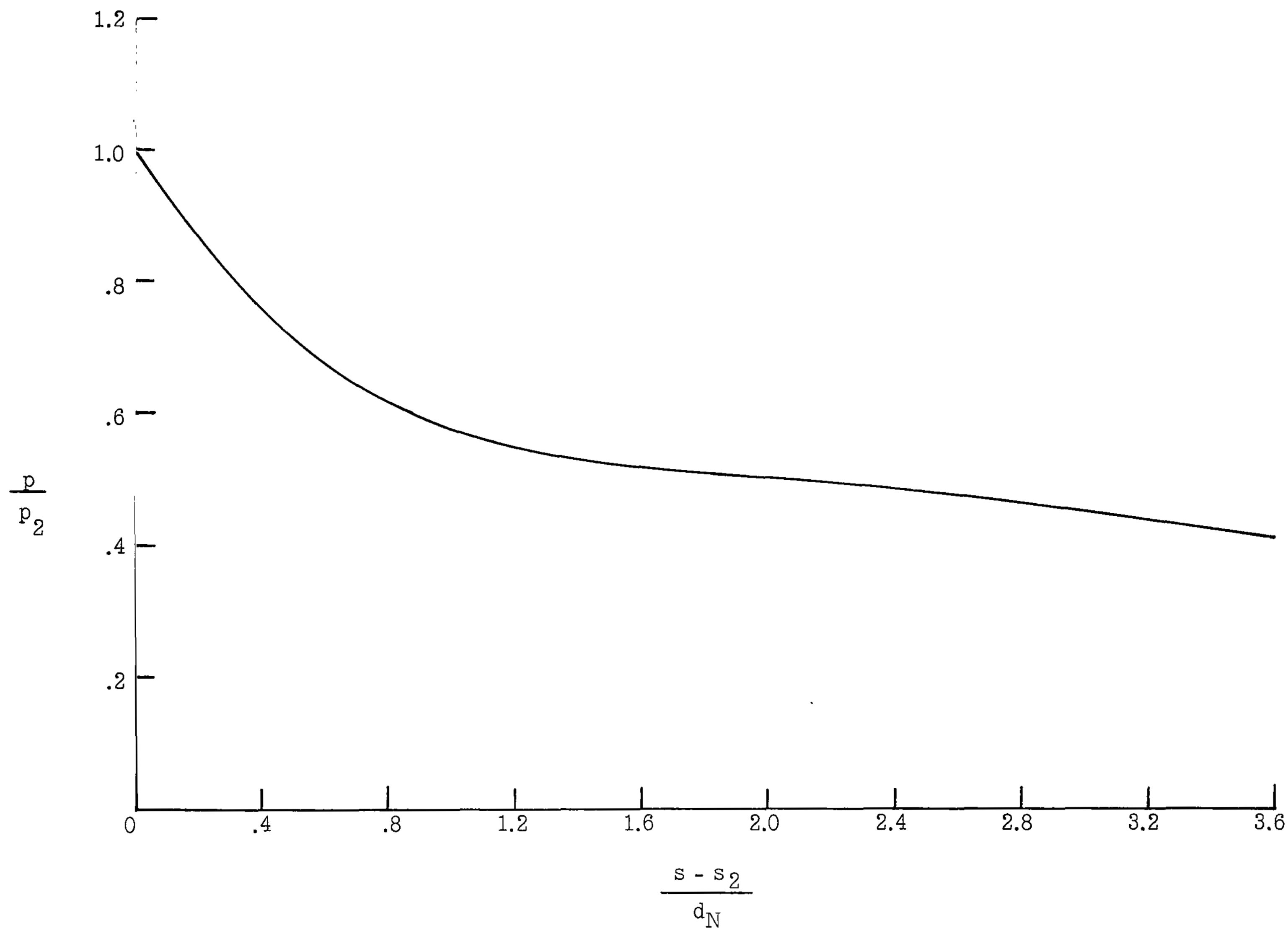
RATE FORMULAS – Concluded

j	Reaction	μ_j, g/mol	D_j	σ_j, cm^2
22	$N_2 + NO^+ \rightleftharpoons N_2{}^+ + NO$	14.483	268.94	20.00×10^{-16}
23	$N_2 + N^+ \rightleftharpoons N_2{}^+ + N$	9.333	44.19	
24	$N_2 + O^+ \rightleftharpoons N_2{}^+ + O$	10.182	83.70	
25	$N_2 + H^+ \rightleftharpoons N_2{}^+ + H$	.966	84.12	
26	$N + NO^+ \rightleftharpoons N^+ + NO$	9.545	224.75	
27	$O + NO^+ \rightleftharpoons O^+ + NO$	10.435	185.24	
28	$H + NO^+ \rightleftharpoons H^+ + NO$	.968	184.82	
29	$N + O^+ \rightleftharpoons N^+ + O$	7.467	39.51	
30	$N + H^+ \rightleftharpoons N^+ + H$	.933	39.94	
31	$O + H^+ \rightleftharpoons O^+ + H$	.941	.43	
