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FAST COMPUTER PROGRAM FOR NONEQUILIBRIUM ROCKET PLUME PREDICTIONS

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AeroChem Research Laboratories, Incorporated

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FOREWORD

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NOMENCLATURE

a	defined by Eq. (15b)
$a_{\frac{1}{2}}$	defined by Eq. (33)
a'	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)
$\overline{K}$	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)
$\overline{r}_{\frac{1}{2}}$	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 ($< \approx 70$ 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.

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*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, $\dot{w}_i$, 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

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

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

$$
\begin{aligned}
(F_i)_{n+1,m} - (\dot{w}_i)_{n+1,m}\,\Delta x/(\rho u)_{n,m}
&= \frac{\Delta x}{m(\Delta\Psi)^3}\left\{\left(\frac{Le}{Pr}a\right)_{n,m+\frac{1}{2}}\left[(F_i)_{n,m+1} - (F_i)_{n,m}\right]\right. \\
&\quad \left. + \left(\frac{Le}{Pr}a\right)_{n,m-\frac{1}{2}}\left[(F_i)_{n,m-1} - (F_i)_{n,m}\right]\right\} \\
&\quad + (F_i)_{n,m}
\end{aligned}
\tag{16a}
$$

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

$$
\begin{aligned}
(F_i)_{n+1,0} - (\dot{w}_i)_{n+1,0}\,\Delta x/(\rho u)_{n,0}
&= \frac{4\Delta x}{(\Delta\Psi)^2}\left(\frac{\mu Le}{Pr}\right)_{n,0}\left[(F_i)_{n,1} - (F_i)_{n,0}\right] \\
&\quad + (F_i)_{n,0}
\end{aligned}
\tag{16b}
$$

Momentum

$$
\begin{aligned}
u_{n+1,m} &= \frac{\Delta x}{m(\Delta\Psi)^3}\left\{a_{n,m+\frac{1}{2}}\left[u_{n,m+1} - u_{n,m}\right]\right. \\
&\quad \left. + a_{n,m-\frac{1}{2}}\left[u_{n,m-1} - u_{n,m}\right]\right\} - \frac{\Delta x}{(\rho u)_{n,m}}\left(\frac{dp}{dx}\right)_{n+1,} + u_{n,m}
\end{aligned}
\tag{17a}
$$

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

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

$$+ u_{n,0} \qquad (17b)$$

<u>Energy</u>

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

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

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

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

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

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

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

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

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

$$
\begin{aligned}
(F_iF_j)_{n+1} &= (F_iF_j)_n + F_{jn}\left[(F_i)_{n+1} - (F_i)_n\right] + F_{in}\left[(F_j)_{n+1} - (F_j)_n\right] \\
&= -\underline{\underline{(F_iF_j)_n}} + \underline{(F_j)_n}\,(F_i)_{n+1} + \underline{(F_i)_n}\,(F_j)_{n+1}
\end{aligned}
\qquad (19)
$$

$$
\begin{aligned}
(F_iF_jF_k)_{n+1} = -\underline{\underline{2(F_iF_jF_k)_n}} &+ \underline{(F_jF_k)_n}\,(F_i)_{n+1} + \underline{(F_iF_k)_n}\,(F_j)_{n+1} \\
&+ \underline{(F_iF_j)_n}\,(F_k)_{n+1}.
\end{aligned}
\qquad (20)
$$

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),

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

---

*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

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

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

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

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

---

* 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) $A + B \rightleftharpoons C + D$

(2) $A + B + M \rightleftharpoons C + M$

(3) $A + B \rightleftharpoons C + D + E$

(4) $A + B \rightleftharpoons C$

(5) $A + M \rightleftharpoons C + D + M$

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

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

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,*

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

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]

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

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,

$$\mu = \rho \epsilon = \alpha 0.00137\ x\ \rho_o \left| u_o - u_e \right| \tag{28a}$$

Developed region,

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

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

Model 4

Initial region,

$$\mu = \rho \epsilon = \alpha 0.00137 x\ \rho_e \left| u_o - u_e \right| \tag{29a}$$

Developed region,

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

Model 5* (Ting/Libby)[19]

Initial region,

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

Developed region,

$$\mu = \rho\,\epsilon = \alpha K\, r_{\frac{1}{2}} \left| u_o - u_e \right| \rho \left(\frac{\rho_o}{\rho}\right)^2 \left(\frac{\text{[illegible]}}{1}\right)^2 \tag{26}$$

Model 6 (Donaldson/Gray)[20]

