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FAST COMPUTER PROGRAM FOR NONEQUILIBRIUM ROCKET PLUME PREDICTIONS

R. R. Mikatarian, et al

AeroChem Research Laboratories, Incorporated

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R.R. Mikatarian, C.J. Kau and H.S. Pergament

AeroChem Research Laboratories, Inc.
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FOREWORD

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ABSTRACT

A fast computer program for predicting nonequilibrium rocket plume properties is described. The analytical model assumes parallel turbulent (or laminar) mixing between concentric chemically reacting streams and can also be used for studying chemical lasers and re-entry wakes. The equations for free shear layer mixing with nonequilibrium chemistry are solved via a mixed implicit/explicit finite difference scheme which efficiently predicts flow properties and composition, even when many chemical reactions are near equilibrium. The stability problems inherent in fully explicit finite difference schemes are shown to be eliminated, and stable integration step sizes are shown to be increased by up to 4 orders of magnitude. Computer run times for typical afterburning rocket plume calculations are shown to be decreased by more than one order of magnitude over the original (fully explicit) AeroChemaxisymmetric mixing with nonequilibrium chemistry program. Both the analysis and computer program write-up are presented, including a sample calculation and a FORTRAN listing.

NOMENCLATURE

a	defined by Eq. (15b)
$a_{\frac{1}{2}}$	defined by Eq. (33)
a^g	attenuation per unit length
A	constant in expression for k_f (see Eq. (23))
$b_{\frac{1}{2}}$	defined under Eq. (25b)
B	activation energy (see Eq. (23))
c_p	specific heat of mixture ($\sum_i X_i c_{p_i}$)
c_{p_i}	specific heat of ith species
e	electronic charge
F_i	defined as X_i/W (= Y_i/W_i)
FDL	factor used for the external control of integration step size
g_i	Gibbs free energy of ith species at standard state (1 atm)
ΔG	change in standard Gibbs free energy for a reaction, $\sum_i (g_i)_{\text{products}} - \sum_i (g_i)_{\text{reactants}}$
h	enthalpy of mixture
h_i	enthalpy of ith species
h_{298_i}	heat of formation of ith species at T = 298 K
k_f	forward rate coefficient
K	eddy viscosity coefficient (see Section VI)
$\bar{K}$	eddy viscosity coefficient for Donaldson/Gray model (see Eq. (32))
K_p	equilibrium constant
Le	Lewis number (laminar or turbulent)
m_e	electron mass
$M_{\frac{1}{2}}$	Mach number at half radius, defined under Eq. (32)
N	temperature exponent in reaction rate equation (Eq. (23))
n_e	electron density
Q	arbitrary dependent variable (see Eqs. (13) - (15))

Q_e	electron-neutral collision cross section
p	static pressure
Pr	Prandtl number (laminar or turbulent)
r	coordinate normal to jet centerline
r_i	inner mixing zone radius
r_j	jet radius
$r_{\frac{1}{2}}$	defined under Eq. (28b)
$\bar{r}_{\frac{1}{2}}$	defined under Eq. (27)
R	universal gas constant
T	static temperature
u	x component of velocity
v	r component of veclocity
v_e	electron velocity
$\dot{w}_i$	molar rate of production of ith species
$\dot{w}^{(j)}$	molar rate of production from jth reaction
W	molecular weight of mixture $(\sum_i F_i)^{-1}$
W_i	molecular weight of ith species
x	coordinate parallel to jet centerline
Δx	$x_{n+1} - x_n$
X_i	mole fraction of ith species
Y_i	mass fraction of ith species

Greek

α	constant for external control of eddy viscosity (see Eqs. (25) - (31))
$\Delta\Psi$	$\psi_{m+1} - \psi_m$
ϵ	eddy diffusivity for turbulent flow; defined as μ/ρ
η	defined by Eq. (25)
μ	viscosity (or eddy viscosity for turbulent flow)
ν_e	electron-neutral collision frequency
ρ	density
σ	electrical conductivity

Ψ	stream function
ω	signal frequency

Subscripts

e	evaluated at edge of mixing layer (free stream)
e^-	electrons
i	ith species
j	value at nozzle (jet) exit
m	Ψ index in grid network
n	x index in grid network
o	evaluated at axis of symmetry, $r = 0$

Miscellaneous

$\lvert\ \rvert$	absolute value
$\left(\frac{\partial}{\partial \beta}\right)_\gamma$	partial derivative with respect to β; γ being held constant
$\sum_i$	summation over i species

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I. INTRODUCTION

The need to accurately determine electromagnetic wave/plume interactions[1,2] has motivated the development of several programs[3-6] to predict the electrical properties of turbulent rocket exhaust plumes.* Each program uses the same gas dynamic model (parallel mixing between two concentric streams), but only the AeroChem program of Mikatarian and Pergament accounts for nonequilibrium chemistry effects; the others[3-5] assume local thermochemical equilibrium to prevail. Attempts to account for transverse radar attenuation data (taken with focused microwaves) under simulated altitude conditions using equilibrium chemistry programs generally fail. Indeed, it has been demonstrated by Pergament and Jensen[7,8] that finite-rate chemical kinetics must be incorporated into rocket plume calculations to accurately predict plume temperatures, electrical properties, etc.

Conceptually the numerical solution of the equations describing axisymmetric mixing with nonequilibrium chemistry presents few difficulties. A fully explicit finite difference scheme[4] yields an accurate solution to the problem. Unfortunately, however, on many occasions the stability requirements associated with the explicit integration scheme are found to so severely limit maximum step sizes (e.g. on the order of 10^{-5} to 10^{-10} ft) that computer solutions become economically prohibitive.† This "stiffness" in the equations,[9,10] (which results in small step sizes) is found to be restricted to nonequilibrium flows where one or more of the chemical reactions is at or near-equilibrium, a situation typical of relatively low altitude (< ≈ 70 kft) afterburning plumes.

In this computer program we utilize a new numerical technique to solve the partial differential equations (in finite-difference form) describing turbulent (or laminar) shear flows with nonequilibrium chemistry: Implicit differences are used in the solution of the species conservation equations‡

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*References 3 and 5 are unclassified descriptions of the solution techniques used in the Naval Weapons Center and Lockheed Propulsion Company codes. Further information on these codes may be found in the classified literature.

†For frozen (non-reactive) flow the governing equations can be integrated quite rapidly using explicit differences.

‡This appears to be the first program to utilize implicit differences for free shear layers with nonequilibrium chemistry, although such schemes have been applied to one-dimensional nonequilibrium nozzle flows.[11,12]

and explicit differences are used for the momentum and energy equations. This mixed implicit/explicit scheme eliminates the instability problems which characterize fully explicit schemes and allows integration step sizes to be increased by orders of magnitude without sacrificing accuracy. Those rocket exhaust plume predictions which could not be made with the original AeroChem program[4] (which uses the fully explicit scheme) because the stable step size approached 10^{-10} ft, are quite easily handled by the new program. Most importantly, for the more typical case in which average step sizes range from 10^{-4} to 10^{-2} ft, the new program reduced computer run times by at least an order of magnitude. (A detailed comparison between rocket plume calculations using the original fully explicit difference scheme and the new mixed implicit/explicit scheme is given in Appendix D.)

The gas dynamic model assumes parallel mixing between the rocket exhaust products and surrounding air (either quiescent or moving), and allows for non-uniform initial conditions at the nozzle exit plane.* Lewis and Prandtl numbers are assumed to be constant, and pressure is allowed to vary parallel to the plume axis. Turbulent transport is described via an appropriate eddy viscosity model and Sutherland's law is used to calculate the viscosity for laminar flow. The program is quite general; it allows any chemical reaction mechanism (and associated rate coefficients) to be used as long as thermodynamic data are available for all species. Thermodynamic data, taken directly from the JANNAF Tables, are input in tabular form.

This report gives the governing partial differential equations and their finite difference formulations, the various eddy viscosity models which may be input to the program, a description of the input data, the output from a sample calculation and a complete FORTRAN listing. The computer output gives detailed axial and radial distributions of velocity, temperature, density and species mole fractions. These results are used to calculate electron densities and electron-neutral collision frequencies which, in turn, are used to determine radar attenuation transverse to the plume and electrical conductivity.

Although the program was written in response to a need for fast predictions of relatively low altitude afterburning rocket plume electrical properties, it can equally well be used for applications to missile base heating and IR radiation problems.

---

*Thus it is possible to account for the effects of an initial boundary layer on the properties in the mixing region.

II. GOVERNING EQUATIONS

A. Conservation Equations and Boundary Conditions

The following equations describe the free-shear layer turbulent or laminar mixing of co-flowing axisymmetric streams undergoing chemical reactions. For turbulent flow all properties are interpreted to be the mean (time-averaged) values. The eddy viscosity, μ, is then described by one of the phenomenological expressions given in Section VI.

Global Continuity

$$\frac{\partial}{\partial x}(\rho u) + \frac{1}{r}\frac{\partial}{\partial r}(\rho v r) = 0 \tag{1}$$

Conservation of Species

$$\rho u \frac{\partial F_i}{\partial x} + \rho v \frac{\partial F_i}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}\left(\frac{Le}{Pr}\mu r \frac{\partial F_i}{\partial r}\right) + \dot{w}_i \tag{2}$$

Conservation of Momentum

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial r} = -\frac{dp}{dx} + \frac{1}{r}\frac{\partial}{\partial r}\left(\mu r \frac{\partial u}{\partial r}\right) \tag{3}$$

Conservation of Energy

$$\rho c_p \left[u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial r}\right] = u\frac{dp}{dx} + \mu\left(\frac{\partial u}{\partial r}\right)^2 + \frac{1}{r}\frac{\partial}{\partial r}\left[\frac{c_p}{Pr}\mu r \frac{\partial T}{\partial r}\right] + \mu\frac{Le}{Pr}\frac{\partial T}{\partial r}\sum_i c_{p_i}\frac{\partial F_i}{\partial r} - \sum_i \dot{w}_i h_i \tag{4}$$

State

$$\rho = \frac{pW}{RT} \tag{5}$$

The conservation equations are solved subject to the following initial and boundary conditions:

$$
\begin{aligned}
x = 0: &\quad u = u(r), \quad F_i = F_i(r), \quad T = T(r) \\
r = 0: &\quad \frac{\partial u}{\partial r} = \frac{\partial T}{\partial r} = \frac{\partial F_i}{\partial r} = 0 \\
r \to \infty: &\quad u \to u_e, \quad F_i \to (F_i)_e, \quad T \to T_e
\end{aligned}
\tag{6}
$$

Pressure is allowed to vary in the axial direction according to,

$$p = c_0 + c_1 x + c_2 x^2 + c_3 x^3 \tag{7}$$

where c_0, c_1, c_2 and c_3 are input coefficients (Card 5, Cols. 21-60).

B. Transformation to Stream Function Coordinates

It is convenient to transform the equations into a streamline coordinate system and utilize the stream function, Ψ, as the radial coordinate. The transformation from cartesian (x, r) coordinates to streamline (x, Ψ) coordinates (which automatically satisfies global continuity, Eq. (1)) is defined by:

$$\Psi \frac{\partial \Psi}{\partial r} = \rho u r \tag{8a}$$

$$\Psi \frac{\partial \Psi}{\partial x} = -\rho v r \tag{8b}$$

From Eqs. (8a) and (8b) we obtain,

$$\left(\frac{\partial}{\partial r}\right)_x = \frac{\rho u r}{\Psi} \left(\frac{\partial}{\partial \Psi}\right)_x \tag{9a}$$

$$\left(\frac{\partial}{\partial x}\right)_r = \left(\frac{\partial}{\partial x}\right)_\Psi - \frac{\rho v r}{\Psi} \left(\frac{\partial}{\partial \Psi}\right)_x \tag{9b}$$

Introducing Eqs. (9a) and (9b) into Eqs. (2), (3), and (4), gives:

Species

$$\frac{\partial F_i}{\partial x} = \frac{1}{\Psi} \frac{\partial}{\partial \Psi} \left[\left(\frac{Le}{Pr}\right) \frac{\mu \rho u r^2}{\Psi} \frac{\partial F_i}{\partial \Psi} \right] + \frac{\dot{w}_i}{u\rho} \tag{10a}$$

and, on the axis of symmetry, $r = \Psi = 0$

$$\frac{\partial F_i}{\partial x} = 2\mu \left(\frac{Le}{Pr}\right) \frac{\partial^2 F_i}{\partial \Psi^2} + \frac{\dot{w}_i}{u\rho} \tag{10b}$$

Momentum

$$\frac{\partial u}{\partial x} = -\frac{1}{\rho u} \frac{dp}{dx} + \frac{1}{\Psi} \frac{\partial}{\partial \Psi} \left[\frac{\mu \rho u r^2}{\Psi} \frac{\partial u}{\partial \Psi} \right] \tag{11a}$$

and, on the axis of symmetry, $r = \Psi = 0$

$$\frac{\partial u}{\partial x} = -\frac{1}{\rho u} \frac{dp}{dx} + 2\mu \frac{\partial^2 u}{\partial \Psi^2} \tag{11b}$$

Energy

$$c_p \frac{\partial T}{\partial x} = \frac{1}{\rho} \frac{dp}{dx} - \frac{1}{\rho u} \sum_i h_i \dot{w}_i + \frac{1}{\Psi} \frac{\partial}{\partial \Psi} \left[\frac{c_p}{Pr} \frac{\mu \rho u r^2}{\Psi} \frac{\partial T}{\partial \Psi} \right] + \frac{\mu \rho u r^2}{\Psi^2} \left[\left(\frac{\partial u}{\partial \Psi}\right)^2 + \frac{Le}{Pr} \frac{\partial T}{\partial \Psi} \sum_i c_{p_i} \frac{\partial F_i}{\partial \Psi} \right] \tag{12a}$$

and, on the axis of symmetry, $r = \Psi = 0$

$$c_p \frac{\partial T}{\partial x} = \frac{1}{\rho} \frac{dp}{dx} + 2\mu \left(\frac{c_p}{Pr}\right) \frac{\partial^2 T}{\partial \Psi^2} - \frac{1}{\rho u} \sum_i h_i \dot{w}_i \tag{12b}$$

C. Finite-Difference Formulation

The governing set of parabolic partial differential equations, (Eqs. (10), (11) and (12)), are first rewritten in finite difference form and then solved using a forward marching technique. The chemistry terms, $\dot{w}_n$, in the species continuity equations are evaluated via implicit-differences; the diffusion terms in the species continuity equations and the complete energy and momentum equations are evaluated via explicit-differences. The following finite-difference formulations[13] are used:

$$\left(\frac{\partial Q}{\partial x}\right)_{n+1,\,m} = \frac{Q_{n+1,\,m} - Q_{n,\,m}}{\Delta x} \tag{13}$$

$$\left(\frac{\partial Q}{\partial \Psi}\right)_{n,\,m} = \frac{Q_{n,\,m+1} - Q_{n,\,m-1}}{2\Delta \Psi} \tag{14a}$$

$$\left[\frac{\partial}{\partial \Psi}\left(a\frac{\partial Q}{\partial \Psi}\right)\right]_{n,\,m} = \frac{a_{n,\,m+\frac{1}{2}}\left[Q_{n,\,m+1} - Q_{n,\,m}\right]}{(\Delta \Psi)^2} - \frac{a_{n,\,m-\frac{1}{2}}\left[Q_{n,\,m} - Q_{n,\,m-1}\right]}{(\Delta \Psi)^2} \tag{14b}$$

where

$$a_{n,\,m\pm\frac{1}{2}} = \frac{a_{n,\,m} + a_{n,\,m\pm1}}{2} \tag{15a}$$

and

$$a = \frac{\mu \rho u r^2}{\Psi} \tag{15b}$$

The difference equations that result from applying Eqs. (13), (14) and (15) to Eqs. (10), (11) and (12) are:

Species

$$(F_i)_{n+1,m} - (\dot{w}_i)_{n+1,m}\,\Delta x/(\rho u)_{n,m}$$

$$= \frac{\Delta x}{m(\Delta\Psi)^3}\left\{\left(\frac{Le}{Pr}a\right)_{n,m+\frac{1}{2}}\left[(F_i)_{n,m+1} - (F_i)_{n,m}\right]\right.$$

$$\left. + \left(\frac{Le}{Pr}a\right)_{n,m-\frac{1}{2}}\left[(F_i)_{n,m-1} - (F_i)_{n,m}\right]\right\} \tag{16a}$$

$$+ (F_i)_{n,m}$$

and, on the axis of symmetry ($m = 0$),

$$(F_i)_{n+1,0} - (\dot{w}_i)_{n+1,0}\,\Delta x/(\rho u)_{n,0}$$

$$= \frac{4\Delta x}{(\Delta\Psi)^2}\left(\frac{\mu Le}{Pr}\right)_{n,0}\left[(F_i)_{n,1} - (F_i)_{n,0}\right]$$

$$+ (F_i)_{n,0} \tag{16b}$$

Momentum

$$u_{n+1,m} = \frac{\Delta x}{m(\Delta\Psi)^3}\left\{a_{n,m+\frac{1}{2}}\left[u_{n,m+1} - u_{n,m}\right]\right.$$

$$\left. + a_{n,m-\frac{1}{2}}\left[u_{n,m-1} - u_{n,m}\right]\right\} - \frac{\Delta x}{(\rho u)_{n,m}}\left(\frac{dp}{dx}\right)_{n+1,} + u_{n,m} \tag{17a}$$

and, on the axis of symmetry, $m = 0$

$$u_{n+1,0} = -\frac{\Delta x}{(\rho u)_{n,0}} \left(\frac{dp}{dx}\right)_{n+1} + \frac{4\mu_{n,0}\Delta x}{(\Delta\Psi)^2} \left[u_{n,1} - u_{n,0}\right] + u_{n,0} \tag{17b}$$

<u>Energy</u>

$$T_{n+1,m} = \frac{\Delta x}{(\rho c_p)_{n,m}} \left(\frac{dp}{dx}\right)_{n+1} + \frac{\Delta x}{4m(\Delta\Psi)^3} \left(\frac{a}{c_p}\right)_{n,m} \left(u_{n,m+1} - u_{n,m-1}\right)^2$$

$$+ \frac{\Delta x}{m(\Delta\Psi)^3 (c_p)_{m,n}} \left\{ \left(\frac{c_p}{Pr} a\right)_{n,m+\frac{1}{2}} \left(T_{n,m+1} - T_{n,m}\right) \right.$$

$$+ \left(\frac{c_p}{Pr} a\right)_{n,m-\frac{1}{2}} \left(T_{n,m-1} - T_{n,m}\right) + \frac{1}{4} \left(\frac{La}{Pr} a\right)_{n,m-1} \sum_i (c_{p_i})_{n,m}$$

$$\left. \left(F_{i_{n,m+1}} - F_{i_{n,m-1}}\right) \left[T_{n,m+1} - T_{n,m-1}\right] \right\}$$

$$+ T_{n,m} - \frac{1}{(\rho u)_{n,m}} \sum_i (h_i \dot{w}_i)_{n,m} \tag{18a}$$

and, on the axis of symmetry, $m = 0$

$$T_{n+1,0} = \frac{\Delta x}{(\rho c_p)_{n,0}} \left(\frac{dp}{dx}\right)_{n+1} + \frac{4\Delta x}{(\Delta\Psi)^2} \left(\frac{\mu}{Pr}\right)_{n,0} \left[T_{n,1} - T_{n,0}\right]$$

$$+ T_{n,0} - \frac{1}{(\rho u)_{n,0}} \sum_i (h_i \dot{w}_i)_{n,0} \tag{18b}$$

The species mole fractions at station n+1, m are determined from the species conservation equations by linearizing the chemistry terms* (i.e. $(\dot{w}_i)_{n+1,m}$) and inverting the resulting matrix. The linearizations involving species F_i and F_j (for a two-body reaction) or F_i, F_j and F_k (for a three-body reaction) at station n+1 (all variables are known at station n), are given by

$$(F_iF_j)_{n+1} = (F_iF_j)_n + F_{jn}\left[(F_i)_{n+1} - (F_i)_n\right] + F_{in}\left[(F_j)_{n+1} - (F_j)_n\right]$$

$$= -\underline{\underline{(F_iF_j)_n}} + \underline{(F_j)_n}\,(F_i)_{n+1} + \underline{(F_i)_n}\,(F_j)_{n+1} \tag{19}$$

$$(F_iF_jF_k)_{n+1} = -\underline{\underline{2(F_iF_jF_k)_n}} + \underline{(F_jF_k)_n}(F_i)_{n+1} + \underline{(F_iF_k)_n}(F_j)_{n+1}$$

$$+ \underline{(F_iF_j)_n}(F_k)_{n+1}. \tag{20}$$

The terms underscored by a single line contribute to the elements of the coefficient matrix, while the terms underscored by a double line contribute to the known column matrix on the right hand side of the matrix equation for the linearized system. Thus the matrix equation takes the form (for N species),

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & & a_{1N} \\ a_{21} & & & & \\ & & & & \\ a_{N1} & & & & a_{NN} \end{bmatrix} \begin{bmatrix} F_1 \\ F_2 \\ \\ F_N \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2 \\ \\ Q_N \end{bmatrix} \tag{21}$$

---

*The chemistry term does not make the energy equation "stiff"; thus when solving for temperature the chemistry term is treated explicitly.

III. SOLUTION OF FINITE DIFFERENCE EQUATIONS

A. Integration Step Size

An exact stability relationship governing the maximum allowable integration step size, $(\Delta x)_{max}$, cannot be obtained due to the nonlinearity of the governing equations. Instead the step-size requirement to satisfy stability can only be estimated. Following Von Neuman[14] a limit is placed on $(\Delta x)_{max}$ such that all dependent variables (u, T, F_i) always remain equal to or greater than zero. Thus the maximum step size at each radial grid point ($m \neq 0$) as established from the species conservation equation* is estimated to be

$$(\Delta x)_{max} = \frac{m\,(\Delta\Psi)^3}{\left[\frac{Le}{Pr}a\right]_{n,\,m+\frac{1}{2}} + \left[\frac{Le}{Pr}a\right]_{n,\,m-\frac{1}{2}}}\ FDL \tag{22a}$$

and on the axis, ($m = 0$),

$$(\Delta x)_{max} = \frac{(\Delta\Psi)^2\,Pr}{4\,Le\,\mu}\ FDL \tag{22b}$$

The actual integration step size, Δx, is taken to be $\frac{1}{3}$ of the smallest value of $(\Delta x)_{max}$ as computed from Eqs. (22a) and (22b). This fraction ($\frac{1}{3}$) was selected on the basis of many trial calculations. Since Eqs. (22a) and (22b) are only approximate an additional factor, FDL, has been incorporated into the program in order to maintain external control (Card 5, Cols. 11-20) on Δx in case smaller step sizes are required to maintain stability of the solution. In addition, the step size can never exceed the input print increment (Card 4, Cols. 21-30).

Should the computed species mole fraction at any radial point become negative (typically, because the chemistry is "fast", and one or more reactions are near-equilibrium), the step size is repeatedly halved until either the species mole fraction becomes positive or the step size becomes less than

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* Applying the same criteria to the momentum and energy equations usually results in larger values of $(\Delta x)_{max}$.

some minimum step size.* In the latter case, the program terminates. After the species mole fraction becomes positive, the next value of Δx is again computed from $\frac{1}{3}(\Delta x)_{max}$. Thus the step size is never determined from the value of Δx needed to satisfy stability for the previous step. This is a somewhat unique approach to specifying Δx for the solution to finite difference equations, and can save substantial computer time. It was adopted because, typical rocket plume calculations show that, when using the mixed implicit/explicit difference scheme, the chemistry only influences stable step sizes in a small region of the flow. Once the program integrates through this region step sizes of $\frac{1}{3}(\Delta x)_{max}$ usually suffice.

B. Edge of Mixing Layer

An additional radial mesh point (at free stream conditions) is added whenever the "next-to-the-last" radial point value of temperature or velocity, differs from the corresponding free stream value by more than a specified percentage of the free stream value. One percent has been selected for velocity and five percent for temperature.

C. Halving the Mesh

The number of grid points cannot be allowed to expand without bounds because of the limited storage capacity of the computer. Therefore, the number of points is halved either when the mesh increases to twice its original size (Card 2, Cols. 1-5) or the number of points exceeds 26. The computer prints all output at the station at which halving occurs.

---

*The minimum step size is an input number (Card 5, Cols 1-10).

IV. CHEMICAL REACTION RATE EQUATIONS

Ten possible reaction types are included in the program:

Reaction Type	
(1)	$A + B \rightleftarrows C + D$
(2)	$A + B + M \rightleftarrows C + M$
(3)	$A + B \rightleftarrows C + D + E$
(4)	$A + B \rightleftarrows C$
(5)	$A + M \rightleftarrows C + D + M$
(6)	$A + B \rightarrow C + D$
(7)	$A + B + M \rightarrow C + M$
(8)	$A + B \rightarrow C + D + E$
(9)	$A + B \rightarrow C$
(10)	$A + M \rightarrow C + D + M$

Reaction types (6)-(10) correspond to reaction types (1)-(5), but proceed in the forward direction only. In Reactions (2), (5), (7) and (10), M is an arbitrary third body. In this program, all species are assumed to have equal third body efficiencies; thus, in evaluating $\dot{w}^{(j)}$, $F_M = (W)^{-1}$. The net rates of production for all reactions are written below, in the form, $\dot{w}^{(j)} = RP^{(j)} - RM^{(j)}$.*

(1) $$\dot{w}^{(j)} = k_f \rho^2 F_A F_B - \frac{k_f \rho^2 F_C F_D}{K_p}$$

(2) $$\dot{w}^{(j)} = \frac{k_f \rho^3 F_A F_B}{W} - \frac{k_f \rho^2 F_C}{K_p WRT}$$

(3) $$\dot{w}^{(j)} = k_f \rho^2 F_A F_B - \frac{k_f \rho^3 F_C F_D F_E RT}{K_p}$$

(4) $$\dot{w}^{(j)} = k_f \rho^2 F_A F_B - \frac{k_f \rho^3 F_C}{K_p RT}$$

(5) $$\dot{w}^{(j)} = \frac{k_f \rho^2 F_A}{W} - \frac{k_f \rho^3 F_C F_D RT}{K_p W}$$

---

* The symbols RP and RM are used on the computer output.

(6) $$\dot{w}^{(j)} = k_f \rho^2 F_A F_B$$

(7) $$\dot{w}^{(j)} = \frac{k_f \rho^3 F_A F_B}{W}$$

(8) $$\dot{w}^{(j)} = k_f \rho^2 F_A F_B$$

(9) $$\dot{w}^{(j)} = k_f \rho^2 F_A F_B$$

(10) $$\dot{w}^{(j)} = \frac{k_f \rho^2 F_A}{W}$$

To reduce round-off and truncation errors $RP^{(j)}$ and $RM^{(j)}$ are computed separately for each reaction. All contributions to the molar rate of production of a given species are then computed and added algebraically to form $\dot{w}_i$.