32	$O + NO^+ \rightleftharpoons N^+ + O_2$	10.435	282.96	
33	$O + N_2{}^+ \rightleftharpoons N^+ + NO$	10.182	94.74	
34	$N + NO^+ \rightleftharpoons O^+ + N_2$	9.545	46.31	
35	$N + NO^+ \rightleftharpoons N_2{}^+ + O$	9.545	130.01	
36	$H + NO^+ \rightleftharpoons N^+ + OH$	.968	314.40	
37	$NO + O^+ \rightleftharpoons N^+ + O_2$	10.435	99.84	
38	$NO + H^+ \rightleftharpoons N^+ + OH$	.968	129.16	
39	$N_2 + O^+ \rightleftharpoons N^+ + NO$	10.182	178.44	
40	$H_2 + NO^+ \rightleftharpoons N^+ + H_2O$	1.875	287.63	

TABLE III.- PARAMETERS IN DROPLET DRAG-COEFFICIENT EXPRESSION

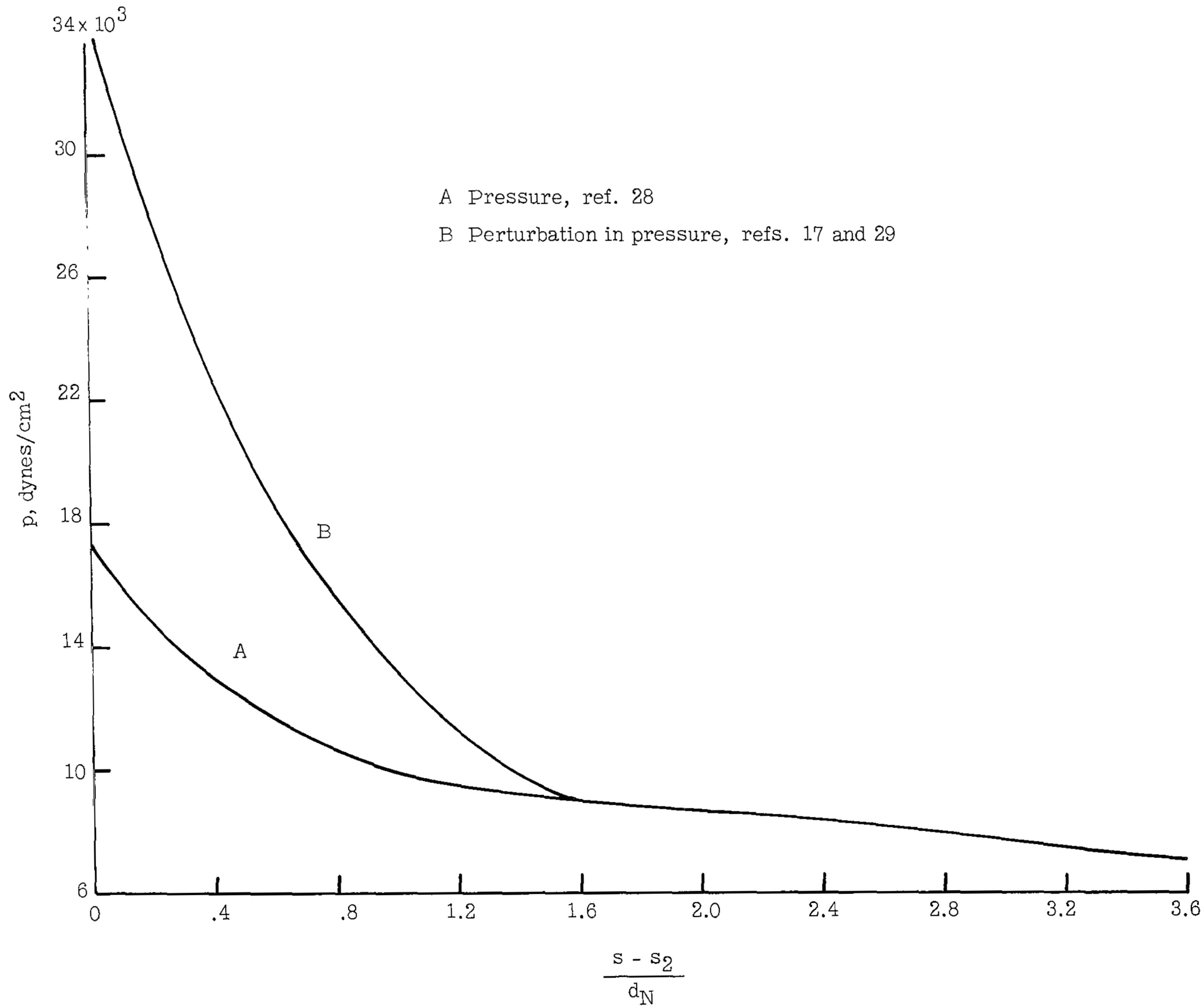
[Values taken from ref. 5]