Initial region,

$$\mu = \rho\,\epsilon = \alpha \overline{K} \left(r_{\frac{1}{2}} - r_i\right) \rho \left| u_o - u_e \right| / 2 \tag{31a}$$

$$\begin{aligned} &\text{For } M_{\frac{1}{2}} \leq 1.2 \quad \overline{K} = 0.0468 + M_{\frac{1}{2}} \left[- 0.0460\, M_{\frac{1}{2}} + 0.0256\, M_{\frac{1}{2}}^2 \right] \\ &\phantom{\text{For }} M_{\frac{1}{2}} > 1.2 \quad \overline{K} = 0.0248 \end{aligned} \tag{32}$$

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,

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

where $W_{\frac{1}{2}}$ and $T_{\frac{1}{2}}$ are evaluated at the half radius. In Eq. (31a), r_1 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,

$$\mu = \rho\,\epsilon = \alpha \overline{K}\, r_{\frac{1}{2}} \rho \left| u_o - u_e \right| / 2 \tag{31b}$$

---

*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

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

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	$1.45\ (10^{-23}) v_e + 8.7\ (10^{-16})$

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

C. Transverse Radar Attenuation

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

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,

$$A = 2 \int_0^{\infty} a' \, dr \qquad \text{db} \qquad (38)$$

where r is in inches.

D. Electrical Conductivity

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

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

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*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
	6-10	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

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*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) Pressure Coefficients (see Section II)	E10.3
	31-40	c_1 (atm/ft)	E10.3
	41-50	c_2 (atm/ft^2)	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	$\Delta\Psi$, $\left(\frac{\text{lbm}}{32.2}\ \text{sec}^{-1}\right)^{\frac{1}{2}}$ 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	E10.3
	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.

Card No.	Column	Description	Format
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, $\left[\frac{\mathrm{lbm}}{32.2}\ \mathrm{sec}^{-1}\right]^{\frac{1}{2}}$
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).

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APPENDIX A

A FAST COMPUTER PROGRAM FOR NONEQUILIBRIUM ROCKET PLUME PREDICTIONS

Fortran Listing

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PROGRAM     MAIN                                  CDC 6600 FTN V3.0-P312 OPT=2  08/07/72  14.54.49.     PAGE    1