The forward rate coefficient, k_f, is expressed in the form,

$$k_f = AT^{-N} \exp(B/RT) \tag{23}$$

and K_p is determined from,

$$\ln K_p = -\Delta G/RT \tag{24}$$

The rate coefficients are divided into seven types:

Rate Coefficient Type*

(1) $k_f = A$

(2) $k_f = AT^{-1}$

(3) $k_f = AT^{-2}$

(4) $k_f = AT^{-\frac{1}{2}}$

(5) $k_f = A \exp(B/RT)$

(6) $k_f = AT^{-1} \exp(B/RT)$

(7) $k_f = AT^{-\frac{3}{2}}$

*Rate coefficient data for typical rocket plume reactions may be found, e.g., in Ref. 15.

V. THERMODYNAMIC DATA

The thermodynamic properties (specific heat, Gibbs free energy and enthalpy) for each species are taken directly from the JANNAF Thermochemical Tables,[16] and input to the program as c_{p_i}, $-\left(\frac{g_i - h_{298_i}}{T}\right)$ and $(h_i - h_{298})$ in tabular form as a function of temperature (Card 11). Linear interpolation is used to define thermodynamic properties at the local temperature.

VI. TRANSPORT PROPERTIES

A. Turbulent Eddy Viscosity Models

The following eddy viscosity models[17-20] are incorporated into the program:

Model 1 (Ferri)[17]

Initial region,*

$$\mu = \rho \epsilon = \alpha 0.00137 \times \left| \rho_o u_o - \rho_e u_e \right| \tag{25a}$$

Developed region,

$$\mu = \rho \epsilon = \alpha K b_{\frac{1}{2}} \left| \rho_o u_o - \rho_e u_e \right| \tag{25b}$$

where $b_{\frac{1}{2}}$ is the value of r where $\rho u = (\rho_o u_o + \rho_e u_e)/2$ and K is the eddy viscosity coefficient, usually taken to be 0.025.†

---

*Defined as region upstream of axial position where $(u_o - u_e)/(u_j - u_e) = 0.95$.

†Most of the models contain a numerical coefficient K which must be determined empirically. The value K = 0.025, taken from Schlicting,[18] has been incorporated directly into the program. This can be changed by the program input data via an appropriate value for the additional constant, α, Eqs. (25-31) (Card 4, Cols. 61-70).

Model 2 (Ting/Libby)[19]

$$\mu = \rho \epsilon = \alpha K \bar{r}_{\frac{1}{2}} \; | u_o - u_e | \; \rho \left(\frac{\rho_o}{\rho}\right)^2 \left(\frac{\eta}{r}\right)^2 \tag{26}$$

where

$$\eta^2 = 2 \int_0^r (\rho_o/\rho) \, r' \, d r' \tag{27}$$

and $\bar{r}_{\frac{1}{2}}$ is the value of η where $u = (u_o + u_e)/2$

Model 3

Initial region,

$$\mu = \rho \epsilon = \alpha 0.00137 \times \rho_o \, | u_o - u_e | \tag{28a}$$

Developed region,

$$\mu = \alpha K r_{\frac{1}{2}} \rho_o \, | u_o - u_e | \tag{28b}$$

where $r_{\frac{1}{2}}$ is the value of r where $u = (u_o - u_e)/2$

Model 4

Initial region,

$$\mu = \rho \epsilon = \alpha 0.00137 \times \rho_e \, | u_o - u_e | \tag{29a}$$

Developed region,

$$\mu = \rho \epsilon = \alpha K r_{\frac{1}{2}} \rho \epsilon \, | u_o - u_e | \tag{29b}$$

Model 5* (Ting/Libby)[19]

Initial region,

$$\mu = \rho\epsilon = \alpha 0.00137 \times |u_j - u_e| \rho\left(\frac{\rho_j}{\rho}\right)^2 \qquad (30)$$

Developed region,

$$\mu = \rho\epsilon = \alpha K \bar{r}_{\frac{1}{2}} |u_o - u_e| \rho\left(\frac{\rho_o}{\rho}\right)^2 \left(\frac{u}{u_1}\right)^2 \qquad (26)$$

Model 6 (Donaldson/Gray)[20]

Initial region,

$$\mu = \rho\epsilon = \alpha\bar{K}(r_{\frac{1}{2}} - r_i)\rho |u_o - u_e|/2 \qquad (31a)$$

$$\text{For } M_{\frac{1}{2}} \le 1.2 \quad \bar{K} = 0.0468 + M_{\frac{1}{2}}\left[-0.0460 M_{\frac{1}{2}} + 0.0256 M_{\frac{1}{2}}^2\right]$$

$$M_{\frac{1}{2}} > 1.2 \quad \bar{K} = 0.0248 \qquad (32)$$

where $M_{\frac{1}{2}}$ is the value of the Mach number where $u = (u_o + u_e)/2$ (i.e., the half radius). The speed of sound at the half radius, $a_{\frac{1}{2}}$ is expressed by,

$$a_{\frac{1}{2}} = \left[\frac{c_p}{c_p - (R/W_{\frac{1}{2}})} \frac{RT_{\frac{1}{2}}}{W_{\frac{1}{2}}}\right]^{\frac{1}{2}} \qquad (33)$$

where $W_{\frac{1}{2}}$ and $T_{\frac{1}{2}}$ are evaluated at the half radius. In Eq. (31a), r_i is the inner mixing zone radius and is defined as the value of r where $(u - u_e)/(u_j - u_e) = 0.95$.

Developed region,

$$\mu = \rho\epsilon = \alpha\bar{K} r_{\frac{1}{2}} \rho |u_o - u_e|/2 \qquad (31b)$$

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*In the program, the specification of Model 5 means that Eq. (30) will be used in the initial region and Model 2 (Eq. 26) will be used in the developed region. This is important for re-starting a problem in the developed region for which Model 5 was selected to run from x = 0. In this case, Model 2 must be specified on Card 2, Cols. 11-15.

B. Laminar Flow

Sutherland's Law[21] is used to describe the viscosity as a function of temperature.

$$\mu = 9.8 \times 10^{-7}\, T^{3/2} / (T + 111) \qquad lb_m/ft\text{-}sec \qquad (34)$$

VII. PLUME ELECTRICAL PROPERTIES

Electron density, electron-neutral collision frequency, unit radar attenuation and electrical conductivity are computed at all radial points for each axial print-out station.

A. Electron Density

$$n_e = 0.733\,(10^{22})\, X_{e^-}\, p\, T^{-1} \qquad m^{-1} \qquad (35)$$

where p is in atm and T in degrees K.

B. Collision Frequency

$$\nu_e = 4.57\,(10^{27})\, p\, T^{-\frac{1}{2}} \sum X_i\, Q_{e_i} \quad sec^{-1} \qquad (36)$$

where p is in atm, T in degrees K and Q_{e_i} in cm^2. The electron-neutral collision cross sections[22] used in the calculations and given in the following table are those which characterize typical solid propellant exhaust plumes. If other species contribute to the value of ν_e, the program must be modified.

Species	Q_{ei}, cm^2
CO	$2.03\ (10^{-23})v_e^{\dagger} + 2.46\ (10^{-16})$
CO_2	$4.7\ (10^{-8})v_e^{-1}$
H_2O	$5.9\ v_e^{-2}$
HCl	$1.85\ v_e^{-2}$
N_2	$3.29\ (10^{-23})v_e$
H_2	$1.45\ (10^{-23})v_e + 8.0\ (10^{-16})$

$\dagger\ v_e = 6.21\ (10^5)\ T^{\frac{1}{2}}$ cm/sec

C. Transverse Radar Attenuation

$$a' = 1.17\ \frac{n_e/\nu_e}{[1 + (\omega/\nu_e)^2]} \quad \text{db/in} \tag{37}$$

where n_e is in ml^{-1}, ν_e in sec^{-1} and ω is rad/sec.* The program then computes transverse (normal to the axis) radar attenuation along a "line-of-site" (i.e. radar beam "spot size" much smaller than the electrical plume diameter) from,

$$A = 2\int_0^{\infty} a'\ dr \quad \text{db} \tag{38}$$

where r is in inches.

D. Electrical Conductivity

$$\sigma = 2.54(10^4)\ \frac{e^2\ n_e}{\nu_e\ m_e} \quad \text{mho/in} \tag{39}$$

where e is 1.6×10^{-19} coulomb and m_e is 9.1×10^{-31} kg.

*Attenuation calculations can be made for a maximum of six signal frequencies.

VIII. PROGRAM OPERATION

A. Machine

The program, as listed in Appendix A, must be run on a CDC computer since a library routine named SECOND (called in subroutine TICK) is used to sense elapsed time from the start of execution. This routine enables the continuing solution cards to be punched when the execution time exceeds the time input on Card 2, Cols. 36-40--if punch options 2 or 3 are selected (Card 2, Cols. 31-35). The program may be run on a different machine by removing the subroutine and replacing it with the dummy routine shown below:

```
SUBROUTINE TICK (JJJ)
JJJ = 0
RETURN
END
```

When this is done the maximum execution time input on Card 2, Cols. 36-40 will not trigger the punch option.

Input and output are on the standard tape units (i.e. 5 for READ, 6 for WRITE and 7 for PUNCH).

B. Sense Switch Control

1. Sense Switch 1 - When Sense Switch 1 is on, the current values of x, T_o, and $n_{e,o}$ are printed on-line.

2. Sense Switch 3 - When Sense Switch 3 is on, the case is terminated and all output is printed at the current axial station.

C. Program Optimization

It is recommended that the program be compiled using the highest level of optimization. On the CDC 6600 this corresponds to the FAST OBJECT CODE MODE.

IX. PROGRAM INPUT DATA

The input data cards are explained below. A listing of the computer program, a sample input data sheet and a sample output are given in Appendices A, B and C, respectively.

Card No.	Columns	Description	Format
1	1-72	Run identification	12A6
2	1-5	Initial number of grid points* in ψ coordinate (26 maximum)	I5
	6-16	Number of species (24 maximum)	I5
	11-15	Viscosity option key If -1: Laminar (Eq. 34) 0: μ = constant 1: Model 1 (Eq. 25) 2: Model 2 (Eq. 26) 3: Model 3 (Eq. 28) 4: Model 4 (Eq. 29) 5: Model 5 (Eqs. 26 and 30) 6: Model 6 (Eq. 31)	I5
	16-20	Number of reactions (40 maximum)	I5
	21-25	$\dot{w}_i$ output option If 0: $\dot{w}_i$ for each species is not output 1: $\dot{w}_i$ for each species is output at all radial points whose temperature is greater than the kinetics cut-off temperature (Card 6, Cols. 61-70)	I5

*Recommended number, 13

Card No.	Columns	Description	Format
2	26-30	RP, RM output option If 0: RP, RM for each reaction is not output 1: RP, RM for each reaction is output at all radial points whose temperature is greater than the kinetics cut-off temperature (Card 6, Cols. 61-70)	I5
	31-35	Card punch option If 0: No cards punched 1: Cards with radial distributions of electron density and collision frequency at all printout stations are punched 2: Cards for continuing a given solution are punched 3: Both the above sets of cards are punched	I5
	36-40	Maximum computer execution time (min) (If card punch option 1, 2 or 3 is selected, cards will be punched after this amount of computer time)*	I5
	41-45	Pressure option If 0: Pressure is a constant 1: Pressure is a function of axial distance	I5
3	1-10 . . . 51-60	Signal frequencies (MHz) - 6 maximum - for which transverse attenuation calculations will be made (see Section VII). Leave blank if no attenuation calculations desired	E10.3

*In practice if this option is selected, the calculations will terminate at an execution time 30 seconds less than this value.

Card No.	Columns	Description	Format
4	1-10	Initial value of x (ft)	E10.3
	11-20	Final value of x (ft)	E10.3
	21-30	Print increment (ft)	E10.3
	31-40	Lewis number	E10.3
	41-50	Prandtl number	E10.3
	51-60	Nozzle (jet) radius (ft)	E10.3
	61-70	α, factor used to vary eddy viscosity* (see Section VI)	E10.3
5	1-10	Δx_{min}, Minimum integration step size (ft)†	E10.3
	11-20	FDL, diffusion step size factor‡	E10.3
	21-30	c_0 (atm)	E10.3
	31-40	c_1 (atm/ft)	E10.3
	41-50	c_2 (atm/ft^2) Pressure Coefficients (see Section II)	E10.3
	51-60	c_3 (atm/ft^3)	E10.3
6	1-10	Pressure at initial value of x(atm)	E10.3
	11-20	Temperature at jet centerline (K)	E10.3
	21-30	Temperature at edge of jet (K) (free stream value)	E10.3

*Set $\alpha = 1.0$ if no changes to eddy viscosity coefficient are desired.

†Recommended value, 1×10^{-10} ft.

‡Set FDL = 1.0 if maximum integration step size criterion discussed in Section III is to be used.

Card No.	Column	Description	Format
6	31-40	Velocity at jet centerline (ft/sec)	E10.3
	41-50	Velocity at edge of jet (ft/sec) (free stream value)	E10.3
	51-60	$\Delta\Psi$, $\left(\frac{lbm}{32.2}\ sec^{-1}\right)^{\frac{1}{2}}$	E10.3
		If $\Delta\Psi = 0$ (or blank) the program computes $\Delta\Psi$ assuming velocity, temperature and species mole fractions are constant at initial station	
		If $\Delta\Psi$ is specified, cards 7.1 to 9.13 are read next. If $\Delta\Psi$ is not specified, card 10.1 is the next card read with cards 7.1 through 9.13 being omitted	
	61-70	Kinetics cut-off temperature (kinetics are frozen at temperatures below this value*)	E10.3

NOTE: For the purpose of illustration it is assumed that there are 13 initial grid points in the Ψ coordinate.

7.1	1-10	T(1), Temperature (K) at jet centerline, r = 0	E10.3
	⋮		
	61-70	T(7)	
7.2	1-10	T(8)	E10.3
	⋮		
	51-60	T(13), Temperature (K) in free stream	
8.1	1-10	u(1), Velocity (ft/sec) at jet centerline, r = 0	E10.3
	⋮		
	61-70	u(7)	
8.2	1-10	u(8)	E10.3
	⋮		
	51-60	u(13)	

*If blank or zero, 400 K is used.

Card No.	Column	Description	Format
NOTE: For the purpose of illustration it is assumed that there are 8 species			
9.1.1	1-10	Mole fraction of 1st species at jet center-line, r = 0	E10.3
	⋮		
	61-70	Mole fraction of 7th species at jet center-line, r = 0	E10.3
9.1.2	1-10	Mole fraction of 8th species at jet center-line, r = 0	E10.3
9.2.1	1-10	Mole fraction of 1st species at next grid point	E10.3
	⋮		
	61-70	Mole fraction of 7th species at next grid point	
9.2.2	1-10	Mole fraction of 8th species of next grid point	E10.3
9.13.1	1-10	Mole fraction of 1st species at 13 grid point (free stream)	E10.3
	⋮		
	61-70	Mole fraction of 7th species at 13th grid point (free stream)	
9.13.2	1-10	Mole fraction of 8th species at 13th grid point (free stream)	E10.3
NOTE: Card Type 10 is not required if Card Types 7, 8 and 9 are input.			
10.1.1	1-10	Mole fraction of 1st species at jet center-line, r = 0	E10.3
	⋮		
	61-70	Mole fraction of 7th species at jet center-line, r = 0	
10.1.2	1-10	Mole fraction of 8th species at jet center-line, r = 0	

Card No.	Column	Description	Format
10.2.1	1-10	Mole fraction of 1st species in free stream	E10.3
	. . .		
	61-70	Mole fraction of 7th species in free stream	
10.2.2	1-10	Mole fraction of 8th species in free stream	

NOTE: The following cards contain the thermodynamic data.* The first card contains the species name, molecular weight and heat of formation. The second and remaining cards contain the temperature and corresponding specific heat, free energy and enthalpy for that species. Two temperatures and corresponding thermodynamic data are placed on each card. The input table can contain up to a maximum of 30 temperature points. The data are input exactly as presented in the JANNAF tables.[16]

Card No.	Column	Description	Format
11.1.1	1- 6	Name of first species	A6
	7-16	Molecular weight	E10.3
	17-26	Heat of formation, h_{298_i} (kcal/mole)	E10.3
11.1.2	1-10	First temperature point (K)	E10.3
	11-20	c_{p_i} (cal/mole-K)	E10.3
	21-30	$-\left(\frac{g_i - h_{298_i}}{T}\right)$ (cal/mole K)	E10.3
	31-40	$h_i - h_{298_i}$ (kcal/mole)	E10.3
	41-50	Second temperature point (K)	E10.3
	51-60	c_{p_i} (cal/mole-K)	E10.3
	61-70	$-\left(\frac{g_i - h_{298_i}}{T}\right)$ (cal/mole-K)	E10.3

*The order of the species must be identical to the order on Card Types 9 or 10.

Card No.	Column	Description	Format
11.1.2	71-80	$h_i - h_{298_i}$ (kcal/mole)	E10.3
11.1.3	⋮	Third temperature point	
11.2.1	⋮	Name of second species	

NOTE: The chemical reaction mechanism for a particular probem is input on the last set of cards, one card for each reaction. (See Section IV.) No particular order is required.

12.1	1-6	Species A	A6
	7	+ sign	
	8-13	Species B (or M)	A6
	14	+ sign	
	15-20	Blank or M	6x
	21	= sign	
	22-27	Species C	A6
	28	+ sign (if needed)	
	29-34	Species D (or M)	A6
	35	+ sign (if needed)	
	36-41	Species E (or M)	A6
	42-48	Blank	
12.1	49-50	Reaction type, 1 to 10 (see Section IV)	I2
	51	Rate coefficient type, 1 to 7 (see Section IV)	I1
	52-59	A, Pre-exponential factor cm-molecule-sec units	E8.2
	60-63	N, Temperature exponent	F4.1
	64-72	B, Activation energy cal/mole	F9.1
12.2	⋮	Next Reaction	

X. PROGRAM OUTPUT

A. Description

Sample output sheets for the input data given in Appendix B are shown in Appendix C. The first page contains the key program input parameters, initial distributions of velocity, temperature and species mole fractions and the chemical reaction mechanism and rate coefficients. The succeeding pages contain printouts at axial stations corresponding to the print increment (Card 4, Cols. 21-30). Following the listing of electrical properties (last page of output), the integration step size and corresponding axial position are given for each integration step up to the next print station.

B. Units

A mixed system of units appears on the program output for ease in making additional calculations and for program check-out.

COLLISION FREQUENCY	electron-neutral collision frequency, sec^{-1}.
DELTA X	integration step size, ft
DENSITY	g/cm^3
ELECTRICAL CONDUCTIVITY	mho/in
ELECTRON DENSITY	ml^{-1}
ENTHALPY	mixture static enthalpy, cal/g
HALF RADIUS/R	nondimensional radial distance to point where $u = (u_o + u_e)/2$, ft (viscosity option 6 only)
INNER MIXING ZONE RADIUS/R	nondimensional radial distance to point where $(u-u_e)/(u_j - u_e) = 0.95$, (viscosity option 6 only)
MACH NO.	Mach number
MACH NUMBER AT HALF RADIUS	Mach number at point where $u = (u_o + u_e)/2$ (viscosity option 6 only)
MINIMUM STEP SIZE	$(\Delta x)_{min}$, ft

MIXING RATE COEFFICIENT	defined by Eq. (31a) or Eq. (31b) (viscosity option 6 only)
MOLE FRACTIONS	species mole fractions
NET RATE OF PRODUCTION (W-DOT/RHO*U)	$\dot{w}_i/\rho u$, mole/g-ft
PRESS	pressure, atm
PSI	stream function, $\left[\frac{\text{lbm}}{32.2}\ \text{sec}^{-1}\right]^{\frac{1}{2}}$
PT	radial grid point number
R	nozzle radius
REACTION J	refers to reactions listed on first page of output
RM	negative molar rate of production for jth reaction (see Section IV), mole/ml-sec
RP	positive molar rate of production for jth reaction (see Section IV), mole/ml-sec
SIGN. FREQ.	signal frequency for attenuation calculations, mHz
TEMPERATURE	K
TRANSVERSE ATTENUATION	db
UNIT ATTENUATION	db/in
VELOCITY	axial velocity, ft/sec
VISCOSITY	μ, lbm/ft-sec
X	axial distance, ft
X/R	nondimensional axial distance
Y/R	nondimensional radial distance from axis

C. Card Output

1. Continuing Solution - Due to the large amount of input data required to continue a solution (after being terminated at a given value of x) the program will punch all input except the thermodynamic data and chemical reaction mechanism if this option is selected (Card 2, Cols. 31-35). However, a new final value of x (Card 4, Cols. 11-20) must be input manually if the problem was initially terminated by reaching the old maximum distance. Cards will also be produced if maximum time (Card 2, Cols. 36-40) is exceeded, by using the proper option.

2. Electron Density and Collision Frequency - The complete radial distribution of electron density and collision frequency at all printout stations will be punched if this option is selected (Card 2, Cols. 31-35).

XI. REFERENCES

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APPENDIX A

A FAST COMPUTER PROGRAM FOR NONEQUILIBRIUM ROCKET PLUME PREDICTIONS

Fortran Listing

```
      PROGRAM MAIN  (TEPEC,CCTPUT,PUNCH,TAPE5=INPUT,TAPE6=OUTPUT,
     1    TAPE7=PUNCH)
C*****************************************************************
C***********                                                   **
C***********              A FAST COMPUTER PROGRAM              **
C***********       FOR NONEQUILIBRIUM ROCKET PLUME PREDICTIONS **
C***********              AEROCHEM RESEARCH LABORATORIES       **
C***********                 PRINCETON, N. J.                  **
C***********                                                   **
C*****************************************************************
C
C
      DIMENSION A(30),RHO(30),Y(30),T(30),PSI(30),RT(30),SUM(30),AR(25),
     1HSTAT(30),H(25,30),ALPHA(25,30),RALPHA(25,30),CP(25,30),SIGMA(30),
     2          WTMOLE(25),CPBAR(30),C(25,9),AID(25),ETA(30),RATIO(30),
     3RU(30),U(30),TITLE(12),XLE(18),XMU(30)          ,G(25),WTMIX(30),
     4RC(40,3),IRRR(40,5),WP(25),WM(25),WDOT(25,30),SAVET(30),SAVEU(30),
     5          IRR(40),FREQ(30),SAVEA(25,30),          PC(4),ZID(5),
     6          ECC(30),HOUT(30),YOUT(30),PHOOUT(30),XMUOUT(30),XLT(30),
     7T4(30),TFDG(30),IRT(40),RP(40,30),RM(40,30)
     8 ,CM(25,25,26), DX(25,26) ,CM1(25,25),DX1(25)
      DIMENSION XAME(6), ISAVE(6), FREQA(6), ALOG(50,6)
      DIMENSION TTB(30)    ,CPTB(25,30),HTB(25,30),UTB(25,30),HF(25)
      COMMON  A       , RHO     , Y       , T       , PSI     , RT
      COMMON  SUM     , AR      , HSTAT   , H       , ALPHA   , RALPHA
      COMMON  CP      , SIGMA           , WTMOLE  , CPBAR   , C
      COMMON  AID     , ETA     , RATIO   , RU      , U       , TITLE
      COMMON  XLE     , XMU     ,           G       , WTMIX   , WDOT
      COMMON  SAVEU   , SAVET   , WM      , WP      , RC
      COMMON            SAVEA   ,           PC      , X       , XMAX
      COMMON  PRNT    , DXMIN   , DX      , FDL     , DELPSI  , [illegible]
      COMMON  XB2     , P       , ZID     , FREQ    , ECC     , DDPX
      COMMON  YOUT    , HOUT    , PHOOUT  , IRRP    , IRR     , IFINIS
      COMMON  IPAGE   , NPSI    , MY      , NS      , NR      , IFDGL
      COMMON  ITURB   , IPRESS  , NPSI    , IIEST   , IIFR    , IFEC
      COMMON  IRT     , XMUOUT  , XLT     , T4      , TFDG    , IOUT
      COMMON  IOUT1   , IOUT2   ,RP       , RM      , ISAVE   , IPUNCH
      COMMON IKINET,NFREQA,ALOG,FREQA,00100,00200,00300,00400
C**** SETTING XAME FOR THOSE SPECIES INVOLVED IN COLLISION FREQ. CALC.
      DATA XAME(1)/6HCO    /
      DATA XAME(2)/6HCO2   /
      DATA XAME(3)/6HH2O   /
      DATA XAME(4)/6HH2    /
      DATA XAME(5)/6HN2    /
      DATA XAME(6)/6HHCL   /
      AV=6.025E23
    4 IFINIS=0
      DO 9999 I=1,8596
 9999 A(I)=0.0
      DO 300 I = 1,6
  300 ISAVE(I) = 0
      R=82.06
      READ  (5,333)(TITLE(I),I=1,12)
C     NS= NO. OF SPECIES
C     NR= NO. OF REACTIONS
```

```
      READ(5,100) MPSI,NS,ITURB,NI,IOUT1,IOUT2,IPUNCH,ITIME,IPRESS,NT
      READ (5,111)  (FREQA(I), I=1,6)
      DO 113 I=1,6
      IF (FREQA(I)) 113, 114, 113
  113 CONTINUE
      I=7
  114 NFREQA = I-1
      NPSI=MPSI-1
      READ  (5,1000)X,XMAX,PRNT,XLF(1),SIGMA(1),RJ,XK2
      DX=0.1*RJ
C     INPUT MINIMUM STEPSIZE LIMIT (DXMIN)
      READ(5,1000) DXMIN,FDL,      PC(1),PC(2),PC(3),PC(4)
      READ  (5,1000)P,T(1),T(MPSI),U(1),U(MPSI),DELPSI,TKINET
      IF(TKINET.EQ.0.0) TKINET = 400.0
C**** THE VALUE OF 30 SECONDS IS TO ALLOW FOR COMPILE TIME
      ILIMIT = 60*ITIME-30
      IDIFFT = 0
      CALL TICK(ISECST)
      IF((ISECST+60*ITIME).GT.86400) IDIFFT = 86400-ISECST
      UNIT = U(1)
      IQ77 = 2
      USUR01 = 0.0
C     TURBULENCE MODELS
      IF (ITURB - 3) 8600,9010,9010
 8600 IF (ITURB - 1) 9011,9010,9011
 9010 USUR01 = 0.95*   (U(1)-U(MPSI)) + U(MPSI)
 9011 CONTINUE
      IF(DELPSI) 3011,3012,3011
 3012 READ  (5,1000)(ALPHA(J,1),J=1,NS)
      READ  (5,1000)(ALPHA(J,MPSI),J=1,NS)
      MMOD=MPSI-2
      DO 4001 I=1,MMOD
      T(I)=T(1)
      U(I)=U(1)
      DO 4001 J=1,NS
 4001 ALPHA(J,I)=ALPHA(J,1)
      DO 4002 J=1,NS
 4002 ALPHA(J,NPSI)=ALPHA(J,MPSI)
      GO TO 3015
 3011 READ  (5,1000)(T(I),I=1,MPSI)
      READ  (5,1000)(U(I),I=1,MPSI)
      DO 7 I=1,MPSI
    7 READ  (5,1000)(ALPHA(J,I),J=1,NS)
C     NEW THERMO DATA DATA INPUT IN JANNAF TABLE FORM
 3015 DO 1991 I=1,NS
      READ(5,222) ATD(I),WTMOLE(I),HF(I)
      DO 10 IT=1, N1,2
      READ(5,102) TTB(IT),  CPTB(I,IT),GTB(I,IT),HTB(I,IT)
     1   ,TTB(IT+1)   ,CPTB(I,IT+1), GTB(I,IT+1),HTB(I,IT+1)
      GTB(I,IT)= -GTB(I,IT)*TTB(IT)  +HF(I) *1000.
      GTB(I,IT+1)= -GTB(I,IT+1)*TTB(IT+1)  +HF(I)*1000.
      HTB(I,IT)=(HTB(I,IT)+HF(I))*1000.
      HTB(I,IT+1)=(HTB(I,IT+1)+ HF(I))*1000.
   10 CONTINUE
      IF(WTMOLE(I)-1.0) 1972,1991,1991
```