M	$C_{D,C}$	$C_{D,FM}$	$\bar{A}$	n
0.5	0.520	7.80	0.315	0.410
.6	.551	6.50	.240	.460
.7	.586	5.57	.182	.500
.8	.625	4.92	.141	.545
.9	.666	4.45	.110	.590
1.0	.712	4.10	.090	.620
1.2	.801	3.60	.065	.670
1.4	.880	3.23	.055	.690
1.6	.929	2.98	.049	.710
1.8	.955	2.80	.047	.715
2.0	.971	2.68	.046	.720
2.4	.981	2.48	.0455	.725
2.8	.969	2.36	.0455	.725
3.2	.949	2.28	.0453	.730
4	.919	2.17	.0452	.730
5	.910	2.10	.0451	.735
6	.910	2.05	.0449	.735
8	.910	2.02	.0448	.740
10	.910	2.00	.0447	.745
12	.910	2.00	.0447	.745



(a) Nondimensional pressure distribution.

Figure 1.- Pressure along the body streamline over a spherically blunted 9° half-angle cone.



(b) Dimensional pressure distribution.

Figure 1.- Concluded.

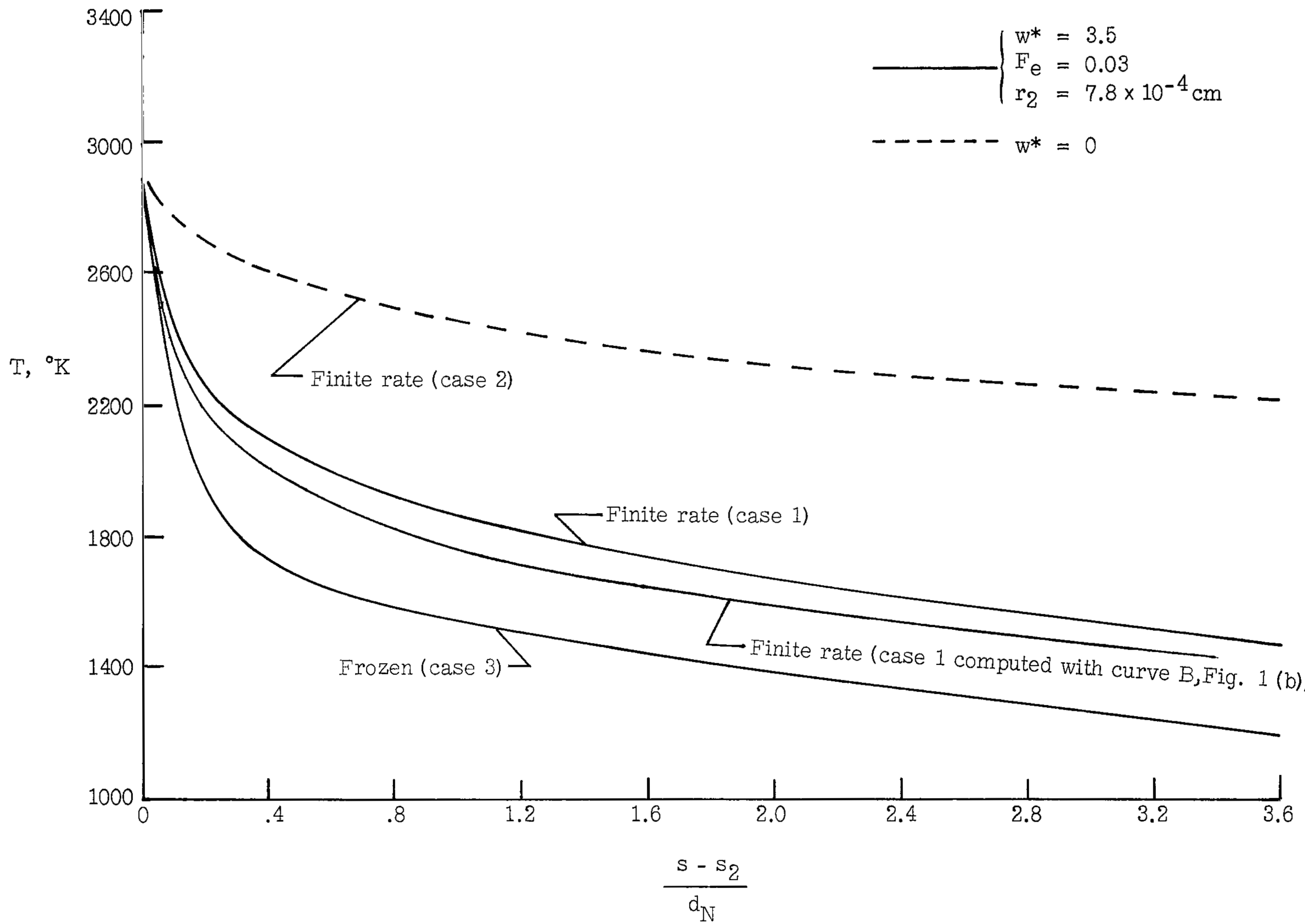


Figure 2.- Temperature along body streamline at an altitude of 47.55 km. (Except as noted, results obtained by using curve A of fig. 1(b).)