            PROGRAM MAIN   (INPUT,OUTPUT,PUNCH,TAPE5=INPUT,TAPE6=OUTPUT,          MAIN       2
           1     TAPE7=PUNCH)                                                     MAIN       3
      C*******************************************************************        MAIN       4
      C***********                                                      **        MAIN       5
      C***********              A FAST COMPUTER PROGRAM                 **        MAIN       6
      C***********       FOR NONEQUILIBRIUM ROCKET PLUME PREDICTIONS    **        MAIN       7
      C***********           AEROCHEM RESEARCH LABORATORIES             **        MAIN       8
      C***********                PRINCETON, N. J.                      **        MAIN       9
      C***********                                                      **        MAIN      10
      C*******************************************************************        MAIN      11
      C                                                                           MAIN      12
      C                                                                           MAIN      13
            DIMENSION A(30),RHO(30),Y(30),T(30),PSI(30),RT(30),SUM(30),AR(25),    MAIN      14
           1HSTAT(30),H(25,30),ALPHA(25,30),RALPHA(25,30),CP(25,30),SIGMA(30),    MAIN      15
           2          WTMOLE(25),CPBAR(30),C(25,9),AID(25),ETA(30),RATIO(30),    MAIN      16
           3RU(30),U(30),TITLE(12),XLF(10),XMU(30)           ,G(25),WIMIX(30),    MAIN      17
           4RC(40,3),IRRR(40,5),WP(25),WM(25),WDOT(25,30),SAVET(30),SAVEU(30),    MAIN      18
           5          IRR(40),FREQ(30),SAVEA(25,30),              PC(4),ZID(5),    MAIN      19
           6          ECC(30),HOUT(30),YOUT(30),RHOOUT(30),XMUOUT(30),XLT(30),    MAIN      20
           7T4(30),TEDG(30),IRT(40),RP(40,30),RM(40,30)                           MAIN      21
           8 ,CM(25,25,26), QX(25,26) ,CM1(25,25),QX1(25)                          MAIN      22
            DIMENSION XAME(6), ISAVE(6), FREQA(6), ALOG(50,6)                     MAIN      23
            DIMENSION TTB(30)     ,CPTB(25,30),HTB(25,30),UTB(25,30),HF(25)       MAIN      24
            COMMON  A       , RHO     , Y       , T       , PSI     , RT          MAIN      25
            COMMON  SUM     , AR      , HSTAT   , H       , ALPHA   , RALPHA      MAIN      26
            COMMON  CP      , SIGMA             , WTMOLE  , CPBAR   , C           MAIN      27
            COMMON  AID     , ETA     , RATIO   , RU      , U       , TITLE       MAIN      28
            COMMON  XLF     , XMU     ,           G       , WIMIX   , WDOT        MAIN      29
            COMMON  SAVEU   , SAVET   , WM      , WP      , RC                    MAIN      30
            COMMON            SAVEA   ,           PC      , X       , XMAX        MAIN      31
            COMMON  PRNT    , DXMIN   , DX      , FOL     , DELPSI  , I           MAIN      32
            COMMON  XR2     , P       , ZID     , FREQ    , ECC     , DPDX        MAIN      33
            COMMON  YOUT    , HOUT    , RHOOUT  , IRRR    , IRR     , IFINIS      MAIN      34
            COMMON  IPAGE   , NPSI    , MY      , NS      , NR      , IEDGE       MAIN      35
            COMMON  ITURB   , IPRESS  , NPSI    , ITEST   , ITER    , IECC        MAIN      36
            COMMON  IRT     , XMUOUT  , XLT     , T4      , TEDG    , IOUT        MAIN      37
            COMMON  IOUT1   , IOUT2   ,RP       , RM      , ISAVE   , IPUNCH      MAIN      38
            COMMON IKINET,NFREQA,ALOG,FREQA,Q0100,Q0200,Q0300,Q0400               MAIN      39
      C**** SETTING XAME FOR THOSE SPECIES INVOLVED IN COLLISION FREQ. CALC.      MAIN      40
            DATA XAME(1)/6HCO     /                                               MAIN      41
            DATA XAME(2)/6HCO2    /                                               MAIN      42
            DATA XAME(3)/6HH2O    /                                               MAIN      43
            DATA XAME(4)/6HH2     /                                               MAIN      44
            DATA XAME(5)/6HN2     /                                               MAIN      45
            DATA XAME(6)/6HHCL    /                                               MAIN      46
            AV=6.025E23                                                           MAIN      47
          4 IFINIS=0                                                              MAIN      48
            DO 9999 I=1,8596                                                      MAIN      49
       9999 A(I)=0.0                                                              MAIN      50
            DO 300 I = 1,6                                                        MAIN      51
        300 ISAVE(I) = 0                                                          MAIN      52
            R=82.06                                                               MAIN      53
            READ  (5,333)(TITLE(I),I=1,12)                                        MAIN      54
      C     NS= NO. OF SPECIES                                                    MAIN      55
      C     NR= NO. OF REACTIONS                                                  MAIN      56
```