A-2

```
 1972 IECC=1                                                            MAIN      112
 1991 CONTINUE                                                          MAIN      113
      DO 301 J = 1,6                                                    MAIN      114
      DO 301 I = 1,NS                                                   MAIN      115
      IF(AID(I).EQ.XAME(J)) ISAVE(J) = 1                                MAIN      116
  301 CONTINUE                                                          MAIN      117
      DO 1992 I=1,NR                                                    MAIN      118
      READ  (5,444)(7ID(J),J=1,5),IRR(I),IRT(I),(RC(I,K),K=1,3)         MAIN      119
      DO 1993 J=1,5                                                     MAIN      120
      IRR(I,J)=0                                                        MAIN      121
      DO 1993 L=1,NS                                                    MAIN      122
      IF(7ID(J)-AID(L)) 1993,1994,1993                                  MAIN      123
 1994 IRR(I,J)=L                                                        MAIN      124
 1993 CONTINUE                                                          MAIN      125
 1992 CONTINUE                                                          MAIN      126
      DO 912 I=1,MPSI                                                   MAIN      127
      WTVR=0.0                                                          MAIN      128
      DO 632 J=1,NS                                                     MAIN      129
  632 WTVR=WTVR+ALPHA(J,I)*WTHOLE(J)                                    MAIN      130
      DO 633 J=1,NS                                                     MAIN      131
  633 ALPHA(J,I)=ALPHA(J,I)/WTVR                                        MAIN      132
  912 CONTINUE                                                          MAIN      133
      IF(DELPSI) 903,3041,903                                           MAIN      134
 3041 DUM=0.0                                                           MAIN      135
      DO 5001 J=1,NS                                                    MAIN      136
 5001 DUM=DUM+ALPHA(J,1)                                                MAIN      137
      XMD=MMOD-1                                                        MAIN      138
      DELPSI=SQRT(P*U(1)/42.285/T(1)/DUM)*RJ/XMD                        MAIN      139
  903 DO 20 I=1,29                                                      MAIN      140
      XI=I-1                                                            MAIN      141
      PSI(I)=XI*DELPSI                                                  MAIN      14
      XLE(I)=XLE(1)                                                     MAIN      14
   20 SIGMA(I)=SIGMA(1)                                                 MAIN      144
      DO 90 I=MPSI,29                                                   MAIN      145
      RT(I)=T(MPSI)                                                     MAIN      146
      T(I)=T(MPSI)                                                      MAIN      147
      DO 80 J=1,NS                                                      MAIN      148
      RALPHA(J,I)=ALPHA(J,MPSI)                                         MAIN      149
   80 ALPHA(J,I)=ALPHA(J,MPSI)                                          MAIN      150
      RU(I)=U(MPSI)                                                     MAIN      151
   90 U(I)=U(MPSI)                                                      MAIN      152
      CALL INOUT                                                        MAIN      153
      PPUNCH = P                                                        MAIN      154
      P=2117.0*P                                                        MAIN      155
      DPDX=0.0                                                          MAIN      156
C      PRESSURE OPTION.  IF IPRESS= 0,  PRESSURE                        MAIN      157
C          IS CONSTANT AND = TO P. IF IPRESS = 1, COEFFICIENTS CALLED   MAIN      158
C          PC(1),PC(2),PC(3),PC(4) ARE INPUT.                           MAIN      159
C          EQUATION USED IS P = PC(1) + PC(2)*X + PC(3)*X*X + PC(4)*X*X*X MAIN      160
    2 IF(IPRESS) 821,822,821                                            MAIN      161
  821 P=(PC(1)+X*(PC(2)+X*(PC(3)+X*PC(4))))*2117.0                      MAIN      162
      DPDX=(PC(2)+X*(2.0*PC(3)+X*3.0*PC(4)))*2117.0                     MAIN      163
      PPUNCH = P/2117.0                                                 MAIN      164
  822 DO 31 I=1,MPSI                                                    MAIN      165
      WTMIX(I)=0.0                                                      MAIN      166
```

```
      DO 30 J=1,NS                                                      MAIN     167
   30 WTMIX(I)=WTMIX(I)+ALPHA(J,I)                                      MAIN     168
      RHO(I)=P/89517.501/T(I)/WTMIX(I)                                  MAIN     169
   31 RHOOUT(I)=RHO(I)/1.94                                             MAIN     170
      DO 805 I=1,MPSI                                                   MAIN     171
C     FREE STREAM VELOCITY WILL BE SET TO 1.0 FPS IF ZERO IS ENTERED    MAIN     172
      U(I) = AMAX1(1.0,U(I))                                            MAIN     173
      TFDG(I)=AMAX1((T(I)-100.00)                                       MAIN     174
      T4(I)=TFDG(I)**4                                                  MAIN     175
      XLT(I)=ALOG(TFDG(I))                                              MAIN     176
      CPBAR(I)=0.0                                                      MAIN     177
      HSTAT(I)=0.0                                                      MAIN     178
      TX=T(I)                                                           MAIN     179
      CALL TKEY(TX  ,TTB,ITKEY,SDT,HDT,HT)                              MAIN     180
      IF (ITKEY.EQ.0) GO TO 9                                           MAIN     181
      DO 805 J=1,NS                                                     MAIN     182
      CP(J,I)=0.0                                                       MAIN     183
      H(J,I)=0.0                                                        MAIN     184
      CALL LIPLN(ITKEY,J,CPTB,SDT,HDT,AX)                               MAIN     185
      CP(J,I)=AX*45055.31                                               MAIN     186
      CALL LIPLN(ITKEY,J, HTB,SDT,HDT,AX)                               MAIN     187
      H(J,I)=AX*45055.31                                                MAIN     188
      HSTAT(I)=HSTAT(I)+H(J,I)*ALPHA(J,I)                               MAIN     189
  805 CPBAR(I)=CPBAR(I)+CP(J,I)*ALPHA(J,I)                              MAIN     190
      ETA(1)=0.0                                                        MAIN     191
      Y(1)=0.0                                                          MAIN     192
      ETA(2)=DELPSI/SQRT(RHO(1)*U(2))                                   MAIN     193
      Y(2)=DELPSI/SQRT(RHO(2)*U(2))                                     MAIN     194
      DO 25 I=3,MPSI                                                    MAIN     195
      ETA(I)=SQRT(ETA(I-2)**2+DELPSI*(PSI(I)/U(I)+4.0*PSI(I-1)/U(I-1)+P5 MAIN     196
     1(I-2)/U(I-2))/1.5/RHO(1))                                         MAIN     197
      TEMP = (Y(I-2)**2+DELPSI*(PSI(I)/RHO(I)/U(I)+4.0*PSI(I-1)/RHO(I-1) MAIN     198
     1    /U(I-1)+PSI(I-2)/RHO(I-2)/U(I-2))/1.5)                        MAIN     199
      IF(TEMP.LT.0.0) CALL OUTPUT                                       MAIN     200
   25 Y(I) = SQRT(TEMP)                                                 MAIN     201
C**** HAS MIXING REGION INTERSECTED X AXIS YET, YES IF 0 OR -           MAIN     202
      IF (ITURB-6) 8010,8011,8010                                       MAIN     203
 8010 IF (U(1) - USUR01) 9000,9000,900)                                 MAIN     204
C     MODEL 6 COMMON CALCULATIONS                                       MAIN     205
 8011 Q01 = (U(1)+U(MPSI))/2.0                                          MAIN     206
      DO 8012 I=2,MPSI                                                  MAIN     207
      IF ((Q01-U(I))*(Q01-U(I-1))) 8013,8013,8012                       MAIN     208
 8012 CONTINUE                                                          MAIN     209
 8013 Q02 = (Q01-U(I-1))/(U(I)-U(I-1))                                  MAIN     210
      Q0100 = Y(I-1)+(Y(I)-Y(I-1))*Q02                                  MAIN     211
      Q030 = T(I-1)+(T(I)-T(I-1))*Q02                                   MAIN     212
      Q03 = CPBAR(I-1)+(CPBAR(I)-CPBAR(I-1))*Q02                        MAIN     213
      Q04 = 1.0/(WTMIX(I-1)+(WTMIX(I)-WTMIX(I-1))*Q02)                  MAIN     214
      Q05 = 89517.501/Q04                                               MAIN     215
      Q06 = Q03/(Q03-Q05)                                               MAIN     216
      Q07 = SQRT(Q06*Q05*Q030)                                          MAIN     217
      Q0300 = Q01/Q07                                                   MAIN     218
      Q08 = (ABS(U(1)-U(MPSI)))/2.0                                     MAIN     219
      IF (Q0300-1.2) 8014,8014,8015                                     MAIN     220
 8014 Q0400 =(.0468+Q0300*((Q0300*(-.0460))+.0256*(Q0300*Q0300)))*XK2   MAIN     221
```

```
      GO TO 8016                                                        MAIN
 8015 QQ400 = .0248EXK2                                                 MAIN
 8016 IF ((U(1)-USUB01)*(U(1)-U(MPSI))) 8020,8020,8800                  MAIN
 8020 IF (USUB01-9000.0) 8021,8021,8900                                 MAIN
 8021 USUB01 = 10000.0                                                  MAIN
      WRITE (6,9900) X                                                  MAIN
      GO TO 8900                                                        MAIN
C     MODEL 6 BEFORE MIXING ZONE REACHES AXIS                           MAIN
 8800 QQ9 = 0.95*   (U(1)-U(MPSI)) + U(MPSI)                            MAIN
      DO 8802 I = 2,MPSI                                                MAIN
      IF ((QQ9-U(I))*(QQ9-U(I-1))) 8804,8804,8802                       MAIN
 8802 CONTINUE                                                          MAIN
 8804 QQ200 = Y(I-1)+(Y(I)-Y(I-1))*(QQ9-U(I-1))/(U(I)-U(I-1))           MAIN
      QQ10 = QQ400*QQ8*(QQ100-QQ200)                                    MAIN
      DO 8810 I = 1,MPSI                                                MAIN
 8810 XMU(I) = QQ10*RHO(I)                                              MAIN
      GO TO 98                                                          MAIN
C     MODEL 6 AFTER MIXING ZONE REACHES AXIS                            MAIN
 8900 QQ11 = QQ400*QQ100*QQ8                                            MAIN
      DO 8910 I = 1,MPSI                                                MAIN
 8910 XMU(I) = QQ11*RHO(I)                                              MAIN
      QQ200 = 0.0                                                       MAIN
      GO TO 98                                                          MAIN
 9000 IQ77 = 9                                                          MAIN
      USUB01 = 0.0                                                      MAIN
      WRITE (6,9900)X                                                   MAIN
 9001 LL = ITURB + 1077                                                 MAIN
C      EDDY VISCOSITY  MODELS                                           MAIN
      GO TO (91,99,8666,78,8667,8668,9003,91,99,45,78,26,33,78),LL      MAIN
C      MODEL 1 BEFORE MIXING ZONE REACHES AXIS                          MAIN
 8666 XMU(I)=0.00137*(X+1.0E-05)*ABS(RHO(I)*U(I)-RHO(MPSI)*U(MPSI))     MAIN
      GO TO 37                                                          MAIN
C      MODEL 3 BEFORE MIXING ZONE REACHES AXIS                          MAIN
 8667 XMU(I)=0.00137*(X+1.0E-05)*RHO(I)*ABS(U(I)-U(MPSI))               MAIN
      GO TO 37                                                          MAIN
C      MODEL 4 BEFORE MIXING ZONE REACHES AXIS                          MAIN
 8668 XMU(I)=0.00137*(X+1.0E-05)*RHO(MPSI)*ABS(U(I)-U(MPSI))            MAIN
      GO TO 37                                                          MAIN
   91 DO 92 I=1,MPSI                                                    MAIN
C     MODEL 0 LAMINAR FLOW                                              MAIN
   92 XMU(I)=3.05E-8*T(I)**1.5/(T(I)+111.0)                             MAIN
      GO TO 98                                                          MAIN
   45 DUM=.5*(RHO(1)*U(1)+RHO(MPSI)*U(MPSI))                            MAIN
      DO 52 J=1,MPSI                                                    MAIN
      I=MPSI-J+1                                                        MAIN
      IF(RHO(I)*U(I)-DUM) 52,52,51                                      MAIN
   52 CONTINUE                                                          MAIN
C     MODEL 1 AFTER MIXING ZONE REACHES AXIS                            MAIN
   51 Z=Y(I)+(Y(I)-Y(I+1))*(RHO(I)*U(I)-DUM)/(RHO(I)*U(I)-RHO(I+1)*U(I+1 MAIN
     1))                                                                MAIN
      XMU(I)=XK2*Z*ABS(RHO(1)*U(1)-RHO(MPSI)*U(MPSI))*0.025             MAIN
      GO TO 37                                                          MAIN
   99 DO 39 I=1,MPSI                                                    MAIN
   39 XMU(I)=XK2*0.025                                                  MAIN
      GO TO 98                                                          MAIN
```

```
   78 RD=(U(1)+U(MPSI))/2.0                                          MAIN     277
      DO 47 I=2,MPSI                                                 MAIN     278
      IF ((RD-U(I))*(RD-U(I-1))) 48,48,47                            MAIN     279
   47 CONTINUE                                                       MAIN     280
   48 RHALVE=ETA(I-1)+(ETA(I)-ETA(I-1))*(RD-U(I-1))/(U(I)-U(I-1))    MAIN     281
      DUMMY=XK2*RHALVE*ABS(U(1)-U(MPSI))*0.025                       MAIN     282
      XMU(1)=DUMMY*RHO(1)                                            MAIN     283
      DO 79 I=2,MPSI                                                 MAIN     284
C     MODEL 2 BEFORE MIXING ZONE REACHES AXIS                        MAIN     285
   79 XMU(I)=DUMMY*(RHO(1)*ETA(I)/Y(I))**2/RHO(I)                    MAIN     286
      GO TO 98                                                       MAIN     287
C     MODEL 2 AFTER MIXING ZONE REACHES AXIS                         MAIN     288
   26 RD=(U(1)+U(MPSI))/2.0                                          MAIN     289
      DO 27 I=2,MPSI                                                 MAIN     290
      IF ((RD-U(I))*(RD-U(I-1))) 28,28,27                            MAIN     291
   27 CONTINUE                                                       MAIN     292
   28 RHALVE=Y(I-1)+(Y(I)-Y(I-1))*(RD-U(I-1))/(U(I)-U(I-1))          MAIN     293
C     MODEL 3 AFTER MIXING ZONE REACHES AXIS                         MAIN     294
      XMU(1)=XK2*RHALVE*RHO(1)*ABS(U(1)-U(MPSI))*0.025               MAIN     295
      DO 29 I=1,MPSI                                                 MAIN     296
   29 XMU(I)=XMU(1)                                                  MAIN     297
      GO TO 98                                                       MAIN     298
   33 RD=(U(1)+U(MPSI))/2.0                                          MAIN     299
      DO 34 I=2,MPSI                                                 MAIN     300
      IF ((RD-U(I))*(RD-U(I-1))) 35,35,34                            MAIN     301
   34 CONTINUE                                                       MAIN     302
   35 RHALVE=Y(I-1)+(Y(I)-Y(I-1))*(RD-U(I-1))/(U(I)-U(I-1))          MAIN     303
C     MODEL 4 AFTER MIXING ZONE REACHES AXIS                         MAIN     304
      XMU(1)=XK2*RHALVE*RHO(MPSI)*ABS(U(1)-U(MPSI))*0.025            MAIN     305
   37 DO 36 I=1,MPSI                                                 MAIN     306
   36 XMU(I)=XMU(1)                                                  MAIN     307
      GO TO 98                                                       MAIN     308
C      MODEL 5 BEFORE MIXING ZONE REACHES AXIS                       MAIN     309
 9003 XMU(1) = 0.00137*(X+1.0E-05)*ABS(UNIT-U(MPSI))*RHO(1)          MAIN     310
      DO 9004 I = 2,MPSI                                             MAIN     311
      XMU(I)=0.00137*(X+1.0E-05)*ABS(UNIT-U(MPSI))*(RHO(1)**2/RHO(I)) MAIN    312
 9004 CONTINUE                                                       MAIN     313
   98 A(1)=0.0                                                       MAIN     314
C     CALCULATE A                                                    MAIN     315
      DO 44 I=2,MPSI                                                 MAIN     316
   44 A(I)=XMU(I)*RHO(I)*U(I)*Y(I)*Y(I)/PSI(I)                       MAIN     317
      DO 899 L=1,NPSI                                                MAIN     318
      RRT=1.986*T(L)                                                 MAIN     319
      ROOTT=SQRT(T(L))                                               MAIN     320
      TX=T(L)                                                        MAIN     321
      CALL TKEY(TX  ,TTB,ITKEY,SDT,HDT,NT)                           MAIN     322
      IF (ITKEY.EQ.0) GO TO 9                                        MAIN     323
      DO 855 I=1,NS                                                  MAIN     324
      G(I)=0.0                                                       MAIN     325
      WP(I)=0.0                                                      MAIN     326
      WM(I)=0.0                                                      MAIN     327
      QX(I,L)=0.0                                                    MAIN     328
      DO 872 J=1,NS                                                  MAIN     329
  872 CM(I,J,L)=0.0                                                  MAIN     330
      CALL LIPLN(ITKEY,I, GTA,SDT,HDT,AX)                            MAIN     331
```

```
      G(I)=AX                                                           MAIN
  855 CONTINUE                                                          MAIN
C     REACTION CALCULATION                                              MAIN
C     REACTION KINETICS CONTINUE DOWN TO 400 DEGREES K                  MAIN
C        UNLESS TKINET IS SET TO A VALUE OTHER THAN 400. K              MAIN
C     REACTION KINETICS FOR ALL REACTIONS CONTINUE DOWN TO TKINET       MAIN
      IF(T(L)-TKINET) 3256,3256,3259                                    MAIN
 3259 CONTINUE                                                          MAIN
      DO 862 I=1,NR                                                     MAIN
      RP(I,L)=0.0                                                       MAIN
      RM(I,L)=0.0                                                       MAIN
      KK = IRT(I)                                                       MAIN
C     REACTION CONSTANT TYPE                                            MAIN
      GO TO (841,842,843,844,845,846,847),KK                            MAIN
  841 RATE=RC(I,1)*AV                                                   MAIN
      GO TO 849                                                         MAIN
  842 RATE=RC(I,1)/T(L)*AV                                              MAIN
      GO TO 849                                                         MAIN
  843 RATE=RC(I,1)/T(L)/T(L)*AV                                         MAIN
      GO TO 849                                                         MAIN
  844 RATE=RC(I,1)/ROOTT*AV                                             MAIN
      GO TO 849                                                         MAIN
  845 RATE=RC(I,1)*EXP(RC(I,3)/RRT)*AV                                  MAIN
      GO TO 849                                                         MAIN
  846 RATE=RC(I,1)*EXP(RC(I,3)/RRT)/T(L)*AV                             MAIN
      GO TO 849                                                         MAIN
  847 RATE=RC(I,1)/T(L)/ROOTT*AV                                        MAIN
  849 CONTINUE                                                          MAIN
      K=IRR(I)                                                          MAIN
C     TYPE OF REACTION                                                  MAIN
      GO TO(864,865,866,870,871,834,835,836,837,838),K                  MAIN
  870 J1=IRRR(I,1)                                                      MAIN
      J2=IRRR(I,2)                                                      MAIN
      J3=IRRR(I,3)                                                      MAIN
      E = (G(J1)+G(J2)-G(J3))/RRT                                       MAIN
      IF(ABS(E).LT.80.0) GO TO 700                                      MAIN
      IF(E.LT.0.0) E= EXP(-80.0)                                        MAIN
      IF(E.GT.0.0) E = EXP(80.0)                                        MAIN
      GO TO 701                                                         MAIN
  700 E = EXP(E)                                                        MAIN
  701 CONTINUE                                                          MAIN
       CRR=RATE*RHOOUT(L)                                               MAIN
      RP(I,L)=CRR*RHOOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)                     MAIN
      RM(I,L)=CRR*ALPHA(J3,L)/E/R/T(L)                                  MAIN
      DO 771 J=1, 3                                                     MAIN
      SIGN=1.0                                                          MAIN
      IF (J.GT.2) SIGN=-1.0                                             MAIN
      IROW= IRRR(I,J)                                                   MAIN
      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)            MAIN
      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)            MAIN
      CM(IROW,J3,L)= CM(IROW,J3,L) -SIGN*RM(I,L)/ALPHA(J3,L)            MAIN
  771 QX(IROW,L)= QX(IROW,L)+ SIGN*RP(I,L)                              MAIN
      GO TO 868                                                         MAIN
  871 J1=IRRR(I,1)                                                      MAIN
      J2=25                                                             MAIN
```

```
      J3=IRRR(I,3)                                                      MAIN     387
      J4=IRRR(I,4)                                                      MAIN     388
      E = (G(J1)-G(J3)-G(J4))/RRT                                       MAIN     389
      IF( ABS(E).LT.80.0) GO TO 702                                     MAIN     390
      IF( E.LT.0.0) E = EXP(-80.0)                                      MAIN     391
      IF( E.GT.0.0) E = EXP(80.0)                                       MAIN     392
      GO TO 703                                                         MAIN     393
  702 E = EXP(E)                                                        MAIN     394
  703 CONTINUE                                                          MAIN     395
       CRR=RATE*RHOOUT(L)*RHOOUT(L)*WTMIX(L)                            MAIN     396
      RP(I,L)=CRR*ALPHA(J1,L)                                           MAIN     397
      RM(I,L)=CRR*RT(L)*RHOOUT(L)*ALPHA(J3,L)*ALPHA(J4,L)/E             MAIN     398
      DO 772 J=1, 4                                                     MAIN     399
      SIGN=1.0                                                          MAIN     400
      IF (J.GT.2) SIGN=-1.0                                             MAIN     401
      IROW= IRRR(I,J)                                                   MAIN     402
      IF(J.EQ.2) IROW=25                                                MAIN     403
      CM(IROW,J1,L)= CM(IROW,J1,L)+SIGN*CRR                             MAIN     404
      CM(IROW,J3,L)= CM(IROW,J3,L)-SIGN*RM(I,L)/ALPHA(J3,L)             MAIN     405
      CM(IROW,J4,L)= CM(IROW,J4,L)-SIGN*RM(I,L)/ALPHA(J4,L)             MAIN     406
  772 QX(IROW,L)= QX(IROW,L)- SIGN*RM(I,L)                              MAIN     407
      GO TO 867                                                         MAIN     408
  864 J1=IRRR(I,1)                                                      MAIN     409
      J2=IRRR(I,2)                                                      MAIN     410
      J3=IRRR(I,3)                                                      MAIN     411
      J4=IRRR(I,4)                                                      MAIN     412
      E = (G(J1)+G(J2)-G(J3)-G(J4))/RRT                                 MAIN     413
      IF(ABS(E).LT.80.0) GO TO 704                                      MAIN     414
      IF(E.LT.0.0) E = EXP(-80.0)                                       MAIN     415
      IF(E.GT.0.0) E = EXP(80.0)                                        MAIN     416
      GO TO 705                                                         MAIN     417
  704 E = EXP(E)                                                        MAIN     418
  705 CONTINUE                                                          MAIN     419
       CRR=RATE*RHOOUT(L)*RHOOUT(L)                                     MAIN     420
      RP(I,L)=CRR*ALPHA(J1,L)*ALPHA(J2,L)                               MAIN     421
      RM(I,L)=CRR*ALPHA(J3,L)*ALPHA(J4,L)/E                             MAIN     422
      DO 773 J=1, 4                                                     MAIN     423
      SIGN=1.0                                                          MAIN     424
      IF (J.GT.2) SIGN=-1.0                                             MAIN     425
      IROW= IRRR(I,J)                                                   MAIN     426
      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)            MAIN     427
      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)            MAIN     428
      CM(IROW,J3,L)= CM(IROW,J3,L) -SIGN*RM(I,L)/ALPHA(J3,L)            MAIN     429
      CM(IROW,J4,L)= CM(IROW,J4,L)-SIGN*RM(I,L)/ALPHA(J4,L)             MAIN     430
  773 QX(IROW,L)= QX(IROW,L)+ SIGN*(RP(I,L)-RM(I,L))                    MAIN     431
      GO TO 867                                                         MAIN     432
  865 J1=IRRR(I,1)                                                      MAIN     433
      J2=IRRR(I,2)                                                      MAIN     434
      J3=IRRR(I,3)                                                      MAIN     435
      E = (G(J1)+G(J2)-G(J3))/RRT                                       MAIN     436
      IF(ABS(E).LT.80.0) GO TO 706                                      MAIN     437
      IF(E.LT.0.0) E=EXP(-80.0)                                         MAIN     438
      IF(E.GT.0.0) E=EXP(80.0)                                          MAIN     439
      GO TO 707                                                         MAIN     440
  706 E = EXP(E)                                                        MAIN     441
```

```
  707   CONTINUE                                                          MAIN     442
         CRR=RATE*RHOOUT(L)*RHOOUT(L)*WTMIX(L)*AV                         MAIN     443
        RP(I,L)=CRR*RHOOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)                     MAIN     444
        RM(I,L)=CRR*ALPHA(J3,L)/(E*R*T(L))                                MAIN     445
        DO 774 J=1,3                                                      MAIN     446
        SIGN=1.0                                                          MAIN     447
        IF (J.GT.2) SIGN=-1.0                                             MAIN     448
        IROW= IRRR(I,J)                                                   MAIN     449
        CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)            MAIN     450
        CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)            MAIN     451
        CM(IROW,J3,L)= CM(IROW,J3,L) -SIGN*RM(I,L)/ALPHA(J3,L)            MAIN     452
  774   QX(IROW,L)= QX(IROW,L)+ SIGN*(RP(I,L  ))                          MAIN     453
        GO TO 868                                                         MAIN     454
  866   J1=IRRR(I,1)                                                      MAIN     455
        J2=IRRR(I,2)                                                      MAIN     456
        J3=IRRR(I,3)                                                      MAIN     457
        J4=IRRR(I,4)                                                      MAIN     458
        J5=IRRR(I,5)                                                      MAIN     459
        E = (G(J1)+G(J2)-G(J3)-G(J4)-G(J5))/RRT                           MAIN     460
        IF(ABS(E).LT.80.0) GO TO 708                                      MAIN     461
        IF(E.LT.0.0) E=EXP(-80.0)                                         MAIN     462
        IF(E.GT.0.0) E = EXP(80.0)                                        MAIN     463
        GO TO 709                                                         MAIN     464
  708   E = EXP(E)                                                        MAIN     465
  709   CONTINUE                                                          MAIN     466
         CRR=RATE*RHOOUT(L)*RHOOUT(L)                                     MAIN     467
        RP(I,L)=CRR*ALPHA(J1,L)*ALPHA(J2,L)                               MAIN     468
        RM(I,L)=CRR*ALPHA(J3,L)*ALPHA(J4,L)*ALPHA(J5,L)*RHOOUT(L)*R*T(L)/E MAIN     469
        DO 775 J=1, 5                                                     MAIN     470
        SIGN=1.0                                                          MAIN     471
        IF (J.GT.2) SIGN=-1.0                                             MAIN     472
        IROW= IRRR(I,J)                                                   MAIN     473
        CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)            MAIN     474
        CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)            MAIN     475
        CM(IROW,J3,L)= CM(IROW,J3,L) -SIGN*RM(I,L)/ALPHA(J3,L)            MAIN     476
        CM(IROW,J4,L)= CM(IROW,J4,L)-SIGN*RM(I,L)/ALPHA(J4,L)             MAIN     477
        CM(IROW,J5,L)= CM(IROW,J5,L)-SIGN*RM(I,L)/ALPHA(J5,L)             MAIN     478
  775   QX(IROW,L)= QX(IROW,L)+ SIGN*(RP(I,L)-2.*RM(I,L))                 MAIN     479
        GO TO 861                                                         MAIN     480
  837   J1=IRRR(I,1)                                                      MAIN     481
        J2=IRRR(I,2)                                                      MAIN     482
        J3=IRRR(I,3)                                                      MAIN     483
         CRR=RATE*RHOOUT(L)                                               MAIN     484
        RP(I,L)=CRR*RHOOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)                     MAIN     485
        RM(I,L)=0.0                                                       MAIN     486
        DO 776 J=1, 3                                                     MAIN     487
        SIGN=1.0                                                          MAIN     488
        IF (J.GT.2) SIGN=-1.0                                             MAIN     489
        IROW= IRRR(I,J)                                                   MAIN     490
        CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)            MAIN     491
        CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)            MAIN     492
  776   QX(IROW,L)= QX(IROW,L)+ SIGN* RP(I,L)                             MAIN     493
        GO TO 868                                                         MAIN     494
  838   J1=IRRR(I,1)                                                      MAIN     495
        J2=25                                                             MAIN     496
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```
      J3=IRRR(I,3)                                                      MAIN      497
      J4=IRRR(I,4)                                                      MAIN      498
       CRR=RATE*RHOOUT(L)*RHOOUT(L)*WTMIX(L)                            MAIN      499
      RP(I,L)=CRR*ALPHA(J1,L)                                           MAIN      500
      RM(I,L)=0.0                                                       MAIN      501
      DO 777 J=1, 4                                                     MAIN      502
      SIGN=1.0                                                          MAIN      503
      IF (J.GT.2) SIGN=-1.0                                             MAIN      504
      IROW= IRRR(I,J)                                                   MAIN      505
      IF (J.EQ.2) IROW=25                                               MAIN      506
  777 CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*CRR                            MAIN      507
      GO TO 867                                                         MAIN      508
  834 J1=IRRR(I,1)                                                      MAIN      509
      J2=IRRR(I,2)                                                      MAIN      510
      J3=IRRR(I,3)                                                      MAIN      511
      J4=IRRR(I,4)                                                      MAIN      512
       CRR=RATE*RHOOUT(L)*RHOOUT(L)                                     MAIN      513
      RP(I,L)=CRR*ALPHA(J1,L)*ALPHA(J2,L)                               MAIN      514
      RM(I,L)=0.0                                                       MAIN      515
      DO 778 J=1, 4                                                     MAIN      516
      SIGN=1.0                                                          MAIN      517
      IF (J.GT.2) SIGN=-1.0                                             MAIN      518
      IROW= IRRR(I,J)                                                   MAIN      519
      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)            MAIN      520
      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)            MAIN      521
  778 QX(IROW,L)= QX(IROW,L)+ SIGN* RP(I,L)                             MAIN      522
      GO TO 867                                                         MAIN      523
  835 J1=IRRR(I,1)                                                      MAIN      524
      J2=IRRR(I,2)                                                      MAIN      525
      J3=IRRR(I,3)                                                      MAIN      526
       CRR=RATE*RHOOUT(L)*RHOOUT(L)*WTMIX(L)*AV                         MAIN      527
      RP(I,L)=CRR*RHOOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)                     MAIN      528
      RM(I,L)=0.0                                                       MAIN      529
      DO 779 J=1, 3                                                     MAIN      530
      SIGN=1.0                                                          MAIN      531
      IF (J.GT.2) SIGN=-1.0                                             MAIN      532
      IROW= IRRR(I,J)                                                   MAIN      533
      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)            MAIN      534
      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)            MAIN      535
  779 QX(IROW,L)= QX(IROW,L)+ SIGN* RP(I,L)                             MAIN      536
      GO TO 868                                                         MAIN      537
  836 J1=IRRR(I,1)                                                      MAIN      538
      J2=IRRR(I,2)                                                      MAIN      539
      J3=IRRR(I,3)                                                      MAIN      540
      J4=IRRR(I,4)                                                      MAIN      541
      J5=IRRR(I,5)                                                      MAIN      542
       CRR=RATE*RHOOUT(L)*RHOOUT(L)                                     MAIN      543
      RP(I,L)=CRR*ALPHA(J1,L)*ALPHA(J2,L)                               MAIN      544
      RM(I,L)=0.0                                                       MAIN      545
      DO 780 J=1, 5                                                     MAIN      546
      SIGN=1.0                                                          MAIN      547
      IF (J.GT.2) SIGN=-1.0                                             MAIN      548
      IROW= IRRR(I,J)                                                   MAIN      549
      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)            MAIN      550
      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)            MAIN      551
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  780 QX(IROW,L)= QX(IROW,L)+ SIGN* RP(I,L)                          MAIN     552
C     CALCULATE WDOT                                                 MAIN     553
  861 WP(J5)=WP(J5)+PP(I,L)                                          MAIN     554
      WM(J5)=WM(J5)+PM(I,L)                                          MAIN     555
  867 WP(J4)=WP(J4)+RP(I,L)                                          MAIN     556
      WM(J4)=WM(J4)+RM(I,L)                                          MAIN     557
  868 WP(J3)=WP(J3)+PP(I,L)                                          MAIN     558
      WM(J3)=WM(J3)+RM(I,L)                                          MAIN     559
      WP(J2)=WP(J2)+RM(I,L)                                          MAIN     560
      WM(J2)=WM(J2)+RP(I,L)                                          MAIN     561
      WP(J1)=WP(J1)+RM(I,L)                                          MAIN     562
      WM(J1)=WM(J1)+RP(I,L)                                          MAIN     563
  862 CONTINUE                                                       MAIN     564
 3256 CONTINUE                                                       MAIN     565
      DO 897 J=1,NS                                                  MAIN     566
  897 WDOT(J,L)=(WP(J)-WM(J))/RHOOUT(L)/U(L)                         MAIN     567
  899 CONTINUE                                                       MAIN     568
      IOUT=IOUT+1                                                    MAIN     569
      CALL SSWTCH(1,KOOOFX)                                          MAIN     570
       GO TO(62,63),KOOOFX                                           MAIN     571
   62 EOUT=RHO(1)*ALPHA(IECC,1)*3.108E23                             MAIN     572
      PRINT 61,X,T(1),U(1),EOUT,IOUT                                 MAIN     573
   61 FORMAT(3H0X=1PE15.7,3H T=1PE15.7,3H U=1PE15.7,6H E/CC=1PE15.7,7H S MAIN     574
     1TEPS=I5)                                                       MAIN     575
   63 IF(IFINIS) 64,69,64                                            MAIN     576
   64 CALL SSWTCH(3,KOOOFX)                                          MAIN     577
       GO TO(66,65),KOOOFX                                           MAIN     578
   65 IF(X-XMAX) 67,66,66                                            MAIN     579
   67 IF(PRNT-PCNT) 69,69,68                                         MAIN     580
   68 CONTINUE                                                       MAIN     581
      GO TO 5                                                        MAIN     582
   66 IFINIS=2                                                       MAIN     583
   69 CALL OUTPUT                                                    MAIN     584
      PCNT=0.0                                                       MAIN     585
      IF(IFINIS-1) 5,5,6                                             MAIN     586
C      CHECK DIFFUSION STEP SIZE                                     MAIN     587
    5 XD=DELPSI*DELPSI*SIGMA(1)/XMU(1)/XLE(1)/12.0 *FDL              MAIN     588
      DO 511 I=2,NPSI                                                MAIN     589
      DUMMY=A(I+1)+A(I-1)+A(I)+A(I)                                  MAIN     590
      DUMMY=PSI(I)*DELPSI*DELPSI*SIGMA(I)/XLF(I)/DUMMY/1.5*FDL       MAIN     591
  511 XD=AMIN1(XD,DUMMY)                                             MAIN     592
      DX=AMIN1(DX,XD)                                                MAIN     593
      DO 101 I=2,NPSI                                                MAIN     594
      EX1=PSI(I)*DELPSI**2/DX                                        MAIN     595
      EX11=.5*(A(I)+A(I+1))                                          MAIN     596
      EX12=.5*(A(I)+A(I-1))                                          MAIN     597
C     INTEGRATE MOMENTUM EQUATION                                    MAIN     598
      PU(I)=(EX11*(U(I+1)-U(I))+EX12*(U(I-1)-U(I)))/EX1+U(I)         MAIN     599
      PU(I)=PU(I)-DX*DPDX/RHO(I)/U(I)                                MAIN     600
      EX3=0.0                                                        MAIN     601
      EX4=0.0                                                        MAIN     602
      DO 21 J=1,NS                                                   MAIN     603