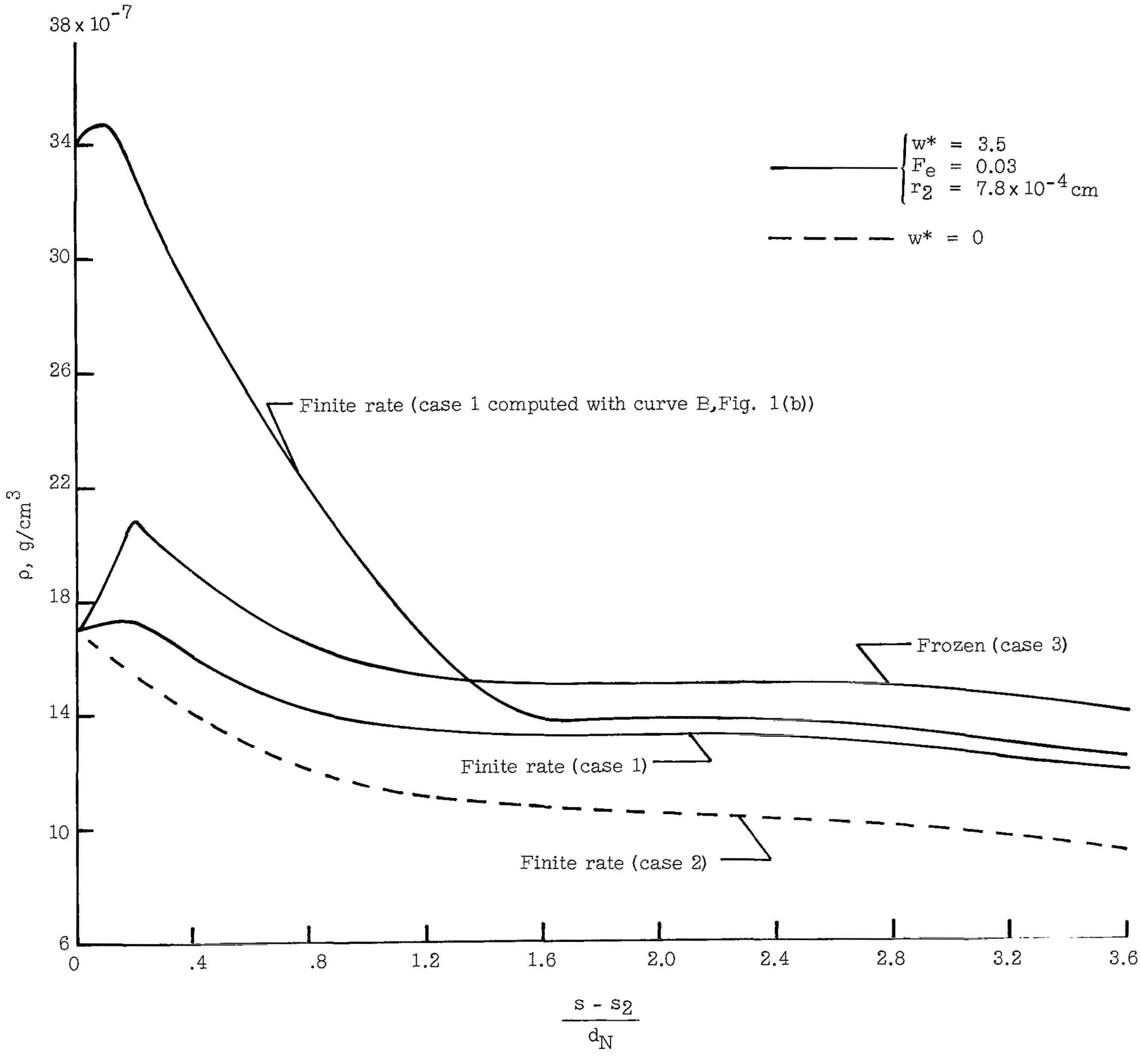


Figure 3.- Density along body streamline at an altitude of 47.55 km. (Except as noted, results obtained by using curve A of fig. 1(b).)