```
      READ(5,100) MPSI,NS,ITURB,IH ,IOUT1,IOUT2,IPUNCH,ITIME,IPRESS,NI   MAIN  57
      READ (5,111)   (FREQA(I), I=1,6)                                   MAIN  58
      DO 113 I=1,6                                                       MAIN  59
      IF (FREQA(I)) 113, 114, 113                                        MAIN  60
  113 CONTINUE                                                           MAIN  61
      I=7                                                                MAIN  62
  114 NFREQA = I-1                                                       MAIN  63
      NPSI=MPSI-1                                                        MAIN  64
      READ  (5,1000)X,XMAX,PRNT,XLF(1),SIGMA(1),RJ,XN2                   MAIN  65
      DX=0.1*RJ                                                          MAIN  66
C     INPUT MINIMUM STEPSIZE LIMIT (DXMIN)                               MAIN  67
      READ(5,1000) DXMIN,FOL,      PC(1),PC(2),PC(3),PC(4)               MAIN  68
      READ  (5,1000)P,T(1),T(MPSI),U(1),U(MPSI),DELPSI,TKINET            MAIN  69
      IF(TKINET.EQ.0.0) TKINET = 400.0                                   MAIN  70
C**** THE VALUE OF 30 SECONDS IS TO ALLOW FOR COMPILE TIME                MAIN  71
      ILIMIT = 60*ITIME-30                                               MAIN  72
      IDIFFT = 0                                                         MAIN  73
      CALL TICK(ISECST)                                                  MAIN  74
      IF((ISECST+60*ITIME).GT.86400) IDIFFT = 86400-ISECST               MAIN  75
      UNIT = U(1)                                                        MAIN  76
      IO77 = 2                                                           MAIN  77
      USUB01 = 0.0                                                       MAIN  78
C     TURBULENCE MODELS                                                  MAIN  79
      IF (ITURB - 3) 8600,9010,9010                                      MAIN  80
 8600 IF (ITURB - 1) 9011,9010,9011                                      MAIN  81
 9010 USUB01 = 0.95*   (U(1)-U(MPSI)) + U(MPSI)                          MAIN  82
 9011 CONTINUE                                                           MAIN  83
      IF(DELPSI) 3011,3012,3011                                          MAIN  84
 3012 READ  (5,1000)(ALPHA(J,1),J=1,NS)                                  MAIN  85
      READ  (5,1000)(ALPHA(J,MPSI),J=1,NS)                               MAIN  86
      MMOD=MPSI-2                                                        MAIN  87
      DO 4001 I=1,MMOD                                                   MAIN  88
      T(I)=T(1)                                                          MAIN  89
      U(I)=U(1)                                                          MAIN  90
      DO 4001 J=1,NS                                                     MAIN  91
 4001 ALPHA(J,I)=ALPHA(J,1)                                              MAIN  92
      DO 4002 J=1,NS                                                     MAIN  93
 4002 ALPHA(J,NPSI)=ALPHA(J,MPSI)                                        MAIN  94
      GO TO 3015                                                         MAIN  95
 3011 READ  (5,1000)(T(I),I=1,MPSI)                                      MAIN  96
      READ  (5,1000)(U(I),I=1,MPSI)                                      MAIN  97
      DO 7 I=1,MPSI                                                      MAIN  98
    7 READ  (5,1000)(ALPHA(J,I),J=1,NS)                                  MAIN  99
C     NEW THERMO DATA DATA INPUT IN JANNAF TABLE FORM                    MAIN 100
 3015 DO 1991 I=1,NS                                                     MAIN 101
      READ(5,222) AID(I),WTMOLE(I),HF(I)                                 MAIN 102
      DO 10 IT=1, N1,2                                                   MAIN 103
      READ(5,102) TTB(IT),  CPTB(I,IT),GTB(I,IT),HTB(I,IT)               MAIN 104
     1   ,TTB(IT+1)   ,CPTB(I,IT+1), GTB(I,IT+1),HTB(I,IT+1)             MAIN 105
      GTB(I,IT)= -GTB(I,IT)*TTB(IT)   +HF(I) *1000.                      MAIN 106
      GTB(I,IT+1)= -GTB(I,IT+1)*TTB(IT+1)   +HF(I)*1000.                 MAIN 107
      HTB(I,IT)=(HTB(I,IT)+HF(I))*1000.                                  MAIN 108
      HTB(I,IT+1)=(HTB(I,IT+1)+ HF(I))*1000.                             MAIN 109
   10 CONTINUE                                                           MAIN 110
      IF(WTMOLE(I)-1.0) 1972,1991,1991                                   MAIN 111
```

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 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
      IRRR(I,J)=0                                                          MAIN     121
      DO 1993 L=1,NS                                                       MAIN     122
      IF(7ID(J)-AID(L)) 1993,1994,1993                                     MAIN     123
 1994 IRRR(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     142
      XLE(I)=XLE(1)                                                        MAIN     143
   20 SIGMA(I)=SIGMA(1)                                                    MAIN     144
      DO 90 I=NPSI,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,NT)                             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)+PS MAIN 196
     1I(I-2)/U(I-2))/1.5/RHO(I))                                        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) - USUP01) 9000,9000,9001                                 MAIN 204
C     MODEL 6 COMMON CALCULATIONS                                       MAIN 205
 8011 QQ1 = (U(1)+U(MPSI))/2.0                                          MAIN 206
      DO 8012 I=2,MPSI                                                  MAIN 207
      IF ((QQ1-U(I))*(QQ1-U(I-1))) 8013,8013,8012                       MAIN 208
 8012 CONTINUE                                                          MAIN 209
 8013 QQ2 = (QQ1-U(I-1))/(U(I)-U(I-1))                                  MAIN 210
      QQ100 = Y(I-1)+(Y(I)-Y(I-1))*QQ2                                  MAIN 211
      QQ30 = T(I-1)+(T(I)-T(I-1))*QQ2                                   MAIN 212
      QQ3 = CPBAR(I-1)+(CPBAR(I)-CPBAR(I-1))*QQ2                        MAIN 213
      QQ4 = 1.0/(WTMIX(I-1)+(WTMIX(I)-WTMIX(I-1))*QQ2)                  MAIN 214
      QQ5 = 89517.501/QQ4                                               MAIN 215
      QQ6 = QQ3/(QQ3-QQ5)                                               MAIN 216
      QQ7 = SQRT(QQ6*QQ5*QQ30)                                          MAIN 217
      QQ300 = QQ1/QQ7                                                   MAIN 218
      QQ8 = (ABS(U(1)-U(MPSI)))/2.0                                     MAIN 219
      IF (QQ300-1.2) 8014,8014,8015                                     MAIN 220
 8014 QQ400 =(.0468+QQ300*((QQ300*(-.0460))+.0256*(QQ300*QQ300)))*XK2   MAIN 221
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```
      GO TO 8016                                                      MAIN
 8015 QQ400 = .0248*XK2                                               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 IO77 = 9                                                        MAIN
      USUB01 = 0.0                                                    MAIN
      WRITE (6,9900)X                                                 MAIN
 9001 LL = ITURB + IO77                                               MAIN
C      EDDY VISCOSITY  MODELS                                         MAIN
      GO TO (91,99,8666,78,8667,8668,9003,91,99,45,78,26,33,70),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(I)*U(I)-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(1)*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, GTR,SDT,HDT,AX)                            MAIN      331
```