      EX3=EX3+H(J,I)*WDOT(J,I)                                       MAIN     604
   21 EX4=EX4+CP(J,I)*(ALPHA(J,I+1)-ALPHA(J,I-1))                    MAIN     605
      EX2=EX1*CPRAR(I)                                               MAIN     606
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      EX5=XLE(I)*A(I)/SIGMA(I)                                          MAIN
      EX6=.5*(EX5+XLE(I+1)*A(I+1)/SIGMA(I+1))                           MAIN
      EX7=.5*(EX5+XLE(I-1)*A(I-1)/SIGMA(I-1))                           MAIN
      EX8=CPBAR(I)*A(I)/SIGMA(I)                                        MAIN
      EX9=.5*(EX8+CPBAR(I+1)*A(I+1)/SIGMA(I+1))                         MAIN
      EX10=.5*(EX8+CPBAR(I-1)*A(I-1)/SIGMA(I-1))                        MAIN
      EX14=EX4*EX5/4.0                                                  MAIN
C     INTEGRATE ENERGY EQUATION                                         MAIN
      RT(I)=(U(I+1)-U(I-1))**2*A(I)/EX2/4.0+DX*DPDX/RHO(I)/CPBAR(I)+T(I) MAIN
     1+((EX9+EX14)*T(I+1)+(EX10-EX14)*T(I-1)-(EX9+EX10)*T(I))/EX2-EX3*DX MAIN
     2/CPBAR(I)                                                         MAIN
      RHOUIX=DX/(RHOOUT(I)* U(I))                                       MAIN
C     INTEGRATE SPECIES EQUATIONS                                       MAIN
      DO 41 J=1,NS                                                      MAIN
   41 QX1(J)      =(EX6*(ALPHA(J,I+1)-ALPHA(J,I))+EX7*(ALPHA(J,I-1)-ALPHA MAIN
     1(J,I)))/EX1+ALPHA(J,I)+  QX(J,I)*RHOUIX                           MAIN
      DO 781 M=1,NS                                                     MAIN
      DO 781 N=1,NS                                                     MAIN
      CM1(M,N)= CM(M,N,I)*RHOUIX                                        MAIN
      IF (M.EQ.N) CM1(M,N)=CM1(M,N) +1.0                                MAIN
  781 CONTINUE                                                          MAIN
      CALL SLDP(QX1,CM1,NS)                                             MAIN
  785 FORMAT (1H , 2I5)                                                 MAIN
      DO 782 J=1, NS                                                    MAIN
  782 RALPHA(J,I)= QX1(J)                                               MAIN
  101 CONTINUE                                                          MAIN
      WRITE(6,786) DX,X                                                 MAIN
  786 FORMAT(1H ,1P2E12.5)                                              MAIN
      EX3=4.0*XMU(1)*DX/DELPSI/DELPSI                                   MAIN
      RHOUIX=DX/(RHOOUT(1)* U(1))                                       MAIN
C     COMPUTE U AT CENTER LINE                                          MAIN
      RU(1)=EX3*(U(2)-U(1))+U(1)-DX*DPDX/RHO(1)/U(1)                    MAIN
      EX4=0.0                                                           MAIN
      DO 200 J=1,NS                                                     MAIN
      EX4=EX4+H(J,1)*WDOT(J,1)                                          MAIN
      RALPHA(J,MPSI)=ALPHA(J,MPSI)                                      MAIN
  200 QX1(J)      =EX3*XLF(1)*(ALPHA(J,2)-ALPHA(J,1))/SIGMA(1)+ALPHA(J,1) MAIN
     1+  QX(J,1)*RHOUIX                                                 MAIN
      DO 783 M=1,NS                                                     MAIN
      DO 783 N=1,NS                                                     MAIN
      CM1(M,N)= CM(M,N,1)*RHOUIX                                        MAIN
      IF (M.EQ.N) CM1(M,N)=CM1(M,N) +1.0                                MAIN
  783 CONTINUE                                                          MAIN
      CALL SLDP(QX1,CM1,NS)                                             MAIN
      DO 784 J=1, NS                                                    MAIN
C     COMPUTE SPECIES AT CENTER LINE                                    MAIN
  784 RALPHA(J,1)= QX1(J)                                               MAIN
C     CALCULATE TEMP. AT CENTER LINE                                    MAIN
      RT(1)=EX3*(T(2)-T(1))/SIGMA(1)+T(1)+DX*DPDX/RHO(1)/CPBAR(1)       MAIN
     1-EX4*DX/CPBAR(1)                                                  MAIN
      RT(MPSI)=T(MPSI)                                                  MAIN
      IF(IEDGE) 230,231,230                                             MAIN
C     COMPUTE TEMP. AND U AT EDGE                                       MAIN
  230 RU(MPSI)=U(MPSI)-DX*DPDX/RHO(MPSI)/U(MPSI)                        MAIN
      RT(MPSI)=T(MPSI)+DX*DPDX/RHO(MPSI)/CPBAR(MPSI)                    MAIN
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      DO 210 I=MPSI,29                                                  MAIN     662
      RU(I)=RU(MPSI)                                                    MAIN     663
      U(I)=RU(MPSI)                                                     MAIN     664
      RT(I)=RT(MPSI)                                                    MAIN     665
  210 T(I)=RT(MPSI)                                                     MAIN     666
  231 CONTINUE                                                          MAIN     667
    1 IFINIS=1                                                          MAIN     668
  921 SAVEX=X                                                           MAIN     669
      SAVEDX=DX                                                         MAIN     670
      DO 941 I=1,29                                                     MAIN     671
      SAVEU(I)=U(I)                                                     MAIN     672
      SAVET(I)=T(I)                                                     MAIN     673
      DO 940 J=1,NS                                                     MAIN     674
      SAVEA(J,I)=ALPHA(J,I)                                             MAIN     675
  940 CONTINUE                                                          MAIN     676
  941 CONTINUE                                                          MAIN     677
      MINIT = 13                                                        MAIN     678
      MHALF = 25                                                        MAIN     679
      NTEST=MPSI-1                                                      MAIN     680
      DO 967 I=1,NTEST                                                  MAIN     681
C      CHECK NEGATIVE MOLE FRACTION                                     MAIN     682
  965 DO 967 J=1,NS                                                     MAIN     683
      IF (RALPHA(J,I)) 995,967,967                                      MAIN     684
  967 CONTINUE                                                          MAIN     685
      X=X+DX                                                            MAIN     686
      PCNT=PCNT+DX                                                      MAIN     687
      DX=XD                                                             MAIN     688
      DO 925 I=1,29                                                     MAIN     689
      DO 926 J=1,NS                                                     MAIN     690
  926 ALPHA(J,I)=RALPHA(J,I)                                            MAIN     691
      T(I)=RT(I)                                                        MAIN     692
  925 U(I)=RU(I)                                                        MAIN     693
      GO TO 999                                                         MAIN     694
  995 IF (DX.LT.DXMIN)  GO TO 8000                                      MAIN     695
  981 DX=SAVEDX/2.0                                                     MAIN     696
      X=SAVEX                                                           MAIN     697
      DO 985 I=1,29                                                     MAIN     698
      DO 982 J=1,NS                                                     MAIN     699
  982 ALPHA(J,I)=SAVEA(J,I)                                             MAIN     700
      T(I)=SAVET(I)                                                     MAIN     701
  985 U(I)=SAVEU(I)                                                     MAIN     702
      GO TO 2                                                           MAIN     703
C     IF MPSI .GE.26 ,MPSI IS HALVED                                    MAIN     704
  999 IF(MPSI-MHALF) 1001,1500,1500                                     MAIN     705
 1001 IF(ABS(U(NPSI)-U(MPSI))/U(MPSI)-.010) 1011,1011,1004              MAIN     706
 1011 IF(ABS(T(NPSI)-T(MPSI))/T(MPSI)-.050) 1002,1002,1004              MAIN     707
 1002 CONTINUE                                                          MAIN     708
      GO TO 2000                                                        MAIN     709
 1004 MPSI=MPSI+1                                                       MAIN     710
      NPSI=MPSI-1                                                       MAIN     711
      DO 1101 I=MPSI,29                                                 MAIN     712
      SAVEU(I)=U(NPSI)                                                  MAIN     713
      RU(I)=U(NPSI)                                                     MAIN     714
      U(I)=U(NPSI)                                                      MAIN     715
      SAVET(I)=T(NPSI)                                                  MAIN     716
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```
      T(I)=T(NPSI)                                                      MAIN      717
      RT(I)=T(NPSI)                                                     MAIN      718
      DO 1102 J=1,NS                                                    MAIN      719
      SAVEA(J,I)=ALPHA(J,NPSI)                                          MAIN      720
      ALPHA(J,I)=ALPHA(J,NPSI)                                          MAIN      721
 1102 RALPHA(J,I)=ALPHA(J,NPSI)                                         MAIN      722
 1101 CONTINUE                                                          MAIN      723
      GO TO 2000                                                        MAIN      724
 1500 IFINIS=0                                                          MAIN      725
      DELPSI=DELPSI+DELPSI                                              MAIN      726
      DO 1600 I=1,MINIT                                                 MAIN      727
      DO 1650 J=1,NS                                                    MAIN      728
 1650 ALPHA(J,I)=ALPHA(J,2*I-1)                                         MAIN      729
      T(I)=T(2*I-1)                                                     MAIN      730
 1600 U(I)=U(2*I-1)                                                     MAIN      731
      MPSI=MINIT                                                        MAIN      732
      NPSI=MPSI-1                                                       MAIN      733
      DO 1700 I=MINIT,29                                                MAIN      734
      DO 1750 J=1,NS                                                    MAIN      735
      ALPHA(J,I)=ALPHA(J,MPSI)                                          MAIN      736
 1750 RALPHA(J,I)=ALPHA(J,MPSI)                                         MAIN      737
      T(I)=T(MPSI)                                                      MAIN      738
      RT(I)=T(MPSI)                                                     MAIN      739
      U(I)=U(MPSI)                                                      MAIN      740
 1700 RU(I)=U(MPSI)                                                     MAIN      741
      DO 1800 I=2,29                                                    MAIN      742
 1800 PSI(I)=PSI(I-1)+DELPSI                                            MAIN      743
      ITER=0                                                            MAIN      744
      ISTEP=0                                                           MAIN      745
      GO TO 2000                                                        MAIN      746
 8000 WRITE (6,8001)                                                    MAIN      747
 8001 FORMAT(68H1NEGATIVE PARAMETER - NOT CORRECTED BY REPEATED HALVING MAIN      748
     1OF STEP SIZE)                                                     MAIN      749
      IFINIS=2                                                          MAIN      750
      GO TO 69                                                          MAIN      751
 2000 CONTINUE                                                          MAIN      752
      CALL TICK(ISECS)                                                  MAIN      753
      IELAPS = ISECS-ISECST                                             MAIN      754
      IF(IELAPS.LT.0) IELAPS = IDIFFT + ISECS                           MAIN      755
      IF(IELAPS.GE.ILIMIT) GO TO 6                                      MAIN      756
      GO TO 2                                                           MAIN      757
  100 FORMAT(14I5)                                                      MAIN      758
  102 FORMAT(8F10.4)                                                    MAIN      759
  111 FORMAT (7(1PE10.3))                                               MAIN      760
  222 FORMAT(A6,7E10.3)                                                 MAIN      761
  333 FORMAT(12A6)                                                      MAIN      762
  444 FORMAT(A6,1X,A6,8X,A6,1X,A6,1X,A6,7X,I2,I1,E8.2,F4.1,F9.1)        MAIN      763
  555 FORMAT(7(1PE10.3))                                                MAIN      764
  666 FORMAT(10I5)                                                      MAIN      765
 1000 FORMAT(7E10.3)                                                    MAIN      766
 9900 FORMAT (39H1 MIXING REGION INTERSECTS AXIS AT X = 1PE15.7)        MAIN      767
    6 IF(IPUNCH.EQ.0.OR.IPUNCH.EQ.1) GO TO 9                            MAIN      768
      PUNCH333,(TITLE(I),I=1,12)                                        MAIN      769
      PUNCH 666,MPSI,NS,ITURB,NR,IOUT1,IOUT2,IPUNCH,ITIMF,IPRESS,NT     MAIN      770
      PUNCH 555,FREQA(1),FREQA(2),FREQA(3),FREQA(4),FREQA(5),FREQA(6)   MAIN      771
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      PUNCH 555,X,XMAX,PRNT,XLE(1),SIGMA(1),RJ,XK2                      MAIN    772
      PUNCH 555, DXMIN, FDL,     PC(1),PC(2),PC(3),PC(4)                MAIN    773
      PUNCH 555,PPUNCH,T(1),T(MPSI),U(1),U(MPSI),DELPSI,TKINET          MAIN    774
      PUNCH  555,(T(I),I=1,MPSI)                                        MAIN    775
      PUNCH  555,(U(I),I=1,MPSI)                                        MAIN    776
      DO 8 I = 1,MPSI                                                   MAIN    777
      PUNCH  555,(RALPHA(J,I),J=1,NS)                                   MAIN    778
    8 CONTINUE                                                          MAIN    779
    9 CONTINUE                                                          MAIN    780
      END                                                               MAIN    781
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```
      SUBROUTINE OUTPUT                                                 OUTPUT     2
      DIMENSION A(30),RHO(30),Y(30),T(30),PSI(30),RT(30),SUM(30),AR(25), OUTPUT     3
     1HSTAT(30),H(25,30),ALPHA(25,30),RALPHA(25,30),CP(25,30),SIGMA(30), OUTPUT     4
     2          WTMOLE(25),CPBAR(30),C(25,9),AID(25),ETA(30),RATIO(30), OUTPUT     5
     3RU(30),U(30),TITLE(12),XLE(30),XMU(30)          ,G(25),WTMIX(30), OUTPUT     6
     4RC(40,3),IRRP(40,5),WP(25),WM(25),WDOT(25,30),SAVET(30),SAVEU(30), OUTPUT     7
     5          IRR(40),EREQ(30),SAVEA(25,30),              PC(4),ZID(5), OUTPUT     8
     6          ECC(30),HOUT(30),YOUT(30),RHOOUT(30),XMUOUT(30),XLT(30), OUTPUT     9
     7T4(30),TFDG(30),IRT(40),RP(40,30),RM(40,30)                        OUTPUT    10
      DIMENSION ISAVE(6), FREQA(6), ALOC(50,6), ATT(6), YATT(50)        OUTPUT    11
      COMMON  A      , RHO    , Y      , T      , PSI    , RT           OUTPUT    12
      COMMON  SUM    , AR     , HSTAT  , H      , ALPHA  , RALPHA       OUTPUT    13
      COMMON  CP     , SIGMA           , WTMOLE , CPBAR  , C            OUTPUT    14
      COMMON  AID    , ETA    , RATIO  , RU     , U      , TITLE        OUTPUT    15
      COMMON  XLE    , XMU             , G      , WTMIX  , WDOT         OUTPUT    16
      COMMON  SAVEU  , SAVET  , WM     , WP     , RC                    OUTPUT    17
      COMMON           SAVEA  ,          PC     , X      , XMAX         OUTPUT    18
      COMMON  PRNT   , DXMIN  , DX     , FDL    , DELPSI , RJ           OUTPUT    19
      COMMON  XK2    , P      , ZID    , FREQ   , ECC    , DPDX         OUTPUT    20
      COMMON  YOUT   , HOUT   , RHOOUT , IRRP   , IRR    , IFINIS       OUTPUT    21
      COMMON  IPAGE  , MPSI   , MY     , NS     , NR     , IEDGE        OUTPUT    22
      COMMON  ITURB  , IPRESS , NPSI   , ITEST  , ITFR   , IECC         OUTPUT    23
      COMMON  IPT    , XMUOUT , XLT    , T4     , TFDG   , IOUT         OUTPUT    24
      COMMON  IOUT1  , IOUT2  ,RP      , RM     , ISAVE  , IPUNCH        OUTPUT    25
      COMMON TKINET,NFREQA,ALOC,FREQA,00100,00200,00300,00400           OUTPUT    26
      DATA ZCO/6HCO    /                                                OUTPUT    27
      DATA ZCO2/6HCO2   /                                               OUTPUT    28
      DATA ZH2O/6HH2O   /                                               OUTPUT    29
      BIG=1.0E30                                                        OUTPUT    30
      DO 5 I=1, NS                                                      OUTPUT    31
      IF (AID(I).EQ.ZCO )  ICO=I                                        OUTPUT    32
      IF (AID(I).EQ.ZCO2) ICO2=I                                        OUTPUT    33
      IF (AID(I).EQ.ZH2O) IH2O=I                                        OUTPUT    34
    5 CONTINUE                                                          OUTPUT    35
      IF(IECC) 531,539,531                                              OUTPUT    36
  531 DO 532 I=1,MPSI                                                   OUTPUT    37
  532 ECC(I)=RHO(I)*ALPHA(IECC,I)*3.108E23                              OUTPUT    38
  539 DO 10 I=1,MPSI                                                    OUTPUT    39
      YOUT(I)=Y(I)/RJ                                                   OUTPUT    40
      XMUOUT(I)=XMU(I)*32.174                                           OUTPUT    41
      HOUT(I)=HSTAT(I)/45055.31                                         OUTPUT    42
      SUM(I)=0.0                                                        OUTPUT    43
      DO 10 J=1,NS                                                      OUTPUT    44
   10 SUM(I)=SUM(I)+ALPHA(J,I)*WTMOLE(J)                                OUTPUT    45
      UD=.05*U(1)+.95*U(MPSI)                                           OUTPUT    46
      DO 83 I=2,MPSI                                                    OUTPUT    47
      IF ((U(I)-UD)*(U(I-1)-UD)) 84,84,83                               OUTPUT    48
   83 CONTINUE                                                          OUTPUT    49
   84 VR=(Y(I)-Y(I-1))*(UD-U(I-1))/(U(I)-U(I-1))+Y(I-1)                 OUTPUT    50
      TD=.05*T(1)+.95*T(MPSI)                                           OUTPUT    51
      DO 85 I=2,MPSI                                                    OUTPUT    52
      IF ((T(I)-TD)*(T(I-1)-TD)) 86,86,85                               OUTPUT    53
   85 CONTINUE                                                          OUTPUT    54
   86 TR=(Y(I)-Y(I-1))*(TD-T(I-1))/(T(I)-T(I-1))+Y(I-1)                 OUTPUT    55
      TR=TR/RJ                                                          OUTPUT    56
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      VR=VR/RJ                                                          OUTPUT    57
      DO 87 J=1,NS                                                      OUTPUT    58
      AR(J)=0.0                                                         OUTPUT    59
      AD=.05*ALPHA(J,1)+.95*ALPHA(J,MPSI)                               OUTPUT    60
      IF(ALPHA(J,MPSI)) 91,92,91                                        OUTPUT    61
   91 DO 88 I=1,MPSI                                                    OUTPUT    62
      IF(ALPHA(J,I)-AD) 88,88,89                                        OUTPUT    63
   88 CONTINUE                                                          OUTPUT    64
   89 AR(J)=Y(I-1)+(Y(I)-Y(I-1))*(AD-ALPHA(J,I-1))/(ALPHA(J,I)-ALPHA(J,I OUTPUT    65
     1-1))                                                              OUTPUT    66
      AR(J)=AR(J)/RJ                                                    OUTPUT    67
      GO TO 87                                                          OUTPUT    68
   92 DO 93 I=1,MPSI                                                    OUTPUT    69
      IF(ALPHA(J,I)-AD) 94,93,93                                        OUTPUT    70
   93 CONTINUE                                                          OUTPUT    71
   94 GO TO 89                                                          OUTPUT    72
   87 CONTINUE                                                          OUTPUT    73
      PCNT=0.0                                                          OUTPUT    74
      IPAGE=IPAGE+1                                                     OUTPUT    75
      WRITE (6,201)X,(TITLE(I),I=1,12),IPAGE                            OUTPUT    76
      WRITE (6,102)                                                     OUTPUT    77
      XORJ=X/RJ                                                         OUTPUT    78
      POUT=P/2117.0                                                     OUTPUT    79
      DPOUT=DPDX/2117.0                                                 OUTPUT    80
      WRITE(6,103) XORJ,DX,POUT                                         OUTPUT    81
      IF (ITURB-6) 8600,8500,8600                                       OUTPUT    82
 8500 WRITE (6,8555)                                                    OUTPUT    83
      QQ101=QQ100/RJ                                                    OUTPUT    84
      QQ201=QQ200/RJ                                                    OUTPUT    85
      WRITE (6,8556) QQ101,QQ201,QQ300,QQ400                            OUTPUT    86
 8555 FORMAT(1H0,8X,4HHALF,21X,12HINNER MIXING,17X,11HMACH NUMBER,16X,11 OUTPUT    87
     *HMIXING RATE/7X,10HRADIUS/R  ,16X,15HZONE RADIUS/R  ,14X,14HAT HAL OUTPUT    88
     *F RADIUS,14X,11HCOEFFICIENT)                                      OUTPUT    89
 8556 FORMAT (4X,1PE14.6,1P3E28.6)                                      OUTPUT    90
 8600 WRITE (6,107)                                                     OUTPUT    91
      WRITE (6,509)                                                     OUTPUT    92
      DO 73 I=1,MPSI                                                    OUTPUT    93
      SS1= 89517.501*WTMIX(I)                                           OUTPUT    94
      SS2= CPBAR(I)/(CPBAR(I)-SS1)                                      OUTPUT    95
      SS=SQRT(SS2*SS1*T(I))                                             OUTPUT    96
      XMACH= U(I)/SS                                                    OUTPUT    97
      IF(IECC) 71,72,71                                                 OUTPUT    98
   71 WRITE (6,207)I,YOUT(I),U(I),T(I),RHOOUT(I),XMACH, HOUT(I), XMUOUT( OUTPUT    99
     1I),ECC(I),PSI(I),I                                                OUTPUT   100
      GO TO 73                                                          OUTPUT   101
   72 WRITE (6,307)I,YOUT(I),U(I),T(I),RHOOUT(I),XMACH, HOUT(I), XMUOUT( OUTPUT   102
     1I)        ,PSI(I),I                                               OUTPUT   103
   73 CONTINUE                                                          OUTPUT   104
      DO 581 I=1,MPSI                                                   OUTPUT   105
      DO 581 J=1,NS                                                     OUTPUT   106
  581 ALPHA(J,I)=ALPHA(J,I)/WTMIX(I)                                    OUTPUT   107
      IRPT=(NS+6)/7                                                     OUTPUT   108
      DO 564 KK=1,IRPT                                                  OUTPUT   109
      I1=1+(KK-1)*7                                                     OUTPUT   110
      I2=7+(KK-1)*7                                                     OUTPUT   111
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      WRITE (6,201)X,(TITLE(I),I=1,12),IPAGE                            OUTPUT    112
      WRITE (6,409)                                                     OUTPUT    113
      WRITE (6,108)(AID(J),J=I1,12)                                     OUTPUT    114
      DO 81 I=1,MPSI                                                    OUTPUT    115
   81 WRITE (6,208)I,YOUT(I),(RALPHA(J,I),J=I1,12),I                    OUTPUT    116
      IF(IOUT1)564,564,74                                               OUTPUT    117
   74 WRITE (6,420)                                                     OUTPUT    118
      WRITE (6,421)(AID(J),J=I1,12)                                     OUTPUT    119
      DO 82 I=1,MPSI                                                    OUTPUT    120
      IF(T(I)-TKINET) 564,564,82                                        OUTPUT    121
   82 WRITE (6,422)I,(WDOT(J,I),J=I1,12),I                              OUTPUT    122
  564 CONTINUE                                                          OUTPUT    123
      IF(IOUT2)567,567,75                                               OUTPUT    124
   75 IRPT=(NR+9)/10                                                    OUTPUT    125
      N=0                                                               OUTPUT    126
      NNR=NR-1                                                          OUTPUT    127
      DO 565 KK=1,IRPT                                                  OUTPUT    128
      LL=0                                                              OUTPUT    129
      N=N+1                                                             OUTPUT    130
      WRITE (6,201)X,(TITLE(I),I=1,12),IPAGE                            OUTPUT    131
   65 I1=1+(N-1)*5                                                      OUTPUT    132
      I2=5+(N-1)*5                                                      OUTPUT    133
      NNN1=I1                                                           OUTPUT    134
      NNN2=I1+1                                                         OUTPUT    135
      NNN3=I1+2                                                         OUTPUT    136
      NNN4=I1+3                                                         OUTPUT    137
      NNN5=I2                                                           OUTPUT    138
      WRITE(6,209)                                                      OUTPUT    139
      WRITE (6,431)NNN1,NNN2,NNN3,NNN4,NNN5                             OUTPUT    140
      WRITE (6,432)                                                     OUTPUT    141
      DO 63 I=1,MPSI                                                    OUTPUT    142
      IF(T(I)-TKINET) 566,566,63                                        OUTPUT    143
   63 WRITE(6,433)I,YOUT(I),(RP(J,I),RM(J,I),J=I1,12),I                 OUTPUT    144
  566 IF(NNR/(5*N))565,565,64                                           OUTPUT    145
   64 IF(LL)565,66,565                                                  OUTPUT    146
   66 N=N+1                                                             OUTPUT    147
      LL=1                                                              OUTPUT    148
      GO TO 65                                                          OUTPUT    149
  565 CONTINUE                                                          OUTPUT    150
  567 CONTINUE                                                          OUTPUT    151
      IF(IPUNCH.EQ.0.OR.IPUNCH.EQ.2) GO TO 568                          OUTPUT    152
      WRITE(7,790) XOR,J,BIG                                            OUTPUT    153
C**** COMPUTE AND OUTPUT THE COLLISION FREQUENCY                        OUTPUT    154
  568 IF (NFREQA) 1065, 1045, 1065                                      OUTPUT    155
 1045 WRITE(6,600)                                                      OUTPUT    156
      WRITE(6,601)                                                      OUTPUT    157
      GO TO 1066                                                        OUTPUT    158
 1065 CONTINUE                                                          OUTPUT    159
      WRITE(6,600)                                                      OUTPUT    160
      WRITE(6,601)                                                      OUTPUT    161
      WRITE (6,1013) (FREQA(J), J=1,NFREQA)                             OUTPUT    162
      WRITE (6,1068)                                                    OUTPUT    163
 1066 DO 602 I=1,NPSI                                                   OUTPUT    164
      FT1 = 1.0/SQRT(T(I))                                              OUTPUT    165
      FT2 = 1.0/FT1                                                     OUTPUT    166
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      FT3 = 1.0/T(I)                                                    OUTPUT   167
      FT4 = T(I)**0.75                                                  OUTPUT   168
      SUMS = 0.0                                                        OUTPUT   169
      DO 603 IDX = 1,6                                                  OUTPUT   170
      IF(ISAVE(IDX).EQ.0) GO TO 603                                     OUTPUT   171
      K = ISAVE(IDX)                                                    OUTPUT   172
      TERM = RALPHA(K,I)                                                OUTPUT   173
      GO TO (604,605,606,607,608,614),IDX                               OUTPUT   174
  604 Q = (1.29E-17)*FT2 + 2.46E-16                                     OUTPUT   175
      GO TO 609                                                         OUTPUT   176
  605 Q = (0.758E-13)*FT1                                               OUTPUT   177
      GO TO 609                                                         OUTPUT   178
  606 Q = (1.53E-11)*FT3                                                OUTPUT   179
      GO TO 609                                                         OUTPUT   180
  607 Q = (9.0E-18)*FT2 + 8.9E-16                                       OUTPUT   181
      GO TO 609                                                         OUTPUT   182
  608 Q = 3.29E-23*6.21E5*FT2                                           OUTPUT   183
      GO TO 609                                                         OUTPUT   184
  614 Q= 1.85*(6.21)**(-2)*(1.0E-10)*FT3                                OUTPUT   185
  609 SUMS = SUMS + Q*TERM                                              OUTPUT   186
  603 CONTINUE                                                          OUTPUT   187
      XNEU = (4.57E27)*SUMS*POUT*FT1                                    OUTPUT   188
      ECON= 0.07157*   ECC(I)/XNEU                                      OUTPUT   189
      IF (NFREQA) 1000, 1001, 1000                                      OUTPUT   190
 1000 CATT = 1.17                                                       OUTPUT   191
      DO 1003 J = 1,NFREQA                                              OUTPUT   192
      ALOC1 = 1. + (6.283*6.283*FREQA(J)*FREQA(J)*1.0E12/(XNEU*XNEU))   OUTPUT   193
 1003 ALOC(I,J) = CATT*ECC(I)/(XNEU*ALOC1)                              OUTPUT   194
      GO TO 1008                                                        OUTPUT   195
 1001 WRITE(6,610) I, YOUT(I),XNEU ,ECON                                OUTPUT   196
      GO TO 1010                                                        OUTPUT   197
 1008 WRITE(6,610) I, YOUT(I),XNEU,ECON,(ALOC(I,J),J=1,NFREQA)          OUTPUT   198
 1010 IF (IPUNCH.EQ.0.OR.IPUNCH.EQ.2) GO TO 602                         OUTPUT   199
      RPT = YOUT(I)                                                     OUTPUT   200
      PPCO = RALPHA(ICO ,I)*POUT                                        OUTPUT   201
      PPCO2= RALPHA(ICO2,I)*POUT                                        OUTPUT   202
      PPH2O= RALPHA(IH2O,I)*POUT                                        OUTPUT   203
      WRITE(7,780) RPT,ECC(I),XNEU,T(I),PPCO,PPCO2,PPH2O                OUTPUT   204
  602 CONTINUE                                                          OUTPUT   205
      IF (NFREQA) 1009, 1015, 1009                                      OUTPUT   206
 1009 DO 1004 J = 1, NFREQA                                             OUTPUT   207
      DO 1005 I = 1, NPSI                                               OUTPUT   208
 1005 YATT(I) =24.0*RJ*ALOC(I,J)                                        OUTPUT   209
      CALL GRATE(ATT(J),YATT,YOUT,NPSI)                                 OUTPUT   210
 1004 CONTINUE                                                          OUTPUT   211
      WRITE (6,1014)(ATT(J),J=1,NFREQA)                                 OUTPUT   212
 1015 CONTINUE                                                          OUTPUT   213
  102 FORMAT(1H0,8X,3HX/R,                                  8X,12HDELTA X OUTPUT   214
     1FEET,4X,10HPRESS(ATM)).                                           OUTPUT   215
  103 FORMAT(4X,1P6E14.6)                                               OUTPUT   216
  107 FORMAT(4H0 PT,5X,3HY/R, 6X,8HVELOCITY,4X,11HTEMPERATURE,5X,7HDENSI OUTPUT   217
     1TY, 6X,8HMACH NO. , 8X,8HENTHALPY,5X,9HVISCOSITY,5X,*ELECTRON*    OUTPUT   218
     2 ,8X,3HPSI,6X,2HPT )                                              OUTPUT   219
  108 FORMAT(3H0PT,3X,5H Y/R ,7(3X,A6,4X),1X,3H PT)                     OUTPUT   220
  201 FORMAT(1H1,//////3H X=1PE15.7,5H FEET,8X,12A6,8X,4HPAGE I4)       OUTPUT   221
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  207 FORMAT(I4,F10.4,1P8E14.6,I4)                                  OUTPUT   222
  208 FORMAT(I3,F9.5,1P7E13.5,I3)                                   OUTPUT   223
  209 FORMAT(1H ,//40X,*REACTION RATES (MOLE/ML-SEC)*//)            OUTPUT   224
  307 FORMAT(I4,F10.4,1P7E14.6,14X,I4)                              OUTPUT   225
  409 FORMAT(1H0,44X,14HMOLE FRACTIONS)                             OUTPUT   226
  420 FORMAT(1H0,35X,36HNET RATE OF PRODUCTION (W-DOT/RHO*U))       OUTPUT   227
  421 FORMAT(3H0PT,8X,7(3X,A6,4X),1X,3H PT)                         OUTPUT   228
  422 FORMAT(I3,9X,1P7E13.5,I3)                                     OUTPUT   229
  431 FORMAT(1H0,2HPT,4X,3HY/R,  8X,5(8HREACTION,I3,11X),2HPT)      OUTPUT   230
  432 FORMAT(19X,5(2HRP, 9X,2HRM,10X))                              OUTPUT   231
  433 FORMAT(I3,1X,1P11E11.4,I4)                                    OUTPUT   232
  509 FORMAT(18X,8HFEET/SEC,4X,11H      K      ,6X,5HGM/CC,22X,6HCAL/GM,12 OUTPUT   233
     1X,9HLB/FT/SEC,3X,*DENSITY(1/ML)*)                             OUTPUT   234
  600 FORMAT(1H1,////// 20X,   *COLLISION*, 3X,*ELECTRICAL*,5X,*UNIT ATT OUTPUT   235
     1ENUATION (DB/IN)*/ 20X,*FREQUENCY*,2X,*CONDUCTIVITY*)         OUTPUT   236
  601 FORMAT(6H    PT, 7X,3HY/R,5X,*(1/SEC)*, 5X,*(MHO/IN)*/)       OUTPUT   237
  610 FORMAT(3X,I3,5X,F7.3,8(2X,1PE10.4))                           OUTPUT   238
  611 FORMAT(3E15.7)                                                OUTPUT   239
  612 FORMAT(E15.7,I5)                                              OUTPUT   240
  780 FORMAT(8(1PE10.3))                                            OUTPUT   241
  790 FORMAT(1PE10.3,60X,E10.3)                                     OUTPUT   242
 1011 FORMAT(1H1,70X,25HLOCAL ATTENUATION (DB/IN))                  OUTPUT   243
 1012 FORMAT(1H0,19X,9HCOLLISION/20X,9HFREQUENCY/3X,2HPT,16X,7H(1/SEC)) OUTPUT   244
 1013 FORMAT(19X,25H  SIGN. FREQ. (MEGACYC)= ,6(1PE10.4,2X))        OUTPUT   245
 1014 FORMAT(19X,13H   TRANSVERSE/24X,20HATTENUATION (DB) =  ,7(1PE10.4, OUTPUT   246
     12X))                                                          OUTPUT   247
 1068 FORMAT (1H0)                                                  OUTPUT   248
 1069 FORMAT (7X,7H(DB/IN))                                         OUTPUT   249
      RETURN                                                        OUTPUT   250
      END                                                           OUTPUT   251
```

```
      SUBROUTINE INOUT                                                  INOUT     2
      DIMENSION A(30),RHO(30),Y(30),T(30),PSI(30),RT(30),SUM(30),AR(25), INOUT     3
     1HSTAT(30),H(25,30),ALPHA(25,30),RALPHA(25,30),CP(25,30),SIGMA(30), INOUT     4
     2          WTMOLE(25),CPBAR(30),C(25,9),AID(25),ETA(30),RATIO(30), INOUT     5
     3RU(30),U(30),TITLE(12),XLE(30),XMU(30)          ,G(25),WTMIX(30), INOUT     6
     4RC(40,3),IRRR(40,5),WP(25),WM(25),WDOT(25,30),SAVET(30),SAVEU(30), INOUT     7
     5          IRR(40),FREQ(30),SAVEA(25,30),          PC(4),ZID(5), INOUT     8
     6          ECC(30),HOUT(30),YOUT(30),RHOOUT(30),XMUOUT(30),XLT(30), INOUT     9
     7T4(30),TFDG(30),IRT(40),RP(40,30),RM(40,30)                       INOUT    10
      DIMENSION ISAVE(6)                                                INOUT    11
      COMMON  A      , RHO    , Y      , T      , PSI    , RT           INOUT    12
      COMMON  SUM    , AR     , HSTAT  , H      , ALPHA  , RALPHA       INOUT    13
      COMMON  CP     , SIGMA           , WTMOLE , CPBAR  , C            INOUT    14
      COMMON  AID    , ETA    , RATIO  , RU     , U      , TITLE        INOUT    15
      COMMON  XLE    , XMU    ,        , G      , WTMIX  , WDOT         INOUT    16
      COMMON  SAVEU  , SAVET  , WM     , WP     , RC                    INOUT    17
      COMMON           SAVEA  ,          PC     , X      , XMAX         INOUT    18
      COMMON  PRNT   , DXMIN  , DX     , FDL    , DELPSI , RJ           INOUT    19
      COMMON  XK2    , P      , ZID    , FREQ   , ECC    , DPDX         INOUT    20
      COMMON  YOUT   , HOUT   , RHOOUT , IRRR   , IRR    , IFINIS       INOUT    21
      COMMON  IPAGE  , MPSI   , MY     , NS     , NR     , IEDGE        INOUT    22
      COMMON  ITURB  , IPRESS , NPSI   , ITEST  , ITER   , IECC         INOUT    23
      COMMON  IRT    , XMUOUT , XLT    , T4     , TFDG   , IOUT         INOUT    24
      COMMON  IOUT1  , IOUT2  ,RP      , RM     , ISAVE  , IPUNCH       INOUT    25
      COMMON TKINET                                                     INOUT    26
      WRITE (6,1901)                                                    INOUT    27
      WRITE (6,1902)                                                    INOUT    28
      WRITE (6,1903)(TITLE(I),I=1,12)                                   INOUT    29
      IF(IPRESS.NE.0) WRITE(6,1904)P                                    INOUT    30
      IF(IPRESS.EQ.0) WRITE(6,1905)P                                    INOUT    31
      WRITE (6,1908)RJ                                                  INOUT    32
      WRITE (6,1909)XLE(1),SIGMA(1)                                     INOUT    33
      WRITE (6,1966)X,XMAX                                              INOUT    34
      WRITE (6,1967)PRNT,DXMIN                                          INOUT    35
      LL=ITURB*2                                                        INOUT    36
      GO TO (1991,1999,1945,1978,1926,1933,9950,8000),LL                INOUT    37
 1991 WRITE (6,1959)                                                    INOUT    38
      GO TO 2999                                                        INOUT    39
 1999 WRITE (6,1960)XK2                                                 INOUT    40
      GO TO 2999                                                        INOUT    41
 1945 WRITE (6,1961)XK2                                                 INOUT    42
      GO TO 2999                                                        INOUT    43
 1978 WRITE (6,1962)XK2                                                 INOUT    44
      GO TO 2999                                                        INOUT    45
 1926 GO TO 2999                                                        INOUT    46
 1933 GO TO 2999                                                        INOUT    47
 8000 WRITE (6,8001)                                                    INOUT    48
 8001 FORMAT(1H0,22X,30HDOSAGE     EDDY VISCOSITY MODEL)                INOUT    49
      GO TO 2999                                                        INOUT    50
 9950 WRITE (6,9951)XK2                                                 INOUT    51
 2999 CONTINUE                                                          INOUT    52
      WRITE (6,1916)                                                    INOUT    53
      WRITE (6,1906)T(1),T(MPSI)                                        INOUT    54
      WRITE (6,1907)U(1),U(MPSI)                                        INOUT    55
      WTMIX(1)=0.0                                                      INOUT    56
```