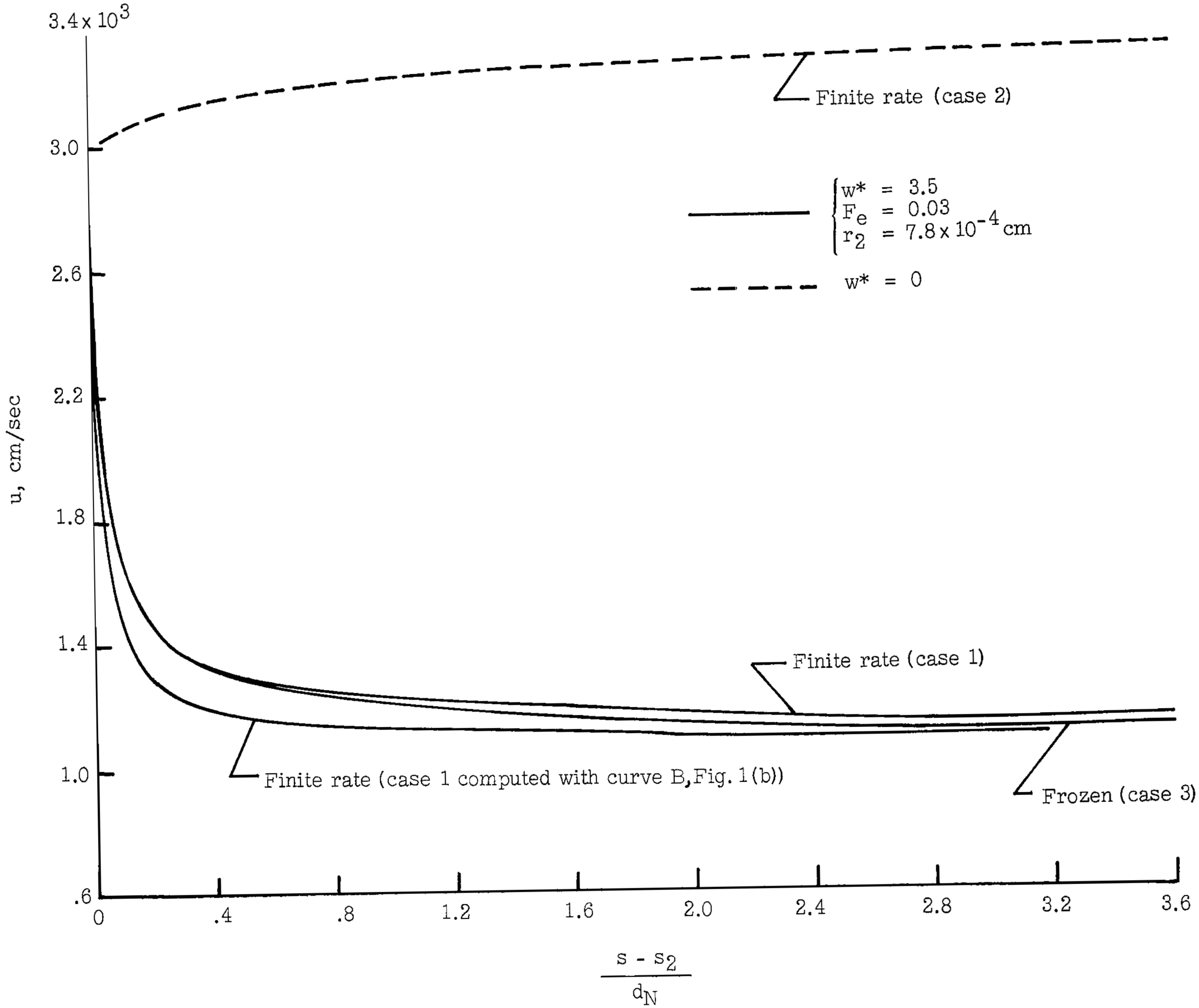


Figure 4.- Velocity along body streamline at an altitude of 47.55 km. (Except as noted, results obtained by using curve A of fig. 1(b).)