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      G(I)=AX                                                            MAIN  332
  855 CONTINUE                                                           MAIN  333
C     REACTION CALCULATION                                               MAIN  334
C     REACTION KINETICS CONTINUE DOWN TO 400 DEGREES K                   MAIN  335
C        UNLESS TKINET IS SET TO A VALUE OTHER THAN 400. K               MAIN  336
C     REACTION KINETICS FOR ALL REACTIONS CONTINUE DOWN TO TKINET        MAIN  337
      IF(T(L)-TKINET) 3256,3256,3259                                     MAIN  338
 3259 CONTINUE                                                           MAIN  339
      DO 862 I=1,NR                                                      MAIN  340
      RP(I,L)=0.0                                                        MAIN  341
      RM(I,L)=0.0                                                        MAIN  342
      KK = IRT(I)                                                        MAIN  343
C     REACTION CONSTANT TYPE                                             MAIN  344
      GO TO (841,842,843,844,845,846,847),KK                             MAIN  345
  841 RATE=RC(I,1)*AV                                                    MAIN  346
      GO TO 849                                                          MAIN  347
  842 RATE=RC(I,1)/T(L)*AV                                               MAIN  348
      GO TO 849                                                          MAIN  349
  843 RATE=RC(I,1)/T(L)/T(L)*AV                                          MAIN  350
      GO TO 849                                                          MAIN  351
  844 RATE=RC(I,1)/ROOTT*AV                                              MAIN  352
      GO TO 849                                                          MAIN  353
  845 RATE=RC(I,1)*EXP(RC(I,3)/RRT)*AV                                   MAIN  354
      GO TO 849                                                          MAIN  355
  846 RATE=RC(I,1)*EXP(RC(I,3)/RRT)/T(L)*AV                              MAIN  356
      GO TO 849                                                          MAIN  357
  847 RATE=RC(I,1)/T(L)/ROOTT*AV                                         MAIN  358
  849 CONTINUE                                                           MAIN  359
      K=IRR(I)                                                           MAIN  360
C     TYPE OF REACTION                                                   MAIN  361
      GO TO(864,865,866,870,871,834,835,836,837,838),K                   MAIN  362
  870 J1=IRRR(I,1)                                                       MAIN  363
      J2=IRRR(I,2)                                                       MAIN  364
      J3=IRRR(I,3)                                                       MAIN  365
      E = (G(J1)+G(J2)-G(J3))/RRT                                        MAIN  366
      IF(ABS(E).LT.80.0) GO TO 700                                       MAIN  367
      IF(E.LT.0.0) E= EXP(-80.0)                                         MAIN  368
      IF(E.GT.0.0) E = EXP(80.0)                                         MAIN  369
      GO TO 701                                                          MAIN  370
700   E = EXP(E)                                                         MAIN  371
701   CONTINUE                                                           MAIN  372
       CRR=RATE*RHOOUT(L)                                                MAIN  373
      RP(I,L)=CRR*RHOOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)                      MAIN  374
      RM(I,L)=CRR*ALPHA(J3,L)/E/R/T(L)                                   MAIN  375
      DO 771 J=1, 3                                                      MAIN  376
      SIGN=1.0                                                           MAIN  377
      IF (J.GT.2) SIGN=-1.0                                              MAIN  378
      IROW= IRRR(I,J)                                                    MAIN  379
      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)             MAIN  380
      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)             MAIN  381
      CM(IROW,J3,L)= CM(IROW,J3,L) -SIGN*RM(I,L)/ALPHA(J3,L)             MAIN  382
  771 QX(IROW,L)= QX(IROW,L)+ SIGN*RP(I,L)                               MAIN  383
      GO TO 868                                                          MAIN  384
  871 J1=IRRR(I,1)                                                       MAIN  385
      J2=25                                                              MAIN  386
```