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```
      WTMIX(MPSI)=0.0                                                   INOUT
      DO 1930 J=1,NS                                                    INOUT
      WTMIX(1)=WTMIX(1)+ALPHA(J,1)                                      INOUT
 1930 WTMIX(MPSI)=WTMIX(MPSI)+ALPHA(J,MPSI)                             INOUT
      DO 1919 J=1,NS                                                    INOUT
      RALPHA(J,1)=ALPHA(J,1)/WTMIX(1)                                   INOUT
      RALPHA(J,MPSI)=ALPHA(J,MPSI)/WTMIX(MPSI)                          INOUT
 1919 WRITE (6,1917)AID(J),RALPHA(J,1),RALPHA(J,MPSI)                   INOUT
      WRITE (6,120)                                                     INOUT
      DO 159 I=1,NR                                                     INOUT
      L=IPR(I)                                                          INOUT
      GO TO(131,132,133,134,135,136,137,138,139,140),L                  INOUT
  131 J1=IRRR(I,1)                                                      INOUT
      J2=IRRR(I,2)                                                      INOUT
      J3=IRRR(I,3)                                                      INOUT
      J4=IRRR(I,4)                                                      INOUT
      WRITE (6,121)I,AID(J1),AID(J2),AID(J3),AID(J4),(RC(I,J),J=1,3)    INOUT
      GO TO 159                                                         INOUT
  132 J1=IRRR(I,1)                                                      INOUT
      J2=IRRR(I,2)                                                      INOUT
      J3=IRRR(I,3)                                                      INOUT
      WRITE (6,122)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)            INOUT
      GO TO 159                                                         INOUT
  133 J1=IRRR(I,1)                                                      INOUT
      J2=IRRR(I,2)                                                      INOUT
      J3=IRRR(I,3)                                                      INOUT
      J4=IRRR(I,4)                                                      INOUT
      J5=IRRR(I,5)                                                      INOUT
      WRITE (6,123)I,AID(J1),AID(J2),AID(J3),AID(J4),AID(J5),(RC(I,J),J= INOUT
     1 1,3)                                                             INOUT
      GO TO 159                                                         INOUT
  134 J1=IRRR(I,1)                                                      INOUT
      J2=IRRR(I,2)                                                      INOUT
      J3=IRRR(I,3)                                                      INOUT
      WRITE (6,124)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)            INOUT
      GO TO 159                                                         INOUT
  135 J1=IRRR(I,1)                                                      INOUT
      J2=IRRR(I,3)                                                      INOUT
      J3=IRRR(I,4)                                                      INOUT
      WRITE (6,125)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)            INOUT
      GO TO 159                                                         INOUT
  136 J1=IRRR(I,1)                                                      INOUT
      J2=IRRR(I,2)                                                      INOUT
      J3=IRRR(I,3)                                                      INOUT
      J4=IRRR(I,4)                                                      INOUT
      WRITE (6,126)I,AID(J1),AID(J2),AID(J3),AID(J4),(RC(I,J),J=1,3)    INOUT
      GO TO 159                                                         INOUT
  137 J1=IRRR(I,1)                                                      INOUT
      J2=IRRR(I,2)                                                      INOUT
      J3=IRRR(I,3)                                                      INOUT
      WRITE (6,127)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)            INOUT
      GO TO 159                                                         INOUT
  138 J1=IRRR(I,1)                                                      INOUT
      J2=IRRR(I,2)                                                      INOUT
      J3=IRRR(I,3)                                                      INOUT
```