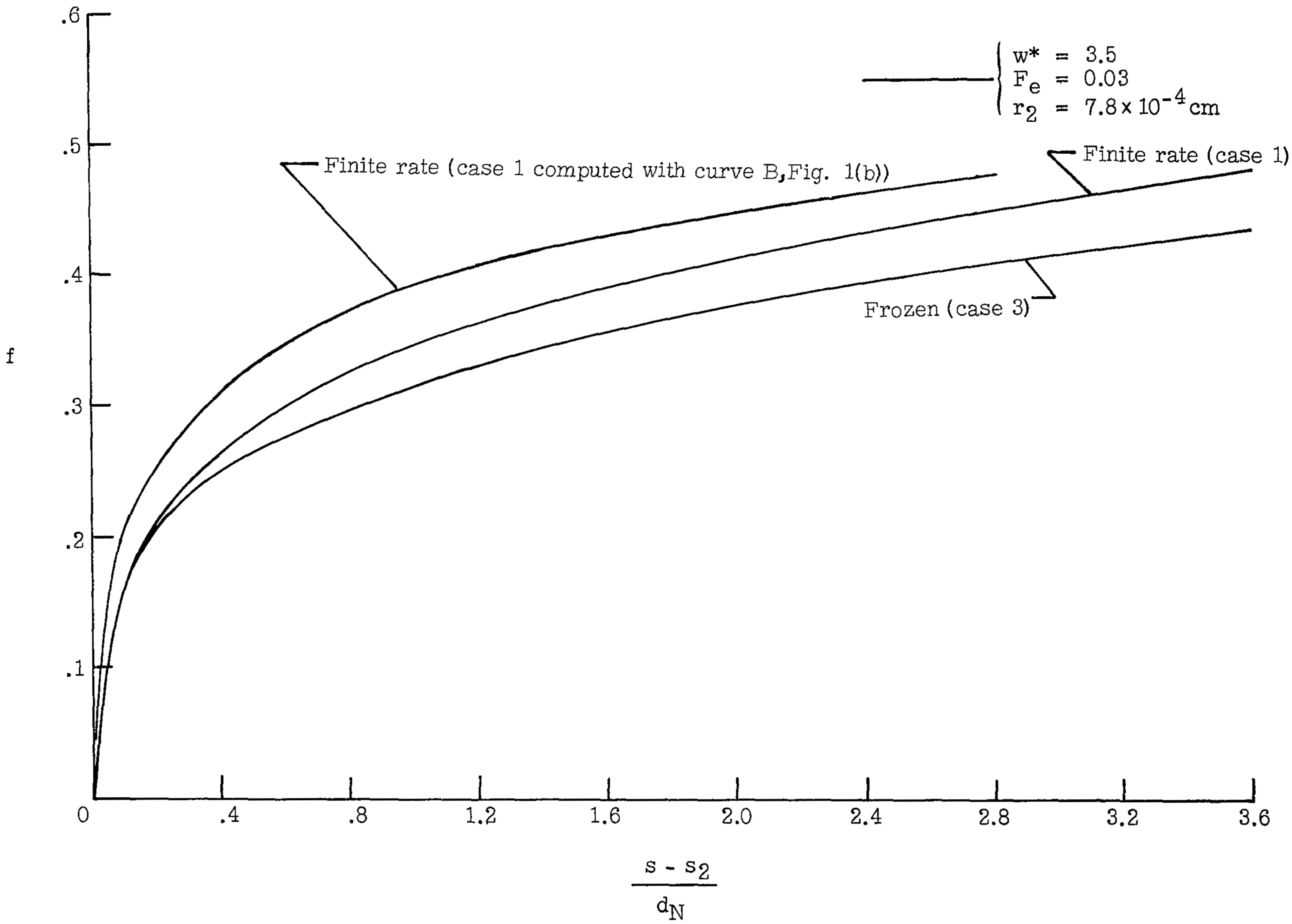


Figure 5.- Fraction of water evaporated along body streamline at an altitude of 47.55 km. (Except as noted, results obtained by using curve A of fig. 1(b).)