```
      J3=IRRR(I,3)
      J4=IRRR(I,4)
      E = (G(J1)-G(J3)-G(J4))/RRT
      IF( ABS(E).LT.80.0) GO TO 702
      IF( E.LT.0.0) E = EXP(-80.0)
      IF( E.GT.0.0) E = EXP(80.0)
      GO TO 703
  702 E = EXP(E)
  703 CONTINUE
       CRR=RATE*RHOOUT(L)*RHOOUT(L)*WTMIX(L)
      RP(I,L)=CRR*ALPHA(J1,L)
      RM(I,L)=CRR*R*T(L)*RHOOUT(L)*ALPHA(J3,L)*ALPHA(J4,L)/E
      DO 772 J=1, 4
      SIGN=1.0
      IF (J.GT.2) SIGN=-1.0
      IROW= IRRR(I,J)
      IF(J.EQ.2) IROW=25
      CM(IROW,J1,L)= CM(IROW,J1,L)+SIGN*CRR
      CM(IROW,J3,L)= CM(IROW,J3,L)-SIGN*RM(I,L)/ALPHA(J3,L)
      CM(IROW,J4,L)= CM(IROW,J4,L)-SIGN*RM(I,L)/ALPHA(J4,L)
  772 QX(IROW,L)= QX(IROW,L)- SIGN*RM(I,L)
      GO TO 867
  864 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      J4=IRRR(I,4)
      E = (G(J1)+G(J2)-G(J3)-G(J4))/RRT
      IF(ABS(E).LT.80.0) GO TO 704
      IF(E.LT.0.0) E = EXP(-80.0)
      IF(E.GT.0.0) E = EXP(80.0)
      GO TO 705
  704 E = EXP(E)
  705 CONTINUE
       CRR=RATE*RHOOUT(L)*RHOOUT(L)
      RP(I,L)=CRR*ALPHA(J1,L)*ALPHA(J2,L)
      RM(I,L)=CRR*ALPHA(J3,L)*ALPHA(J4,L)/E
      DO 773 J=1, 4
      SIGN=1.0
      IF (J.GT.2) SIGN=-1.0
      IROW= IRRR(I,J)
      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)
      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)
      CM(IROW,J3,L)= CM(IROW,J3,L) -SIGN*RM(I,L)/ALPHA(J3,L)
      CM(IROW,J4,L)= CM(IROW,J4,L)-SIGN*RM(I,L)/ALPHA(J4,L)
  773 QX(IROW,L)= QX(IROW,L)+ SIGN*(RP(I,L)-RM(I,L))
      GO TO 867
  865 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      E = (G(J1)+G(J2)-G(J3))/RRT
      IF(ABS(E).LT.80.0) GO TO 706
      IF(E.LT.0.0) E=EXP(-80.0)
      IF(E.GT.0.0) E=EXP(80.0)
      GO TO 707
  706 E = EXP(E)
```