```
      J4=IRRR(I,4)                                                      INOUT     112
      J5=IRRR(I,5)                                                      INOUT     113
      WRITE (6,128)I,AID(J1),AID(J2),AID(J3),AID(J4),AID(J5),(RC(I,J),J= INOUT     114
     11,3)                                                              INOUT     115
      GO TO 159                                                         INOUT     116
  139 J1=IRRR(I,1)                                                      INOUT     117
      J2=IRRR(I,2)                                                      INOUT     118
      J3=IRRR(I,3)                                                      INOUT     119
      WRITE (6,129)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)            INOUT     120
      GO TO 159                                                         INOUT     121
  140 J1=IRRR(I,1)                                                      INOUT     122
      J2=IRRR(I,2)                                                      INOUT     123
      J3=IRRR(I,3)                                                      INOUT     124
      WRITE (6,130)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)            INOUT     125
  159 CONTINUE                                                          INOUT     126
  120 FORMAT(1H0,19X,26HREACTIONS BEING CONSIDERED,6X,19HKR=A*EXP(B/RT)/ INOUT     127
     1T**N,7X,1HA,8X,1HN,9X,1HB,7X,*(MOLECULE-MOL-SEC UNITS)*)          INOUT     128
  121 FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,2H+ ,A6,18X,1PE9.3,2X,0PF4.1,2X INOUT     129
     1,F10.1)                                                           INOUT     130
  122 FORMAT(I9,9X,A6,2H+ ,A6,3H+ M,5X,2H= ,A6,3H+ M,23X,1PE9.3,2X,0PF4. INOUT     131
     11,2X,F10.1)                                                       INOUT     132
  123 FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,2H+ ,A6,2H+ ,A6,10X,1PE9.3,2X,0 INOUT     133
     1PF4.1,2X,F10.1)                                                   INOUT     134
  124 FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,26X,1PE9.3,2X,0PF4.1,2X,F10.1)  INOUT     135
  125 FORMAT(I9,9X,A6,3H+ M,13X,2H= ,A6,2H+ ,A6,3H+ M,15X,1PE9.3,2X,0PF4 INOUT     136
     1.1,2X,F10.1)                                                      INOUT     137
  126 FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,2H+ ,A6,18X,1PE9.3,2X,0PF4.1,2X INOUT     138
     1,F10.1,3X,16HONE WAY REACTION)                                    INOUT     139
  127 FORMAT(I9,9X,A6,2H+ ,A6,3H+ M,5X,2H= ,A6,3H+ M,23X,1PE9.3,2X,0PF4. INOUT     140
     11,2X,F10.1,3X,16HONE WAY REACTION)                                INOUT     141
  128 FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,2H+ ,A6,2H+ ,A6,10X,1PE9.3,2X,0 INOUT     142
     1PF4.1,2X,F10.1,3X,16HONE WAY REACTION)                            INOUT     143
  129 FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,26X,1PE9.3,2X,0PF4.1,2X,F10.1,3 INOUT     144
     1X,16HONE WAY REACTION)                                            INOUT     145
  130 FORMAT(I9,9X,A6,3H+ M,13X,2H= ,A6,2H+ ,A6,3H+ M,15X,1PE9.3,2X,0PF4 INOUT     146
     1.1,2X,F10.1,3X,16HONE WAY REACTION)                               INOUT     147
 1901 FORMAT(1H1,37X,46HAEROCHEM RESEARCH LABORATORIES  PRINCETON N.J.)  INOUT     148
 1902 FORMAT(25X,*A FAST COMPUTER PROGRAM FOR NONEQUILIBRIUM ROCKET PLUM INOUT     149
     1E PREDICTIONS*)                                                   INOUT     150
 1903 FORMAT(1H0,24X,12A6)                                              INOUT     151
 1904 FORMAT(1H0,22X,19HPRESSURE(INITIAL) =1PE15.7,12H ATMOSPHERES)     INOUT     152
 1905 FORMAT(1H0,22X,20HPRESSURE(CONSTANT) =1PE15.7,12H ATMOSPHERES)    INOUT     153
 1906 FORMAT(23X,24HTEMPERATURE(DEG. KELVIN),3X,1PE15.7,4X,1PE15.7)     INOUT     154
 1907 FORMAT(23X,24HVELOCITY    (FEET/SECOND),3X,1PE15.7,4X,1PE15.7)    INOUT     155
 1908 FORMAT(1H0,22X,14HNOZZLE RADIUS=1PE15.7,5H FEET)                  INOUT     156
 1909 FORMAT(1H0,22X,23HLEWIS NUMBER(CONSTANT)=1PE15.7,5X,25HPRANDTL NUM INOUT     157
     1BER(CONSTANT)=1PE15.7)                                            INOUT     158
 1916 FORMAT(1H0,54X,3HJET,16X,4HEDGE)                                  INOUT     159
 1917 FORMAT(23X,13HMOLE FRACTION,3X,A6,5X,1PE15.7,4X,1PE15.7)          INOUT     160
 1959 FORMAT(1H0,22X,40HLAMINAR VISCOSITY MODEL(SUTHERLANDS LAW))       INOUT     161
 1960 FORMAT(1H0,22X,29HCONSTANT VISCOSITY MODEL  MU=1PE15.7)           INOUT     162
 1961 FORMAT(1H0,22X,27HFERRI VISCOSITY MODEL     K=1PE15.7)            INOUT     163
 1962 FORMAT(1H0,22X,31HTING-LIBBY VISCOSITY MODEL    K=1PE15.7)        INOUT     164
 1966 FORMAT(1H0,22X,16HX INITIAL(FEET)=1PE15.7,12X,14HX FINAL(FEET)=1PE INOUT     165
     115.7)                                                             INOUT     166
```