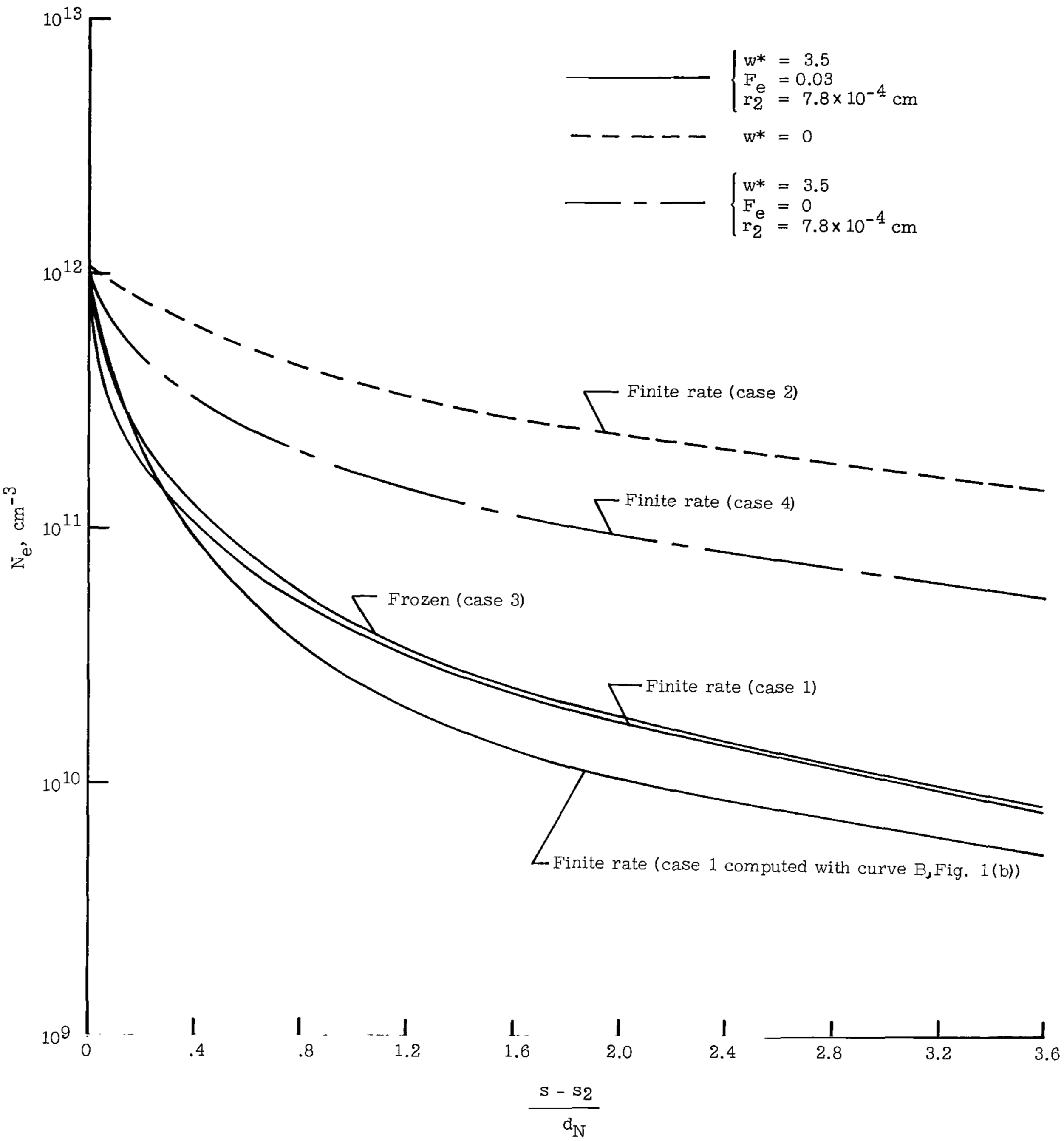


Figure 6.- Electron number density along body streamline at an altitude of 47.55 km. (Except as noted, results obtained by using curve A of fig. 1(b).)