```
      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 OX(IROW,L)= OX(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=PATE*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 OX(IROW,L)= OX(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*PHOOUT(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
            IPOW= 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 OX(IROW,L)= OX(IPOW,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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PROGRAM   MAIN                                CDC 6600 FTN V3.0-P312 OPT=2  08/07/72  12.54.49.      PAGE     10
                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 OX(IROW,L)= OX(IROW,L)+ SIGN* RP(I,L)
C     CALCULATE WDOT
  861 WP(J5)=WP(J5)+RP(I,L)
      WM(J5)=WM(J5)+RM(I,L)
  867 WP(J4)=WP(J4)+RP(I,L)
      WM(J4)=WM(J4)+RM(I,L)
  868 WP(J3)=WP(J3)+RP(I,L)
      WM(J3)=WM(J3)+RM(I,L)
      WP(J2)=WP(J2)+RM(I,L)
      WM(J2)=WM(J2)+RP(I,L)
      WP(J1)=WP(J1)+RM(I,L)
      WM(J1)=WM(J1)+RP(I,L)
  862 CONTINUE
 3256 CONTINUE
      DO 897 J=1,NS
  897 WDOT(J,L)=(WP(J)-WM(J))/RHOOUT(L)/U(L)
  899 CONTINUE
      IOUT=IOUT+1
      CALL SSWTCH(1,K000FX)
       GO TO(62,63),K000FX
   62 EOUT=RHO(1)*ALPHA(IECC,1)*3.108E23
      PRINT 61,X,T(1),U(1),EOUT,IOUT
   61 FORMAT(3H0X=1PE15.7,3H T=1PE15.7,3H U=1PE15.7,6H E/CC=1PE15.7,7H S
     1TEPS=I5)
   63 IF(IFINIS) 64,69,64
   64 CALL SSWTCH(3,K000FX)
       GO TO(66,65),K000FX
   65 IF(X-XMAX) 67,66,66
   67 IF(PRNT-PCNT) 69,69,68
   68 CONTINUE
      GO TO 5
   66 IFINIS=2
   69 CALL OUTPUT
      PCNT=0.0
      IF(IFINIS-1) 5,5,6
C      CHECK DIFFUSION STEP SIZE
    5 XD=DELPSI*DELPSI*SIGMA(1)/XMU(1)/XLE(1)/12.0 *FDL
      DO 511 I=2,NPSI
      DUMMY=A(I+1)+A(I-1)+A(I)+A(I)
      DUMMY=PSI(I)*DELPSI*DELPSI*SIGMA(I)/XLE(I)/DUMMY/1.5*FDL
  511 XD=AMIN1(XD,DUMMY)
      DX=AMIN1(DX,XD)
      DO 101 I=2,NPSI
      EX1=PSI(I)*DELPSI**2/DX
      EX11=.5*(A(I)+A(I+1))
      EX12=.5*(A(I)+A(I-1))
C     INTEGRATE MOMENTUM EQUATION
      PU(I)=(EX11*(U(I+1)-U(I))+EX12*(U(I-1)-U(I)))/EX1+U(I)
      PU(I)=PU(I)-DX*DPDX/RHO(I)/U(I)
      EX3=0.0
      EX4=0.0
      DO 21 J=1,NS
      EX3=EX3+H(J,I)*WDOT(J,I)
   21 EX4=EX4+CP(J,I)*(ALPHA(J,I+1)-ALPHA(J,I-1))
      EX2=EX1*CPRAR(I)
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```
      EX5=XLE(I)*A(I)/SIGMA(I)                                          MAIN       607
      EX6=.5*(EX5+XLE(I+1)*A(I+1)/SIGMA(I+1))                           MAIN       608
      EX7=.5*(EX5+XLE(I-1)*A(I-1)/SIGMA(I-1))                           MAIN       609
      EX8=CPBAR(I)*A(I)/SIGMA(I)                                        MAIN       610
      EX9=.5*(EX8+CPBAR(I+1)*A(I+1)/SIGMA(I+1))                         MAIN       611
      EX10=.5*(EX8+CPBAR(I-1)*A(I-1)/SIGMA(I-1))                        MAIN       612
      EX14=EX4*EX5/4.0                                                  MAIN       613
C     INTEGRATE ENERGY EQUATION                                         MAIN       614
      RT(I)=(U(I+1)-U(I-1))**2*A(I)/EX2/4.0+DX*DPDX/RHO(I)/CPBAR(I)+T(I) MAIN      615
     1+((EX9+EX14)*T(I+1)+(EX10-EX14)*T(I-1)-(EX9+EX10)*T(I))/EX2-EX3*DX MAIN      616
     2/CPBAR(I)                                                         MAIN       617
      RHOUIX=DX/(RHOOUT(I)* U(I))                                       MAIN       618
C     INTEGRATE SPECIES EQUATIONS                                       MAIN       619
      DO 41 J=1,NS                                                      MAIN       620
   41 QX1(J)      =(EX6*(ALPHA(J,I+1)-ALPHA(J,I))+EX7*(ALPHA(J,I-1)-ALPHA MAIN     621
     1(J,I)$)/EX1+ALPHA(J,I)+  QX(J,I)*RHOUIX                           MAIN       622
      DO 781 M=1,NS                                                     MAIN       623
      DO 781 N=1,NS                                                     MAIN       624
      CM1(M,N)= CM(M,N,I)*RHOUIX                                        MAIN       625
      IF (M.EQ.N) CM1(M,N)=CM1(M,N) +1.0                                MAIN       626
  781 CONTINUE                                                          MAIN       627
      CALL SLDP(QX1,CM1,NS)                                             MAIN       628
  785 FORMAT (1H , 2I5)                                                 MAIN       629
      DO 782 J=1, NS                                                    MAIN       630
  782 RALPHA(J,I)= QX1(J)                                               MAIN       631
  101 CONTINUE                                                          MAIN       632
      WRITE(6,786) DX,X                                                 MAIN       633
  786 FORMAT(1H ,1P2E12.5)                                              MAIN       634
      EX3=4.0*XMU(1)*DX/DELPSI/DELPSI                                   MAIN       635
      RHOUIX=DX/(RHOOUT(1)* U(1))                                       MAIN       636
C     COMPUTE U AT CENTER LINE                                          MAIN       637
      RU(1)=EX3*(U(2)-U(1))+U(1)-DX*DPDX/RHO(1)/U(1)                    MAIN       638
      EX4=0.0                                                           MAIN       639
      DO 200 J=1,NS                                                     MAIN       640
      EX4=EX4+H(J,1)*WDOT(J,1)                                          MAIN       641
      RALPHA(J,MPSI)=ALPHA(J,MPSI)                                      MAIN       642
  200 QX1(J)      =EX3*XLF(1)*(ALPHA(J,2)-ALPHA(J,1))/SIGMA(1)+ALPHA(J,1) MAIN     643
     1+  QX(J,1)*RHOUIX                                                 MAIN       644
      DO 783 M=1,NS                                                     MAIN       645
      DO 783 N=1,NS                                                     MAIN       646
      CM1(M,N)= CM(M,N,1)*RHOUIX                                        MAIN       647
      IF (M.EQ.N) CM1(M,N)=CM1(M,N) +1.0                                MAIN       648
  783 CONTINUE                                                          MAIN       649
      CALL SLDP(QX1,CM1,NS)                                             MAIN       650
      DO 784 J=1, NS                                                    MAIN       651
C     COMPUTE-SPECIES AT CENTER LINE                                    MAIN       652
  784 RALPHA(J,1)= QX1(J)                                               MAIN       653
C     CALCULATE TEMP. AT CENTER LINE                                    MAIN       654
      RT(1)=EX3*(T(2)-T(1))/SIGMA(1)+T(1)+DX*DPDX/RHO(1)/CPBAR(1)       MAIN       655
     1-EX4*DX/CPBAR(1)                                                  MAIN       656
      RT(MPSI)=T(MPSI)                                                  MAIN       657
      IF(IEDGE) 230,231,230                                             MAIN       658
C     COMPUTE TEMP. AND U AT EDGE                                       MAIN       659
  230 RU(MPSI)=U(MPSI)-DX*DPDX/RHO(MPSI)/U(MPSI)                        MAIN       660
      RT(MPSI)=T(MPSI)+DX*DPDX/RHO(MPSI)/CPBAR(MPSI)                    MAIN       661
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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     [illegible]
      RU(I)=U(NPSI)                                                MAIN     [illegible]
      U(I)=U(NPSI)                                                 MAIN     [illegible]
      SAVET(I)=T(NPSI)                                             MAIN     [illegible]
```