```
 1967 FORMAT(1H0,22X,16HPRINT INCREMENT=1PE15.7,12X,18HMINIMUM STEP SIZE INOUT     167
     1=1PE15.7)                                                         INOUT     168
 9951 FORMAT(1H0,22X,69HTING-LIBBY VISCOSITY MODEL AFTER MIXING REGION I INOUT     169
     1INTERSECTS X AXIS    K=1PE15.7)                                   INOUT     170
      RETURN                                                            INOUT     171
      END                                                               INOUT     172
170
```

SUBROUTINE GRATE

CDC 6600 FTN V3.0-P312 OPT=2 08/07/72 12.54.49. PAGE 1

```
      SUBROUTINE GRATE(ANSWER,Y,X,N)                                    GRATE      2
      DIMENSION X(30),Y(50)                                             GRATE      3
      SUM = 0.0                                                         GRATE      4
      INTER = N-1                                                       GRATE      5
      I1 = 1                                                            GRATE      6
      I2 = 2                                                            GRATE      7
      DO 1 I = 1,INTER                                                  GRATE      8
      SUM = SUM + (X(I2)-X(I1))*(Y(I2)+Y(I1))                           GRATE      9
      I1 = I1 + 1                                                       GRATE     10
      I2 = I2 + 1                                                       GRATE     11
    1 CONTINUE                                                          GRATE     12
      ANSWER = 0.5*SUM                                                  GRATE     13
      RETURN                                                            GRATE     14
      END                                                               GRATE     15
```

```
SUBROUTINE  TICK                                    CDC 6600 FTN V3.0-P312 OPT=2  08/07/72  12.54.49.     PAGE    1
          SUBROUTINE  TICK(JJJJ)                                                  TICK      2
          CALL SECOND(TIME)                                                       TICK      3
          JJJJ=TIME                                                               TICK      4
          RETURN                                                                  TICK      5
          END                                                                     TICK      6
```

```
      SUBROUTINE SLOP(X,A,N)                                            SLOP
C     THIS PROGRAM FINDS THE SOLUTIONS TO A SET OF N SIMULTANEOUS LINEAR SLOP
C     EQUATIONS BY USING THE GAUSS-GORDAN REDUCTION ALGORITHM WITH THE  SLOP
C      DIAGONAL PIVOT STRATEGY                                          SLOP
      DIMENSION A(25,25),X(25)                                          SLOP
      DO 9 K=1,N                                                        SLOP
      IF (ABS(A(K,K)) .GT. 1.E-10) GO TO 5                              SLOP
      WRITE (6,101)                                                     SLOP
      GO TO 99                                                          SLOP
    5 KP1= K+1                                                          SLOP
      DO 6 J= KP1, N                                                    SLOP
    6 A(K,J)= A(K,J)/A(K,K)                                             SLOP
      X(K)= X(K)/A(K,K)                                                 SLOP
      A(K,K)= 1.0                                                       SLOP
      DO 9 I=1,N                                                        SLOP
      IF (I.EQ.K .OR. A(I,K).EQ.0.) GO TO 9                             SLOP
      DO 8 J=KP1,N                                                      SLOP
    8 A(I,J)= A(I,J)- A(I,K)*A(K,J)                                     SLOP
      X(I)= X(I)- A(I,K)*X(K)                                           SLOP
      A(I,K)=0.                                                         SLOP
    9 CONTINUE                                                          SLOP
   99 CONTINUE                                                          SLOP
  101 FORMAT( * ERROR--- SMALL PIVOT *)                                 SLOP
      RETURN                                                            SLOP
      END                                                               SLOP
```

```
      SUBROUTINE TKEY(T,TTB,ITKEY,SDT,HDT,NT)                           TKEY
      DIMENSION TTB(30)                                                 TKEY
      NT1=NT-1                                                          TKEY
      DO 10 IT=1,NT1                                                    TKEY
      DT= TTB(IT+1)-TTB(IT)                                             TKEY
      SDT=(T-TTB(IT))/DT                                                TKEY
      HDT=(TTB(  IT+1)-T) /DT                                           TKEY
      IF ((SDT*HDT).GE.0.0) GO TO 11                                    TKEY
   10 CONTINUE                                                          TKEY
      WRITE(6,100) T,T                                                  TKEY
      ITKEY=0                                                           TKEY
  100 FORMAT(1H , *   TEMPERATURE OUT OF RANGE *, E14.5,I5)             TKEY
      RETURN                                                            TKEY
   11 ITKEY=IT                                                          TKEY
      RETURN                                                            TKEY
      END                                                               TKEY
```