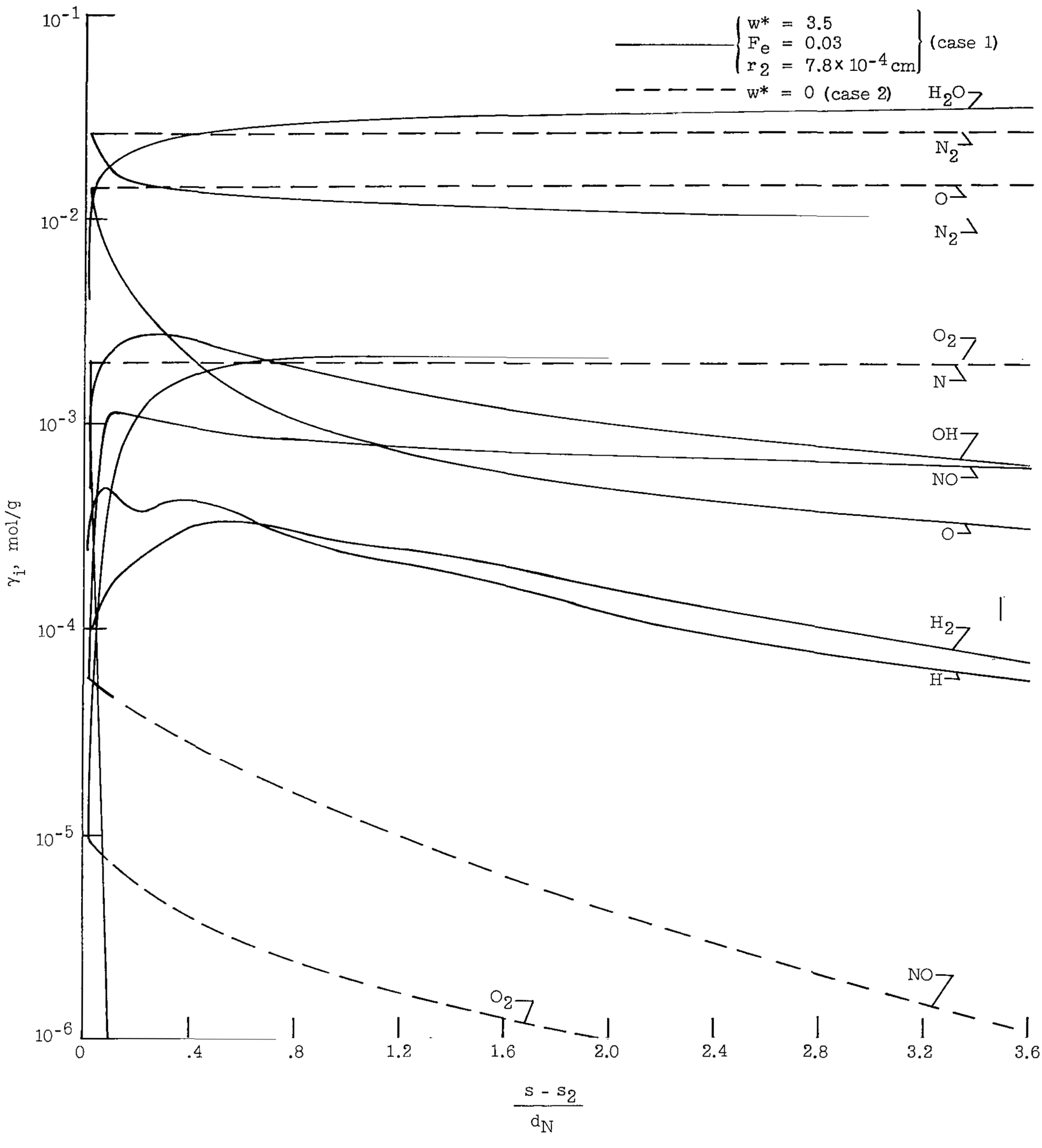


Figure 7.- Concentration of neutral species along body streamline using finite-rate chemistry. Altitude, 47.55 km. (Results computed by using curve A of fig. 1(b).)

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