```
      SUBROUTINE LIPLN (ITKEY,I,ATB,SDT,HDT,AX)                         LIPLN    2
      DIMENSION ATB(25,30)                                              LIPLN    3
      AX= ATB(I,ITKEY)*HDT+ ATB(I,ITKEY+1)*SDT                          LIPLN    4
      RETURN                                                            LIPLN    5
      END                                                               LIPLN    6
```

APPENDIX B

SAMPLE INPUT DATA SHEET

IBM

FORTRAN Coding Form

A FAST COMPUTER PROGRAM FOR
NONEQUILIBRIUM ROCKET PLUME PREDICTIONS

STATEMENT

CARD															
1	SAMPLE TEST CASE														
2	13	17	6	19	1	1	0	60	0	22					
3	9.57	+03													
4	0.0		10.0		1.0		1.0		1.0		0.25		1.0		
5	1.0	-10	2.0												
6	0.1		2000.		300.		7480.		100.				600.		
7, 8, 9	CARD TYPES 7, 8 AND 9 OMITTED														
10.1.1	3.27	-08	5.36	-03	5.04	-02	5.96	-06	5.36	-07	8.14	-02	2.85	-01	
10.1.2	2.35	-01	1.76	-01	2.68	-03	5.16	-07	1.29	-08	6.06	-05	1.19	-03	
10.1.3	1.19	-04	3.40	-02	1.27	-01									
10.2.1	0.0		0.0		0.0		0.0		0.0		0.0		0.0		
10.2.2	0.0		0.0		0.0		0.0		0.0		0.0		0.0		
10.2.3	2.1	-01	0.0		7.9	-01									

IBM

FORTRAN Coding Form

FORTRAN STATEMENT

THERMODYNAMIC DATA CARDS IN THE FOLLOWING ORDER: K, H, HCL, KCL, K^+, H_2, H_2O, CO, CO_2, CL, CL^-, E^-, O, OH, O_2, AL_2O_3, N_2.

11.1.1	K		39.1	21.31					
11.1.2		100.	4.968	42.714	-0.984	200.	4.968	38.751	-0.488
11.1.3		400.	4.968	38.492	0.506	600.	4.968	39.272	1.500
11.1.4		800.	4.968	40.084	2.493	1000.	4.968	40.822	3.487
11.1.5		1200.	4.968	41.481	4.481	1400.	4.970	42.070	5.474
11.1.6		1600.	4.975	42.602	6.469	1800.	4.988	43.084	7.465
11.1.7		2000.	5.013	43.526	8.465	2200.	5.057	43.932	9.471
11.1.8		2400.	5.122	44.310	10.489	2600.	5.213	44.662	11.522
11.1.9		2800.	5.334	44.993	12.576	3000.	5.489	45.305	13.658
11.1.10		3200.	5.685	45.601	14.775	3400.	5.932	45.883	15.935
11.1.11		3600.	6.242	46.153	17.152	3800.	6.630	46.412	18.438
11.1.12		4000.	7.111	46.664	19.810	4200.	7.701	46.908	21.289
11.2.1	2ND SPECIES (H)								
:	:								
11.17.1	18TH SPECIES (N_2)								
:	:								
11.17.12	:								

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CHEMICAL REACTION CARDS:

12.1	KCL	+H		=K	+HCL	15	3.0E-11	4072.
12.2	Φ	+Φ	+M	=Φ2	+M	22	1.0E-29	1.0
12.3	H	+H	+M	=H2	+M	22	1.0E-29	1.0
12.4	Φ	+H	+M	=ΦH	+M	22	1.0E-29	1.0
12.5	H	+ΦH	+M	=H2Φ	+M	22	1.0E-28	1.0
12.6	CΦ	+Φ	+M	=CΦ2	+M	26	5.0E-29	1.0 -4000.
12.7	ΦH	+ΦH		=H2Φ	+Φ	15	1.0E-11	-1000.
12.8	ΦH	+H2		=H2Φ	+H	15	4.0E-11	-5500.
12.9	Φ	+H2		=ΦH	+H	15	3.0E-11	-8200.
12.10	H	+Φ2		=ΦH	+Φ	15	3.0E-10	-16500.
12.11	CΦ	+ΦH		=CΦ2	+H	15	5.0E-13	-600.

IBM

FORTRAN Coding Form

FORTRAN STATEMENT

12.12	H	+HCL		=CL	+H2		15	8.8E-11	-4622.
12.13	HCL	+ΦH		=H2Φ	+CL		15	7.2E-12	-3250.
12.14	ΦH	+CL		=HCL	+Φ		15	3.0E-11	-5000.
12.15	H	+CL	+M	=HCL	+M		22	3.0E-29	
12.16	K+	+E-	+M	=K	+M		27	2.0E-22	1.5
12.17	K+	+CL-		=K	+CL		14	1.0E-08	0.5
12.18	CL	+E-	+M	=CL-	+M		21	3.0E-30	
12.19	H	+CL-		=HCL	+E-		15	1.7E-12	-6210.

APPENDIX C

SAMPLE OUTPUT

AEROCHEM RESEARCH LABORATORIES PRINCETON N.J.
A FAST COMPUTER PROGRAM FOR NONEQUILIBRIUM ROCKET PLUME PREDICTIONS

SAMPLE TEST CASE (8/7/72)

PRESSURE(CONSTANT) = 1.0000000E-01 ATMOSPHERES

NOZZLE RADIUS= 2.5000000E-01 FEET

LEWIS NUMBER(CONSTANT)= 1.0000000E+00 PRANDTL NUMBER(CONSTANT)= 1.0000000E+00

X INITIAL(FEET)= 0. X FINAL(FEET)= 1.0000000E+01

PRINT INCREMENT= 1.0000000E+00 MINIMUM STEP SIZE= 1.0000000E-10

DONALDSON/GRAY VISCOSITY MODEL

		JET	EDGE
TEMPERATURE(DEG. KELVIN)		2.0000000E+03	3.0000000E+02
VELOCITY (FEET/SECOND)		7.4800000E+03	1.0000000E+02
MOLE FRACTION	K	3.2784627E-08	0.
MOLE FRACTION	H	5.3647026E-03	0.
MOLE FRACTION	HCL	5.0467965E-02	0.
MOLE FRACTION	KCL	5.9608140E-06	0.
MOLE FRACTION	K+	5.3647026E-07	0.
MOLE FRACTION	H2	8.1464558E-02	0.
MOLE FRACTION	H2O	2.8512545E-01	0.
MOLE FRACTION	CO	2.3544450E-01	0.
MOLE FRACTION	CO2	1.7683338E-01	0.
MOLE FRACTION	CL	2.6823513E-03	0.
MOLE FRACTION	CL-	5.1659988E-07	0.
MOLE FRACTION	E-	1.2914247E-08	0.
MOLE FRACTION	O	6.0601159E-05	0.
MOLE FRACTION	OH	1.1921228E-03	0.
MOLE FRACTION	O2	1.1921228E-04	2.1000000E-01
MOLE FRACTION	AL2O3	3.4075652E-02	0.
MOLE FRACTION	N2	1.2716243E-01	7.9000000E-01

	REACTIONS BEING CONSIDERED	KP=A*EXP(B/RT)/T**N	A	N	B	(MOLECULE-ML-SEC UNITS)
1	KCL + H = K + HCL		3.000E-11	-0.0	4072.0	
2	O + O + M = O2 + M		1.000E-29	1.0	-0.0	
3	H + H + M = H2 + M		1.000E-29	1.0	-0.0	
4	O + H + M = OH + M		1.000E-29	1.0	-0.0	
5	H + OH + M = H2O + M		1.000E-28	1.0	-0.0	
6	CO + O + M = CO2 + M		5.000E-29	1.0	-4000.0	
7	OH + OH = H2O + O		1.000E-11	-0.0	-1000.0	
8	OH + H2 = H2O + H		4.000E-11	-0.0	-5500.0	
9	O + H2 = OH + H		3.000E-11	-0.0	-8200.0	
10	H + O2 = OH + O		3.000E-10	-0.0	-16500.0	
11	CO + OH = CO2 + H		5.000E-13	-0.0	-600.0	
12	H + HCL = CL + H2		8.800E-11	-0.0	-4622.0	
13	HCL + OH = H2O + CL		7.200E-12	-0.0	-3250.0	
14	OH + CL = HCL + O		3.000E-11	-0.0	-5000.0	
15	H + CL + M = HCL + M		3.000E-29	1.0	-0.0	
16	K+ + E- + M = K + M		2.000E-22	1.5	-0.0	
17	K+ + CL- = K + CL		1.000E-08	.5	-0.0	
18	CL + E- + M = CL- + M		3.000E-30	-0.0	-0.0	
19	H + CL- = HCL + E-		1.700E-12	-0.0	-6210.0	

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X= 0. FEET SAMPLE TEST CASE (8/7/72) PAGE 1

X/R	DELTA X FEET	PRESS(ATM)
0.	2.500000E-02	1.000000E-01

HALF RADIUS/R	INNER MIXING ZONE RADIUS/R	MACH NUMBER AT HALF RADIUS	MIXING RATE COEFFICIENT
1.199084E+00	1.019909E+00	1.775436E+00	2.480000E-02

PT	Y/R	VELOCITY FEET/SEC	TEMPERATURE K	DENSITY GM/CC	MACH NO.	ENTHALPY CAL/GM	VISCOSITY LB/FT/SEC	ELECTRON DENSITY(1/ML)	PSI	PT
1	0.0000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	0.	1
2	.1000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	1.259332E-02	2
3	.2000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	2.518665E-02	3
4	.3000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	3.777997E-02	4
5	.4000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	5.037330E-02	5
6	.5000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	6.296662E-02	6
7	.6000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	7.555994E-02	7
8	.7000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	8.815327E-02	8
9	.8000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	1.007466E-01	9
10	.9000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	1.133399E-01	10
11	1.0000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	1.259332E-01	11
12	1.3982	1.000000E+02	3.000000E+02	1.172305E-04	8.770271E-02	5.116059E-01	2.999450E-02	0.	1.385266E-01	12
13	2.2874	1.000000E+02	3.000000E+02	1.172305E-04	8.770271E-02	5.116059E-01	2.999450E-02	0.	1.511199E-01	13

MOLE FRACTIONS

PT	Y/R	K	H	HCL	KCL	K+	H2	H2O	PT
1	0.00000	3.27844E-08	5.36470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	1
2	.10000	3.27844E-08	5.36470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	2
3	.20000	3.27844E-08	5.36470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	3
4	.30000	3.27844E-08	5.36470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	4
5	.40000	3.27844E-08	5.36470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	5
6	.50000	3.27844E-08	5.36470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	6
7	.60000	3.27844E-08	5.36470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	7
8	.70000	3.27844E-08	5.36470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	8
9	.80000	3.27844E-08	5.36470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	9
10	.90000	3.27844E-08	5.36470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	10
11	1.00000	3.27844E-08	5.36470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	11
12	1.39817	0.	0.	0.	0.	0.	0.	0.	12
13	2.28737	0.	0.	0.	0.	0.	0.	0.	13

NET RATE OF PRODUCTION (W=DOT/RHO*U)

PT	K	H	HCL	KCL	K+	H2	H2O	PT
1	3.69229E-06	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	1
2	3.69229E-06	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	2
3	3.69229E-06	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	3
4	3.69229E-06	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	4
5	3.69229E-06	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	5
6	3.69229E-06	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	6
7	3.69229E-06	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	7
8	3.69229E-06	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	8
9	3.69229E-06	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	9
10	3.69229E-06	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	10
11	3.69229E-06	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	11

X= 0. FEET SAMPLE TEST CASE (8/7/72) PAGE 1

MOLE FRACTIONS

PT	Y/R	CO	CO2	CL	CL-	E-	O	OH	PT
1	0.00000	2.39449E-01	1.76833E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	1
2	.10000	2.39449E-01	1.76833E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	2
3	.20000	2.39449E-01	1.76833E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	3
4	.30000	2.39449E-01	1.76833E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	4
5	.40000	2.39449E-01	1.76833E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	5
6	.50000	2.39449E-01	1.76833E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	6
7	.60000	2.39449E-01	1.76833E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	7
8	.70000	2.39449E-01	1.76833E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	8
9	.80000	2.39449E-01	1.76833E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	9
10	.90000	2.39449E-01	1.76833E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	10
11	1.00000	2.39449E-01	1.76833E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	11
12	1.39817	0.	0.	0.	0.	0.	0.	0.	12
13	2.28737	0.	0.	0.	0.	0.	0.	0.	13

NET RATE OF PRODUCTION (W-DOT/RHO*U)

PT	CO	CO2	CL	CL-	E-	O	OH	PT
1	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	1
2	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	2
3	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	3
4	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	4
5	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	5
6	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	6
7	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	7
8	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	8
9	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	9
10	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	10
11	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	11

SAMPLE TEST CASE (8/7/72)

MOLE FRACTIONS

[illegible]	[illegible]	O2	AL2O3	N2					PT
1	.00000	1.19212E-04	3.40757E-02	1.27162E-01	0.	0.	0.	0.	1
[illegible]	.10000	1.19212E-04	3.40757E-02	1.27162E-01	0.	0.	0.	0.	2
[illegible]	.20000	1.19212E-04	3.40757E-02	1.27162E-01	0.	0.	0.	0.	3
[illegible]	.30000	1.19212E-04	3.40757E-02	1.27162E-01	0.	0.	0.	0.	4
[illegible]	.40000	1.19212E-04	3.40757E-02	1.27162E-01	0.	0.	0.	0.	5
[illegible]	.50000	1.19212E-04	3.40757E-02	1.27162E-01	0.	0.	0.	0.	6
[illegible]	.60000	1.19212E-04	3.40757E-02	1.27162E-01	0.	0.	0.	0.	7
[illegible]	.70000	1.19212E-04	3.40757E-02	1.27162E-01	0.	0.	0.	0.	8
[illegible]	[illegible]	1.19212E-04	3.40757E-02	1.27162E-01	0.	0.	0.	0.	9
[illegible]	[illegible]	1.19212E-04	3.40757E-02	1.27162E-01	0.	0.	0.	0.	10
11	[illegible]	1.19212E-04	3.40757E-02	1.27162E-01	0.	0.	0.	0.	11
[illegible]	[illegible]	2.10000E-01	0.	7.90000E-01	0.	0.	0.	0.	12
[illegible]	[illegible]	2.10000E-01	0.	7.90000E-01	0.	0.	0.	0.	13

NET RATE OF PRODUCTION (W-DOT/RHO*U)

[illegible]	O2	AL2O3	N2					PT
1	-2.56932E-06	0.	0.	0.	0.	0.	0.	1
[illegible]	-2.56932E-06	0.	0.	0.	0.	0.	0.	2
[illegible]	-2.56932E-06	0.	0.	0.	0.	0.	0.	3
[illegible]	-2.56932E-06	0.	0.	0.	0.	0.	0.	4
[illegible]	-2.56932E-06	0.	0.	0.	0.	0.	0.	5
[illegible]	-2.56932E-06	0.	0.	0.	0.	0.	0.	6
[illegible]	-2.56932E-06	0.	0.	0.	0.	0.	0.	7
[illegible]	-2.56932E-06	0.	0.	0.	0.	0.	0.	8
[illegible]	-2.56932E-06	0.	0.	0.	0.	0.	0.	9
10	-2.56932E-06	0.	0.	0.	0.	0.	0.	10
11	-2.56932E-06	0.	0.	0.	0.	0.	0.	11

REACTION RATES (MOLE/ML-SEC)

PT	Y/H	REACTION 1 RP	REACTION 1 RM	REACTION 2 RP	REACTION 2 RM	REACTION 3 RP	REACTION 3 RM	REACTION 4 RP	REACTION 4 RM	REACTION 5 RP	REACTION 5 RM	PT
1	0.	5.9858E-07	1.1564E-07	1.5093E-12	2.1389E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	1
2	1.0000E-01	5.9858E-07	1.1564E-07	1.5093E-12	2.1389E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	2
3	2.0000E-01	5.9858E-07	1.1564E-07	1.5093E-12	2.1389E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	3
4	3.0000E-01	5.9858E-07	1.1564E-07	1.5093E-12	2.1389E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	4
5	4.0000E-01	5.9858E-07	1.1564E-07	1.5093E-12	2.1389E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	5
6	5.0000E-01	5.9858E-07	1.1564E-07	1.5093E-12	2.1389E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	6
7	6.0000E-01	5.9858E-07	1.1564E-07	1.5093E-12	2.1389E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	7
8	7.0000E-01	5.9858E-07	1.1564E-07	1.5093E-12	2.1389E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	8
9	8.0000E-01	5.9858E-07	1.1564E-07	1.5093E-12	2.1389E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	9
10	9.0000E-01	5.9858E-07	1.1564E-07	1.5093E-12	2.1389E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	10
11	1.0000E+00	5.9858E-07	1.1564E-07	1.5093E-12	2.1389E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	11

REACTION RATES (MOLE/ML-SEC)

PT	Y/H	REACTION 6 RP	REACTION 6 RM	REACTION 7 RP	REACTION 7 RM	REACTION 8 RP	REACTION 8 RM	REACTION 9 RP	REACTION 9 RM	REACTION 10 RP	REACTION 10 RM	PT
1	0.	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	1
2	1.0000E-01	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	2
3	2.0000E-01	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	3
4	3.0000E-01	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	4
5	4.0000E-01	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	5
6	5.0000E-01	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	6
7	6.0000E-01	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	7
8	7.0000E-01	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	8
9	8.0000E-01	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	9
10	9.0000E-01	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	10
11	1.0000E+00	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	11

REACTION RATES (MOLE/ML-SEC)

PT	Y/H	REACTION 11		REACTION 12		REACTION 13		REACTION 14		REACTION 15		PT
		RP	RM	RP	RM	RP	RM	RP	RM	RP	RM	
1	0.	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	1
2	1.0000E-01	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	2
3	2.0000E-01	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	3
4	3.0000E-01	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	4
5	4.0000E-01	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	5
6	5.0000E-01	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	6
7	6.0000E-01	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	7
8	7.0000E-01	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	8
9	8.0000E-01	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	9
10	9.0000E-01	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	10
11	1.0000E+00	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	11

REACTION RATES (MOLE/ML-SEC)

PT	Y/H	REACTION 16		REACTION 17		REACTION 18		REACTION 19		REACTION 20		PT
		RP	RM	RP	RM	RP	RM	RP	RM	RP	RM	
1	0.	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	1
2	1.0000E-01	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	2
3	2.0000E-01	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	3
4	3.0000E-01	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	4
5	4.0000E-01	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	5
6	5.0000E-01	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	6
7	6.0000E-01	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	7
8	7.0000E-01	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	8
9	8.0000E-01	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	9
10	9.0000E-01	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	10
11	1.0000E+00	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	11

PT	Y/S	COLLISION FREQUENCY (1/SEC)	ELECTRICAL CONDUCTIVITY (MHO/IN)	UNIT ATTENUATION (DB/IN)
		SIGN. FREQ. (MEGACYC)= 9.7500E+02		
1	0.000	3.0832E+10	1.1017E-02	3.6402E-02
2	.100	3.0832E+10	1.1017E-02	3.6402E-02
3	.200	3.0832E+10	1.1017E-02	3.6402E-02
4	.300	3.0832E+10	1.1017E-02	3.6402E-02
5	.400	3.0832E+10	1.1017E-02	3.6402E-02
6	.500	3.0832E+10	1.1017E-02	3.6402E-02
7	.600	3.0832E+10	1.1017E-02	3.6402E-02
8	.700	3.0832E+10	1.1017E-02	3.6402E-02
9	.800	3.0832E+10	1.1017E-02	3.6402E-02
10	.900	3.0832E+10	1.1017E-02	3.6402E-02
11	1.000	3.0832E+10	1.1017E-02	3.6402E-02
12	1.398	7.3762E+09	0.	0.

TRANSVERSE ATTENUATION (DB) = 2.6149E-01

2.50000E-02	0.
1.90080E-01	2.50000E-02
2.27558E-01	2.15080E-01
1.77170E-01	4.42638E-01
8.85850E-02	4.42638E-01
1.77170E-01	5.31224E-01
1.27594E-01	7.08394E-01
1.00482E-01	8.35977E-01
9.88847E-02	9.36419E-01

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X/R	DELTA X FEET	PRESS(ATM)
4.141214E+00	9.888472E-02	1.000000E-01

HALF RADIUS/R	INNER MIXING ZONE RADIUS/R	MACH NUMBER AT HALF RADIUS	MIXING RATE COEFFICIENT
1.094830E+00	8.188493E-01	1.509756E+00	2.490000E-02

PT	Y/R	VELOCITY FEET/SEC	TEMPERATURE K	DENSITY GM/CC	MACH NO.	ENTHALPY CAL/GM	VISCOSITY LB/FT/SEC	ELECTRON DENSITY(1/ML)	PST	PT
1	0.0000	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907386E-03	4.419308E+09	0.	1
2	.0999	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907386E-03	4.419308E+09	1.259332E-02	2
3	.1998	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907386E-03	4.419308E+09	2.518665E-02	3
4	.2997	7.480000E+03	1.995371E+03	1.752709E-05	2.726314E+00	-1.241199E+03	6.907386E-03	4.419310E+09	3.777997E-02	4
5	.3995	7.479989E+03	1.995371E+03	1.752710E-05	2.726311E+00	-1.241197E+03	6.907389E-03	4.419449E+09	5.037330E-02	5
6	.4994	7.479680E+03	1.995355E+03	1.752724E-05	2.726206E+00	-1.241133E+03	6.907445E-03	4.423511E+09	6.296662E-02	6
7	.5993	7.475278E+03	1.995171E+03	1.752892E-05	2.724674E+00	-1.240205E+03	6.908108E-03	4.484099E+09	7.555994E-02	7
8	.6994	7.437421E+03	1.993991E+03	1.753991E-05	2.711384E+00	-1.232162E+03	6.912437E-03	4.991374E+09	8.815327E-02	8
9	.8007	7.234296E+03	1.989396E+03	1.759384E-05	2.638795E+00	-1.188220E+03	6.929752E-03	7.384200E+09	1.007466E-01	9
10	.9073	6.510506E+03	1.969091E+03	1.777788E-05	2.381637E+00	-1.031756E+03	7.006222E-03	1.317522E+10	1.133399E-01	10
11	1.0310	4.743910E+03	1.827208E+03	1.919058E-05	1.788797E+00	-6.769682E+02	7.562964E-03	1.777640E+10	1.259332E-01	11
12	1.1945	2.300324E+03	1.287576E+03	2.728697E-05	1.014664E+00	-2.773312E+02	1.075373E-02	8.495932E+09	1.385266E-01	12
13	1.4189	9.051555E+02	7.399447E+02	4.751716E-05	5.149041E-01	-9.124333E+01	1.872640E-02	1.356855E+09	1.511199E-01	13
14	1.7194	3.584702E+02	4.491325E+02	7.829308E-05	2.581546E-01	-2.799443E+01	3.085512E-02	9.238785E+08	1.637132E-01	14
15	2.1396	1.659948E+02	3.378280E+02	1.040989E-04	1.372803E-01	-6.838738E+00	4.102512E-02	3.756923E+08	1.763065E-01	15
16	2.6833	1.124715E+02	3.071575E+02	1.144977E-04	9.766968E-02	-9.203940E-01	4.512329E-02	5.995028E+07	1.888999E-01	16
17	3.2422	1.019145E+02	3.010600E+02	1.169176E-04	8.922589E-02	2.905605E-01	4.603755E-02	7.862719E+06	2.014932E-01	17
18	3.7638	1.000000E+02	3.000000E+02	1.172305E-04	8.770271E-02	5.116059E-01	4.620029E-02	0.	2.140865E-01	18
19	4.2521	1.000000E+02	3.000000E+02	1.172305E-04	8.770271E-02	5.116059E-01	4.620029E-02	0.	2.266798E-01	19

MOLE FRACTIONS

PT	Y/R	K	H	HCL	KCL	K+	H2	H2O	PT
1	0.00000	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39186E-07	8.18652E-02	2.84461E-01	1
2	.04988	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39186E-07	8.18652E-02	2.84461E-01	2
3	.14977	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39186E-07	8.18652E-02	2.84461E-01	3
4	.29965	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39186E-07	8.18652E-02	2.84461E-01	4
5	.39953	1.55856E-07	5.08564E-03	5.07714E-02	5.83412E-06	5.39186E-07	8.18647E-02	2.84461E-01	5
6	.49942	1.57035E-07	5.09133E-03	5.07663E-02	5.83368E-06	5.39173E-07	8.18515E-02	2.84457E-01	6
7	.59932	1.59724E-07	5.17653E-03	5.06925E-02	5.82725E-06	5.39012E-07	8.16596E-02	2.84390E-01	7
8	.69941	1.82959E-07	5.91020E-03	5.00578E-02	5.77194E-06	5.37857E-07	8.00444E-02	2.83800E-01	8
9	.80070	2.99163E-07	9.49315E-03	4.67447E-02	5.48223E-06	5.32834E-07	7.20236E-02	2.80084E-01	9
10	.90726	5.91270E-07	1.74667E-02	3.65899E-02	4.57155E-06	5.14889E-07	5.03326E-02	2.61745E-01	10
11	1.03100	8.27781E-07	1.98406E-02	2.09126E-02	2.86265E-06	4.29543E-07	2.28090E-02	2.00135E-01	11
12	1.19652	7.91338E-07	1.11811E-02	6.13179E-03	9.68287E-07	1.96289E-07	6.19345E-03	1.01865E-01	12
13	1.41890	3.88565E-07	3.81955E-03	2.67101E-03	2.63547E-07	6.41387E-08	3.72846E-03	3.62870E-02	13
14	1.71945	8.74338E-08	8.85438E-04	1.17603E-03	1.23100E-07	1.95991E-08	1.65992E-03	1.11777E-02	14
15	2.13955	1.03919E-08	1.51973E-04	3.71461E-04	4.34483E-08	4.87975E-09	5.34077E-04	2.73869E-03	15
16	2.68327	1.26825E-09	1.86231E-05	7.98926E-05	9.08039E-09	9.26440E-10	1.23035E-04	5.07776E-04	16
17	3.20216	1.07638E-10	1.74532E-06	1.28541E-05	1.45620E-09	1.39690E-10	2.06919E-05	7.49219E-05	17
18	3.76375	0.	0.	0.	0.	0.	0.	0.	18
19	4.25210	0.	0.	0.	0.	0.	0.	0.	19

NET RATE OF PRODUCTION (W-DOT/RHO*U)

PT	K	H	HCL	KCL	K+	H2	H2O	PT
1	-6.64882E-11	-5.32473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	1
2	-6.64882E-11	-5.32473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	2
3	-6.64882E-11	-5.32473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	3
4	-6.64670E-11	-5.32383E-07	4.21486E-07	-2.28665E-11	8.93334E-11	5.84642E-06	-5.74383E-06	4
5	-6.51084E-11	-5.25848E-07	4.17983E-07	-2.42414E-11	8.93498E-11	5.83853E-06	-5.73621E-06	5
6	-3.83322E-11	-3.73239E-07	3.37780E-07	-5.14925E-11	8.98247E-11	5.65207E-06	-5.56658E-06	6
7	2.13296E-10	1.39325E-06	-6.64468E-07	-3.10310E-10	9.70143E-11	3.45840E-06	-3.67145E-06	7
8	1.99602E-09	1.47767E-05	-1.13265E-05	-2.16072E-09	1.64700E-10	-1.37331E-05	1.16571E-05	8
9	1.34543E-08	1.14427E-04	-9.91153E-05	-1.41163E-08	6.62017E-10	-1.46223E-04	1.22852E-04	9
10	4.42172E-08	5.04251E-04	-3.49425E-04	-4.75418E-08	3.32462E-09	-6.62950E-04	4.42510E-04	10
11	8.19314E-08	7.77689E-04	-4.37972E-04	-8.93179E-08	7.38658E-09	-8.44388E-04	5.77806E-04	11
12	-3.45776E-07	-4.12008E-04	-2.82496E-04	3.43164E-07	2.61200E-09	-5.51770E-04	4.59941E-04	12
13	-1.72601E-06	8.85255E-05	-1.88459E-05	1.32608E-06	-6.69097E-11	-5.19879E-05	3.83775E-05	13

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MOLE FRACTIONS

PT	Y/R	CO	CO2	CI	CL-	E-	O	OH	PT
1	0.00000	2.35311E-01	1.76973E-01	2.37974E-03	5.20233E-07	1.19973E-08	7.89347E-05	1.70718E-03	1
2	.09988	2.35311E-01	1.76973E-01	2.37974E-03	5.20233E-07	1.19973E-08	7.89347E-05	1.70718E-03	2
3	.19977	2.35311E-01	1.76973E-01	2.37974E-03	5.20233E-07	1.19973E-08	7.89347E-05	1.70718E-03	3
4	.29965	2.35311E-01	1.76973E-01	2.37974E-03	5.20233E-07	1.19973E-08	7.89348E-05	1.70718E-03	4
5	.39953	2.35311E-01	1.76973E-01	2.37984E-03	5.20232E-07	1.19977E-08	7.89442E-05	1.70726E-03	5
6	.49942	2.35299E-01	1.76967E-01	2.38265E-03	5.20209E-07	1.20086E-08	7.92055E-05	1.70949E-03	6
7	.59932	2.35125E-01	1.76895E-01	2.42473E-03	5.19888E-07	1.21720E-08	8.30479E-05	1.74256E-03	7
8	.69941	2.33599E-01	1.76322E-01	2.78895E-03	5.17400E-07	1.35410E-08	1.19987E-04	2.03246E-03	8
9	.89070	2.25181E-01	1.73470E-01	4.44909E-03	5.06121E-07	1.99862E-08	4.33972E-04	3.63397E-03	9
10	.90726	1.95306E-01	1.63158E-01	9.62337E-03	4.73545E-07	3.52964E-08	2.74125E-03	8.84767E-03	10
11	1.03100	1.29695E-01	1.30421E-01	1.35220E-02	3.80963E-07	4.41914E-08	9.70302E-03	1.28187E-02	11
12	1.19452	5.93039E-02	6.41834E-02	9.78882E-03	1.79322E-07	1.48830E-08	7.78412E-03	3.25615E-03	12
13	1.41890	2.29510E-02	2.22697E-02	3.15918E-03	6.20097E-08	1.36597E-09	1.08184E-03	1.52159E-04	13
14	1.71945	7.76035E-03	6.76917E-03	6.97186E-04	1.87894E-08	5.64541E-10	2.70964E-04	1.11768E-04	14
15	2.13956	2.04955E-03	1.65776E-03	1.06490E-04	4.64453E-09	1.72677E-10	5.03626E-05	3.67502E-05	15
16	2.68327	4.01068E-04	3.10788E-04	1.18801E-05	8.89377E-10	2.50529E-11	3.95032E-06	4.26322E-06	16
17	3.24216	6.12012E-05	4.63519E-05	1.01155E-06	1.34655E-10	3.22056E-12	9.24337E-08	3.17798E-07	17
18	3.76375	0.	0.	0.	0.	0.	0.	0.	18
19	4.25210	0.	0.	0.	0.	0.	0.	0.	19

NET RATE OF PRODUCTION (W-DOT/RHO*U)

PT	CO	CO2	CI	CL-	E-	O	OH	PT
1	-5.83544E-06	5.83544E-06	-4.21606E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	1
2	-5.83544E-06	5.83544E-06	-4.21606E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	2
3	-5.83544E-06	5.83544E-06	-4.21606E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	3
4	-5.83547E-06	5.83547E-06	-4.21557E-07	9.39150E-11	-4.58157E-12	-2.46762E-08	-9.42855E-08	4
5	-5.83804E-06	5.83808E-06	-4.16052E-07	9.39173E-11	-4.56748E-12	-2.45845E-08	-9.67891E-08	5
6	-5.90629E-06	5.90629E-06	-3.37822E-07	9.40084E-11	-4.18368E-12	-2.26453E-08	-1.35525E-07	6
7	-6.83180E-06	6.83180E-06	6.64682E-07	9.54614E-11	1.55294E-12	-1.65444E-08	-3.02688E-07	7
8	-1.52409E-05	1.52409E-05	1.13286E-05	1.08138E-10	5.65616E-11	-7.56295E-07	7.01983E-07	8
9	-8.39002E-05	8.39002E-05	9.91292E-05	2.75471E-10	3.86545E-10	-1.16830E-05	3.14289E-05	9
10	-4.89032E-04	4.89032E-04	3.49471E-04	1.96081E-09	1.36381E-09	5.23358E-05	2.86055E-04	10
11	-1.22859E-03	1.22859E-03	4.38056E-04	5.15755E-09	2.22902E-09	5.11271E-04	1.93455E-04	11
12	-6.26208E-04	6.26208E-04	2.82150E-04	2.29516E-09	3.16833E-10	1.10596E-03	8.78162E-04	12
13	-4.82731E-05	4.82731E-05	1.75196E-05	2.30802E-10	-2.97712E-10	-8.95360E-05	-4.24589E-05	13

MOLE FRACTIONS

PT	Y/R	O2	Al2O3	N2					PT
1	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	1
2	.09988	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	2
3	.19977	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	3
4	.29965	1.18411E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	4
5	.39953	1.18522E-04	3.40761E-02	1.27165E-01	0.	0.	0.	0.	5
6	.49942	1.21408E-04	3.40747E-02	1.27193E-01	0.	0.	0.	0.	6
7	.59932	1.59615E-04	3.40543E-02	1.27590E-01	0.	0.	0.	0.	7
8	.69941	4.68254E-04	3.38809E-02	1.30968E-01	0.	0.	0.	0.	8
9	.80070	2.20949E-03	3.29493E-02	1.49122E-01	0.	0.	0.	0.	9
10	.90726	1.06917E-02	2.96278E-02	2.13864E-01	0.	0.	0.	0.	10
11	1.03100	4.72881E-02	2.14991E-02	3.72252E-01	0.	0.	0.	0.	11
12	1.19452	1.28105E-01	1.02065E-02	5.91999E-01	0.	0.	0.	0.	12
13	1.41890	1.82563E-01	3.73755E-03	7.17579E-01	0.	0.	0.	0.	13
14	1.71945	2.01611E-01	1.20090E-03	7.66679E-01	0.	0.	0.	0.	14
15	2.13956	2.07954E-01	3.06417E-04	7.84042E-01	0.	0.	0.	0.	15
16	2.68327	2.09624E-01	5.88364E-05	7.88856E-01	0.	0.	0.	0.	16
17	3.24216	2.09945E-01	8.88949E-06	7.89827E-01	0.	0.	0.	0.	17
18	3.76375	2.10000E-01	0.	7.90000E-01	0.	0.	0.	0.	18
19	4.25210	2.10000E-01	0.	7.90000E-01	0.	0.	0.	0.	19

NET RATE OF PRODUCTION (W-DOT/RHO*U)

PT	O2	Al2O3	N2					PT
1	1.37115E-08	0.	0.	0.	0.	0.	0.	1
2	1.37115E-08	0.	0.	0.	0.	0.	0.	2
3	1.37115E-08	0.	0.	0.	0.	0.	0.	3
4	1.36416E-08	0.	0.	0.	0.	0.	0.	4
5	9.74826E-09	0.	0.	0.	0.	0.	0.	5
6	-9.07713E-08	0.	0.	0.	0.	0.	0.	6
7	-1.42056E-06	0.	0.	0.	0.	0.	0.	7
8	-1.34219E-05	0.	0.	0.	0.	0.	0.	8
9	-1.13249E-04	0.	0.	0.	0.	0.	0.	9
10	-6.34966E-04	0.	0.	0.	0.	0.	0.	10
11	-1.25556E-03	0.	0.	0.	0.	0.	0.	11
12	-1.53513E-03	0.	0.	0.	0.	0.	0.	12
13	2.26721E-05	0.	0.	0.	0.	0.	0.	13

REACTION RATES (MOLE/ML-SEC)

PT	Y/R	REACTION 1		REACTION 2		REACTION 3		REACTION 4		REACTION 5		PT
		RP	RM	RP	RM	RP	RM	RP	RM	RP	RM	
1	0.	5.5927E-07	5.5927E-07	2.5846E-12	1.9969E-13	1.0728E-08	8.3019E-10	1.6651E-10	1.2902E-11	3.6013E-08	2.7928E-09	1
2	9.9884E-02	5.5927E-07	5.5927E-07	2.5846E-12	1.9969E-13	1.0728E-08	8.3019E-10	1.6651E-10	1.2902E-11	3.6013E-08	2.7928E-09	2
3	1.9977E-01	5.5927E-07	5.5927E-07	2.5846E-12	1.9969E-13	1.0728E-08	8.3019E-10	1.6651E-10	1.2902E-11	3.6013E-08	2.7928E-09	3
4	2.9965E-01	5.5927E-07	5.5927E-07	2.5846E-12	1.9970E-13	1.0728E-08	8.3019E-10	1.6651E-10	1.2902E-11	3.6013E-08	2.7928E-09	4
5	3.9953E-01	5.5929E-07	5.5929E-07	2.5852E-12	1.9988E-13	1.0729E-08	8.3018E-10	1.6654E-10	1.2902E-11	3.6016E-08	2.7928E-09	5
6	4.9942E-01	5.5989E-07	5.5988E-07	2.6024E-12	2.0471E-13	1.0753E-08	8.2989E-10	1.6728E-10	1.2917E-11	3.6105E-08	2.7921E-09	6
7	5.9932E-01	5.6879E-07	5.6874E-07	2.8621E-12	2.6846E-13	1.1120E-08	8.2617E-10	1.7840E-10	1.3139E-11	3.7433E-08	2.7845E-09	7
8	6.9941E-01	6.4439E-07	6.4411E-07	5.9885E-12	7.7520E-13	1.4530E-08	7.9872E-10	2.9498E-10	1.5120E-11	4.9966E-08	2.7345E-09	8
9	8.0070E-01	9.8985E-07	9.8819E-07	7.9065E-11	3.4384E-12	3.7834E-08	6.8095E-10	1.7296E-09	2.5647E-11	1.4483E-07	2.5348E-09	9
10	9.0726E-01	1.5670E-06	1.5615E-06	3.2869E-09	1.2611E-11	1.3345E-07	3.7372E-10	2.0943E-08	4.9318E-11	6.7596E-07	1.7893E-09	10
11	1.0310E+00	1.4034E-06	1.3953E-06	5.5540E-08	6.6849E-12	2.3222E-07	2.6593E-11	1.1357E-07	1.1715E-11	1.5004E-06	1.5975E-10	11
12	1.1945E+00	8.6222E-07	8.8376E-07	1.4497E-07	5.8996E-17	2.9910E-07	1.1884E-16	2.0823E-07	6.2388E-17	8.7105E-07	2.3175E-16	12
13	1.4189E+00	7.8882E-07	8.4585E-07	2.5673E-08	5.2076E-31	3.2002E-07	3.0291E-29	9.0640E-08	2.2203E-30	1.2748E-07	4.0202E-31	13

REACTION RATES (MOLE/ML-SEC)

PT	Y/R	REACTION 6		REACTION 7		REACTION 8		REACTION 9		REACTION 10		PT
		RP	RM	RP	RM	RP	RM	RP	RM	RP	RM	
1	0.	1.4040E-08	1.0668E-09	5.0921E-06	5.0964E-06	3.1377E-04	3.1443E-04	5.5050E-06	5.5119E-06	6.3167E-07	6.3346E-07	1
2	9.9884E-02	1.4040E-08	1.0668E-09	5.0921E-06	5.0964E-06	3.1377E-04	3.1443E-04	5.5050E-06	5.5119E-06	6.3167E-07	6.3346E-07	2
3	1.9977E-01	1.4040E-08	1.0668E-09	5.0921E-06	5.0964E-06	3.1377E-04	3.1443E-04	5.5050E-06	5.5119E-06	6.3167E-07	6.3346E-07	3
4	2.9965E-01	1.4040E-08	1.0668E-09	5.0921E-06	5.0965E-06	3.1377E-04	3.1443E-04	5.5051E-06	5.5119E-06	6.3168E-07	6.3346E-07	4
5	3.9953E-01	1.4042E-08	1.0668E-09	5.0926E-06	5.0970E-06	3.1378E-04	3.1444E-04	5.5057E-06	5.5124E-06	6.3229E-07	6.3357E-07	5
6	4.9942E-01	1.4088E-08	1.0665E-09	5.1060E-06	5.1137E-06	3.1414E-04	3.1478E-04	5.5230E-06	5.5257E-06	6.4841E-07	6.3650E-07	6
7	5.9932E-01	1.4744E-08	1.0632E-09	5.3063E-06	5.3593E-06	3.1949E-04	3.1988E-04	5.7773E-06	5.7271E-06	8.6655E-07	6.8041E-07	7
8	6.9941E-01	2.1230E-08	1.0416E-09	7.2262E-06	7.7152E-06	3.6540E-04	3.6378E-04	8.1816E-06	7.6288E-06	2.8987E-06	1.1478E-06	8
9	8.0070E-01	7.4531E-08	9.5788E-10	2.3194E-05	2.7376E-05	5.8868E-04	5.7246E-04	2.6622E-05	2.1933E-05	2.1860E-05	7.4539E-06	9
10	9.0726E-01	4.2101E-07	6.6595E-10	1.3997E-04	1.5734E-04	1.0078E-03	9.5259E-04	1.1741E-04	9.8727E-05	1.9029E-04	1.1679E-04	10
11	1.0310E+00	1.2328E-06	5.2719E-11	3.3451E-04	3.4526E-04	6.8894E-04	6.4056E-04	1.8585E-04	1.6742E-04	8.0008E-04	6.8572E-04	11
12	1.1945E+00	1.1565E-06	2.5910E-17	3.8726E-05	3.4390E-05	5.0702E-05	3.3951E-05	3.1625E-05	2.3847E-05	3.6584E-04	2.6934E-04	12
13	1.4189E+00	1.7904E-07	2.1628E-33	1.9171E-07	2.4680E-08	8.7910E-07	2.9288E-08	7.4650E-07	1.9319E-07	4.5483E-06	5.4977E-06	13

REACTION RATES (MOLE/ML-SEC)

PT	Y/H	REACTION 11 RP	REACTION 11 RM	REACTION 12 RP	REACTION 12 RM	REACTION 13 RP	REACTION 13 RM	REACTION 14 RP	REACTION 14 RM	REACTION 15 RP	REACTION 15 RM	PT
1	0.	3.8821E-05	3.8069E-05	1.5916E-03	1.5915E-03	6.1800E-05	6.1926E-05	7.7607E-06	7.7515E-06	1.5060E-08	1.1655E-09	1
2	9.9884E-02	3.8821E-05	3.8069E-05	1.5916E-03	1.5915E-03	6.1800E-05	6.1926E-05	7.7607E-06	7.7515E-06	1.5060E-08	1.1655E-09	2
3	1.9977E-01	3.8821E-05	3.8069E-05	1.5916E-03	1.5915E-03	6.1800E-05	6.1926E-05	7.7607E-06	7.7515E-06	1.5060E-08	1.1655E-09	3
4	2.9965E-01	3.8821E-05	3.8069E-05	1.5916E-03	1.5915E-03	6.1800E-05	6.1926E-05	7.7607E-06	7.7515E-06	1.5060E-08	1.1655E-09	4
5	3.9953E-01	3.8823E-05	3.8071E-05	1.5916E-03	1.5915E-03	6.1803E-05	6.1928E-05	7.7614E-06	7.7524E-06	1.5061E-08	1.1655E-09	5
6	4.9942E-01	3.8832E-05	3.8111E-05	1.5933E-03	1.5932E-03	6.1878E-05	6.1999E-05	7.7807E-06	7.7773E-06	1.5097E-08	1.1652E-09	6
7	5.9932E-01	3.9602E-05	3.8720E-05	1.6177E-03	1.6176E-03	6.2990E-05	6.3063E-05	8.0719E-06	8.1431E-06	1.5626E-08	1.1610E-09	7
8	6.9941E-01	4.5940E-05	4.3972E-05	1.8247E-03	1.8244E-03	7.2600E-05	7.2262E-05	1.0834E-05	1.1621E-05	2.0569E-08	1.1310E-09	8
9	8.0070E-01	7.9518E-05	6.8919E-05	2.7422E-03	2.7400E-03	1.2155E-04	1.1810E-04	3.2344E-05	3.9291E-05	5.5586E-08	1.0013E-09	9
10	9.0726E-01	1.7113E-04	1.1495E-04	3.9829E-03	3.9859E-03	2.3444E-04	2.2176E-04	1.6423E-04	1.9517E-04	2.2057E-07	6.1725E-10	10
11	1.0310E+00	1.8894E-04	7.8328E-05	2.6217E-03	2.6320E-03	2.0227E-04	1.8880E-04	3.5158E-04	3.8875E-04	4.7460E-07	5.4159E-11	11
12	1.1945E+00	4.1237E-05	3.0862E-06	5.3456E-04	5.4497E-04	2.1781E-05	1.4869E-05	7.3081E-05	9.5069E-05	7.8558E-07	3.0618E-16	12
13	1.4189E+00	1.8981E-06	9.3637E-10	6.3212E-05	6.4365E-05	5.2409E-07	1.7779E-08	7.8507E-07	2.9793E-06	7.9406E-07	7.3814E-29	13

REACTION RATES (MOLE/ML-SEC)

PT	Y/H	REACTION 16 RP	REACTION 16 RM	REACTION 17 RP	REACTION 17 RM	REACTION 18 RP	REACTION 18 RM	REACTION 19 RP	REACTION 19 RM	REACTION 20 RP	REACTION 20 RM	PT
1	0.	1.2014E-12	1.8282E-13	1.4121E-11	2.6851E-11	7.0894E-12	5.6732E-13	2.1103E-10	2.0409E-10	0.	0.	1
2	9.9884E-02	1.2014E-12	1.8282E-13	1.4121E-11	2.6851E-11	7.0894E-12	5.6732E-13	2.1103E-10	2.0409E-10	0.	0.	2
3	1.9977E-01	1.2014E-12	1.8282E-13	1.4121E-11	2.6851E-11	7.0894E-12	5.6732E-13	2.1103E-10	2.0409E-10	0.	0.	3
4	2.9965E-01	1.2014E-12	1.8282E-13	1.4121E-11	2.6851E-11	7.0894E-12	5.6732E-13	2.1103E-10	2.0409E-10	0.	0.	4
5	3.9953E-01	1.2015E-12	1.8282E-13	1.4121E-11	2.6853E-11	7.0900E-12	5.6731E-13	2.1103E-10	2.0409E-10	0.	0.	5
6	4.9942E-01	1.2026E-12	1.8300E-13	1.4120E-11	2.6915E-11	7.1050E-12	5.6720E-13	2.1126E-10	2.0425E-10	0.	0.	6
7	5.9932E-01	1.2191E-12	1.8574E-13	1.4110E-11	2.7856E-11	7.3308E-12	5.6578E-13	2.1467E-10	2.0667E-10	0.	0.	7
8	6.9941E-01	1.3549E-12	2.0986E-13	1.4013E-11	3.6666E-11	9.3970E-12	5.5627E-13	2.4399E-10	2.2662E-10	0.	0.	8
9	8.0070E-01	2.0041E-12	3.2528E-13	1.3676E-11	9.9570E-11	2.3281E-11	5.1891E-13	3.8374E-10	3.1013E-10	0.	0.	9
10	9.0726E-01	3.5828E-12	5.0586E-13	1.2688E-11	4.0057E-10	8.7766E-11	3.9251E-13	6.6346E-10	4.3516E-10	0.	0.	10
11	1.0310E+00	5.2393E-12	1.1266E-13	1.0265E-11	6.8785E-10	1.9323E-10	6.2022E-14	6.2242E-10	2.2120E-10	0.	0.	11
12	1.1945E+00	3.8957E-12	2.0779E-18	5.2976E-12	1.7315E-10	1.3464E-10	2.1972E-18	1.6230E-10	3.8760E-12	0.	0.	12
13	1.4189E+00	1.4130E-12	8.1648E-31	2.3909E-12	9.2604E-13	2.1013E-[illegible]	3.1349E-29	9.6216E-12	5.9951E-16	0.	0.	13

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PT	Y/W	COLLISION FREQUENCY (1/SEC)	ELECTRICAL CONDUCTIVITY (MHO/IN)	UNIT ATTENUATION (DB/IN)
		SIGN. FREQ. (MEGACYC) =		9.7500E+02
1	0.000	3.0885E+10	1.0241E-02	3.3930E-02
2	.100	3.0885E+10	1.0241E-02	3.3930E-02
3	.200	3.0885E+10	1.0241E-02	3.3930E-02
4	.300	3.0885E+10	1.0241E-02	3.3930E-02
5	.400	3.0885E+10	1.0241E-02	3.3931E-02
6	.499	3.0885E+10	1.0251E-02	3.3962E-02
7	.	3.0880E+10	1.0393E-02	3.4424E-02
8	.699	3.0828E+10	1.1588E-02	3.8240E-02
9	.801	3.0486E+10	1.7335E-02	5.6254E-02
10	.907	3.0045E+10	3.2465E-02	9.7411E-02
11	1.031	2.5963E+10	4.9231E-02	1.2159E-01
12	1.195	2.3592E+10	2.5773E-02	5.4420E-02
13	1.419	2.0940E+10	4.6375E-03	7.9316E-03
14	1.719	1.6288E+10	4.0595E-03	4.3819E-03
15	2.141	1.0744E+10	2.5026E-03	1.2239E-03
16	2.683	8.1009E+09	5.2965E-04	1.4841E-04
17	3.242	7.4869E+09	7.5163E-05	1.8043E-05
18	3.764	7.3762E+09	0.	0.

TRANSVERSE
ATTENUATION (DB) = 4.5217E-01

8.37292E-02 1.03530E+00
8.34182E-02 1.11903E+00

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APPENDIX D

COMPARISON BETWEEN MIXED IMPLICIT/EXPLICIT AND FULLY EXPLICIT FINITE DIFFERENCE SCHEMES

APPENDIX D

Comparisons between rocket exhaust plume calculations obtained using the present program (mixed implicit/explicit scheme) and the original AeroChem program[6] (explicit scheme) have been made in order to (i) demonstrate that both schemes yield identical results and (ii) determine the difference in computer run times between the two schemes. The case investigated is a typical solid propellant exhaust containing potassium as the dominant alkali metal impurity. (Typical input data for such a propellant are given in Appendix B.) The programs were run on a CDC 6600 computer. Comparisons between centerline and radial distributions, velocity, temperature and species mole fractions computed via the mixed implicit/explicit and explicit schemes are shown in Figs. D1-D4. The notation $k_1/100$ means that the rate coefficients for $K + HCl \rightarrow KCl + H$ (which is very near equilibrium, even at a pressure of 0.1 atm) was arbitrarily reduced by a factor of 100. This was necessary in order to run the original (explicit) AeroChem program[6] without excessive computer time. Figures D1-D4 show that the two schemes do, in fact, give identical results and we are therefore confident that the new program properly calculates exhaust plume properties.

The principal advantage of the mixed implicit/explicit scheme over the explicit scheme is that stable integration step sizes are much larger. This is clearly demonstrated via the (typical) step size comparison shown in Fig. D5. Thus even though the computational time for each integration step in the present program is about 4 times greater than in the original AeroChem program (primarily because of the matrix inversion subroutine in the present program) the much larger step sizes still give considerable reductions in computer run time.

Table D-I shows a comparison between computer run times for the present and original programs for a typical solid propellant plume at sea level and at 50 kft. For this case, the original AeroChem program cannot be used (in a practical sense) to compute plume properties--primarily because the reaction $K + HCl \rightarrow KCl + H$ is very nearly in equilibrium--resulting in stable integration step sizes of less than about 10^{-8} ft. Thus we record an (essentially) infinite computer run time in Table D-I. However this case can be run using a modified version of the original AeroChem program[6] which keeps the reaction $K + HCl \rightarrow KCl + H$ <u>identically</u> in equilibrium. Run times are noted to be 30 min and 17 min for the sea level and 50 kft cases, respectively. Using the present program reduces these run times to 2.5 and 2.2 min--a very considerable reduction. If, in addition the program is compiled with the 6600 optimized compiler, the run time then is reduced to 1 min for the 50 kft case.

Additional comparisons (made at AFRPL while demonstrating the present program), between the original and present AeroChem programs for other low altitude plumes also showed reductions in computer run times by factors of from 10 to 30.

TABLE D-I

CDC 6600 COMPUTER RUN TIME, MINUTES

10 ft plume; $r_J = 0.25$ ft

		Sea Level	50 kft
Original AeroChem Program[6]	(Explicit)	∞	∞
Original AeroChem Program[6]	(Explicit-modified to put K + HCl → KCl + H in equilibrium)	30	17
Present Program	(Mixed Implicit/Explicit)	2.5	2.2
Present Program	(Mixed Implicit/Explicit using CDC 6600 Optimized Compiler)		1.0

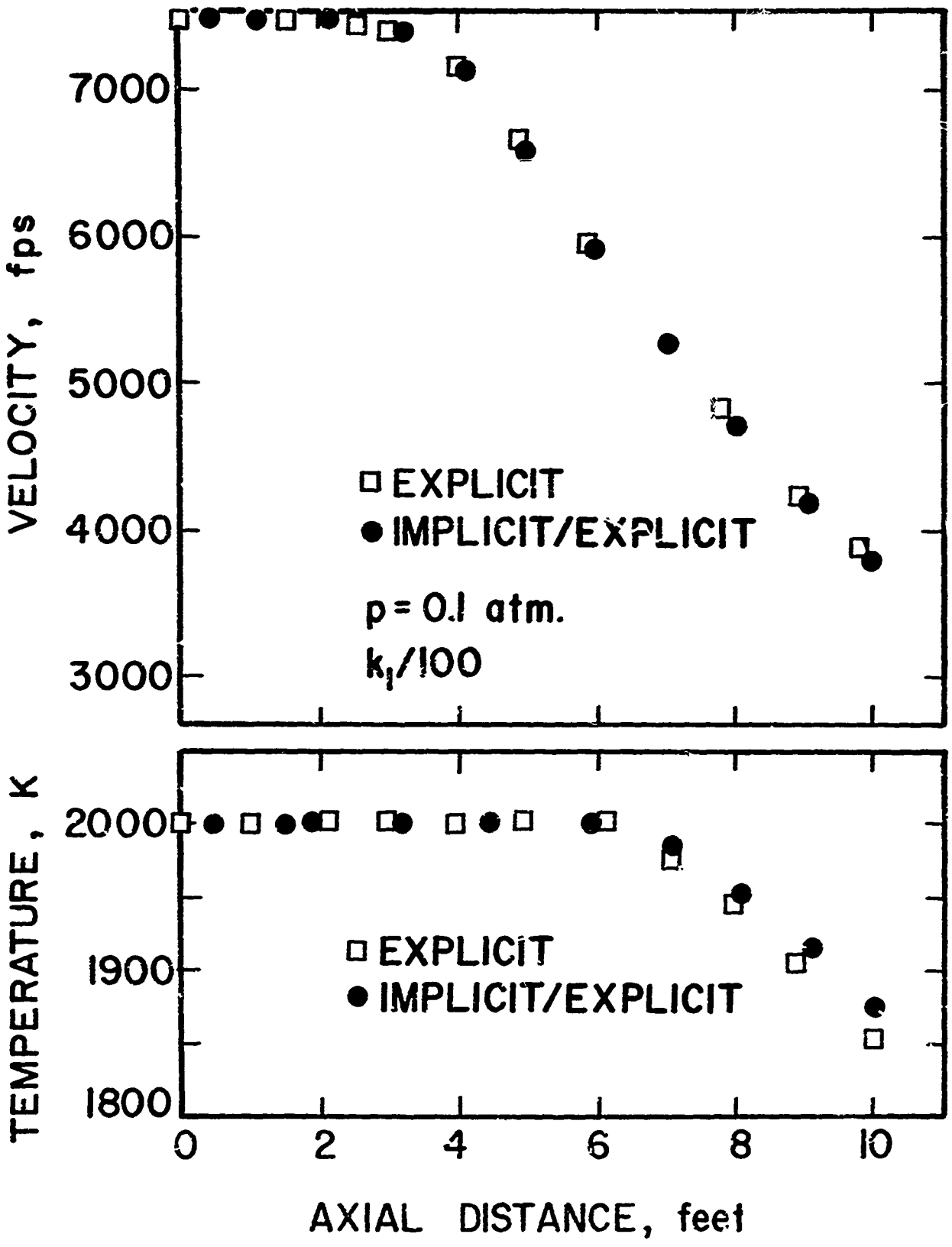

FIG. D1 COMPARISONS BETWEEN CENTERLINE DISTRIBUTIONS OF VELOCITY AND TEMPERATURE COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$r_j = 0.25$ ft

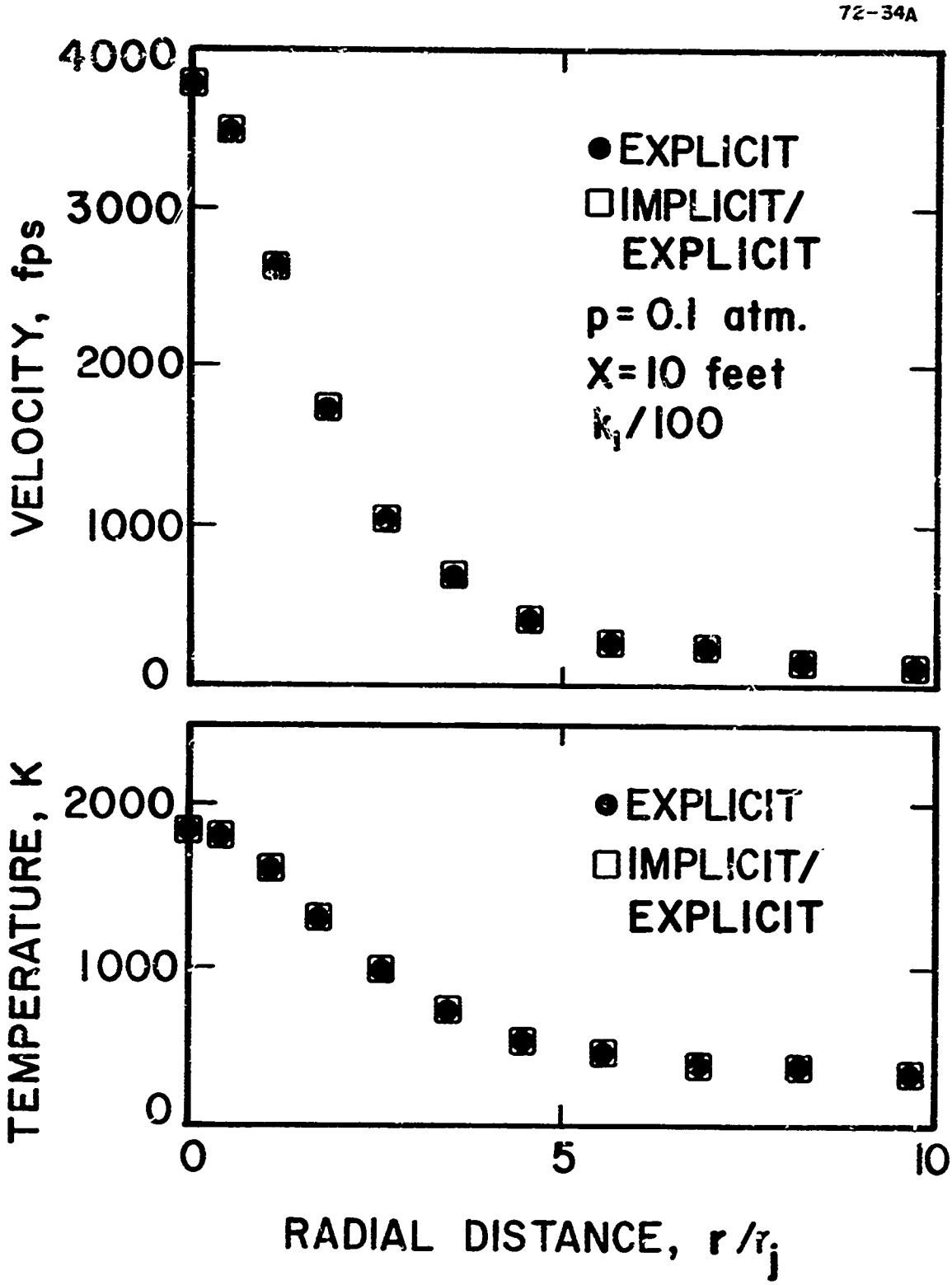

FIG. D2 COMPARISONS BETWEEN RADIAL DISTRIBUTIONS OF VELOCITY AND TEMPERATURE COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$r_j = 0.25$ ft

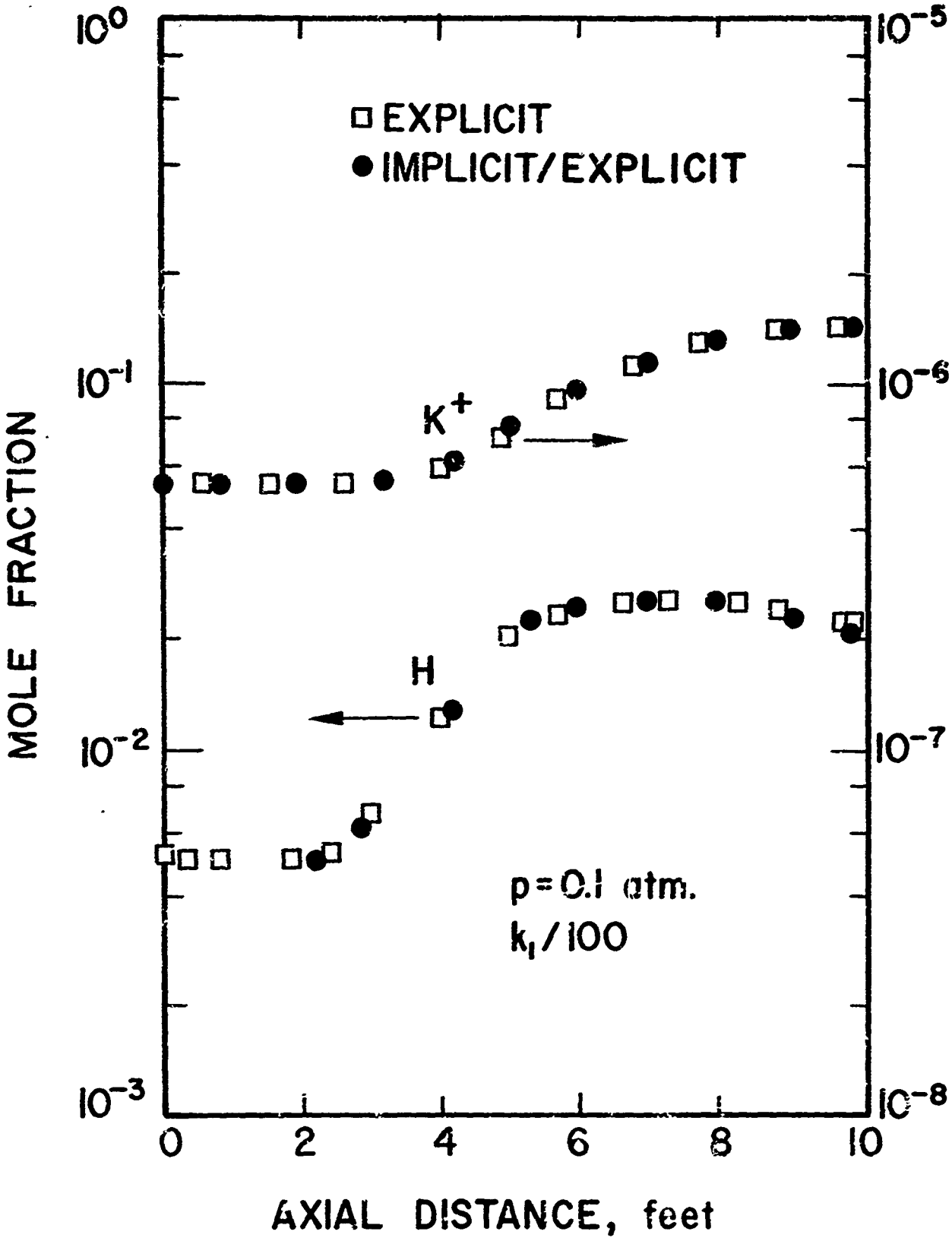

FIG. D3 COMPARISONS BETWEEN CENTERLINE DISTRIBUTIONS OF X_{K^+} AND X_H COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$r_j = 0.25$ ft

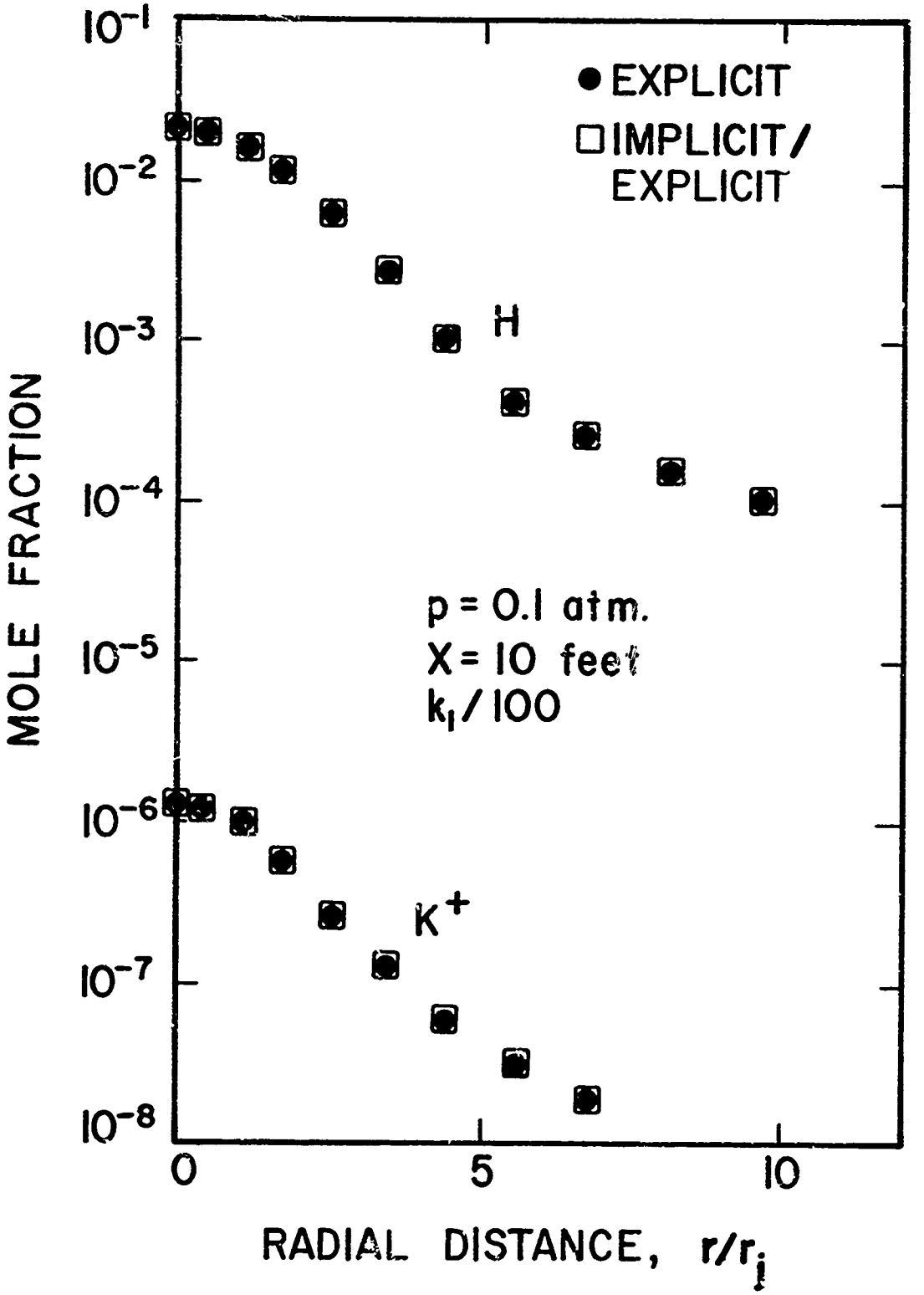

FIG. D4 COMPARISONS BETWEEN RADIAL DISTRIBUTIONS OF X_{K^+} AND X_H COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$r_j = 0.25$ ft

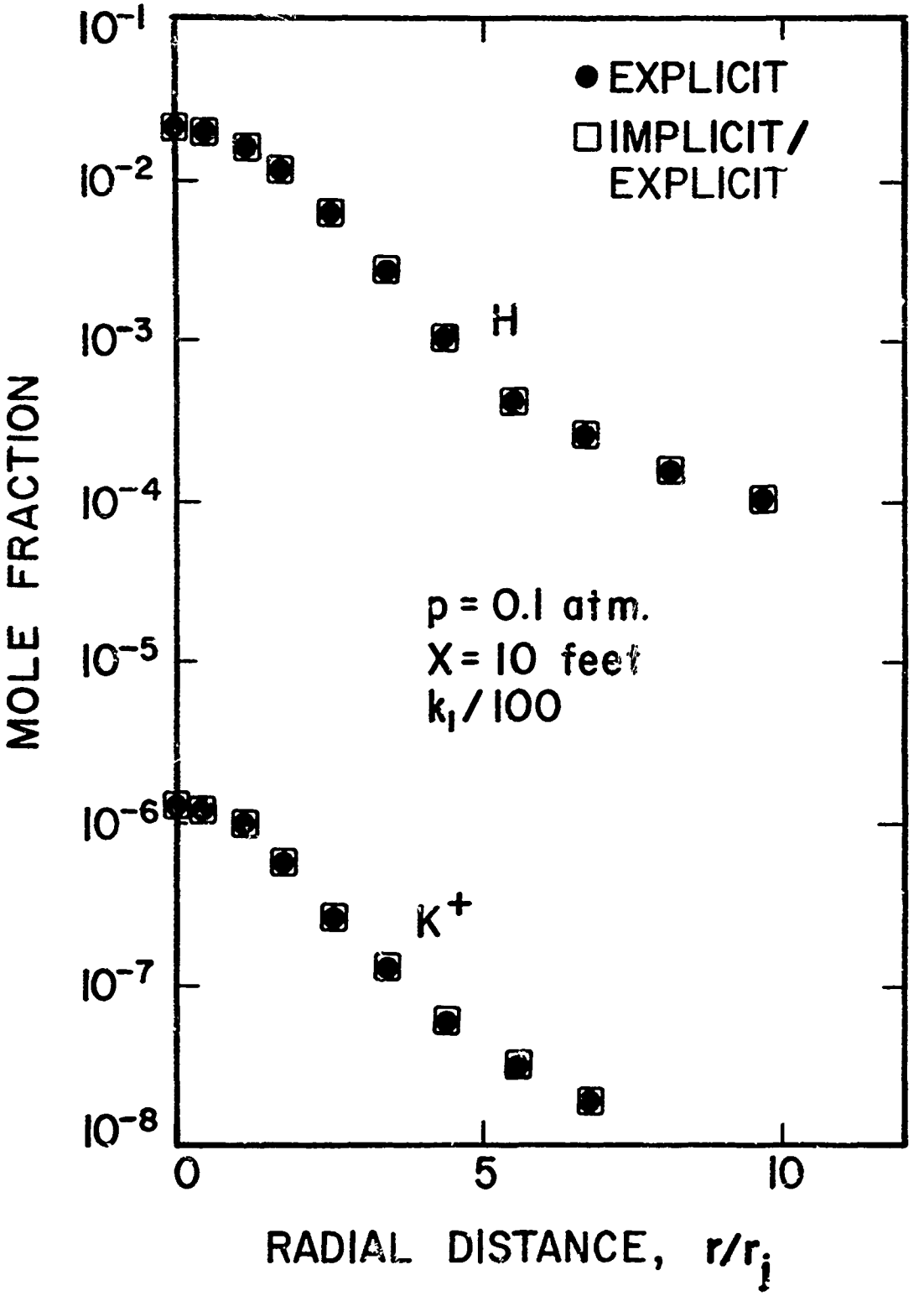

FIG. D4 COMPARISONS BETWEEN RADIAL DISTRIBUTIONS OF X_{K^+} AND X_H COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$r_j = 0.25$ ft