```
           T(I)=T(NPSI)                                                   MAIN
           RT(I)=T(NPSI)                                                  MAIN
           DO 1102 J=1,NS                                                 MAIN
           SAVEA(J,I)=ALPHA(J,NPSI)                                       MAIN
           ALPHA(J,I)=ALPHA(J,NPSI)                                       MAIN
      1102 RALPHA(J,I)=ALPHA(J,NPSI)                                      MAIN
      1101 CONTINUE                                                       MAIN
           GO TO 2000                                                     MAIN
      1500 IFINIS=0                                                       MAIN
           DELPSI=DELPSI+DELPSI                                           MAIN
           DO 1600 I=1,MINIT                                              MAIN
           DO 1650 J=1,NS                                                 MAIN
      1650 ALPHA(J,I)=ALPHA(J,2*I-1)                                      MAIN
           T(I)=T(2*I-1)                                                  MAIN
      1600 U(I)=U(2*I-1)                                                  MAIN
           MPSI=MINIT                                                     MAIN
           NPSI=MPSI-1                                                    MAIN
           DO 1700 I=MINIT,29                                             MAIN
           DO 1750 J=1,NS                                                 MAIN
           ALPHA(J,I)=ALPHA(J,MPSI)                                       MAIN
      1750 RALPHA(J,I)=ALPHA(J,MPSI)                                      MAIN
           T(I)=T(MPSI)                                                   MAIN
           RT(I)=T(MPSI)                                                  MAIN
           U(I)=U(MPSI)                                                   MAIN
      1700 RU(I)=U(MPSI)                                                  MAIN
           DO 1800 I=2,29                                                 MAIN
      1800 PSI(I)=PSI(I-1)+DELPSI                                         MAIN
           ITER=0                                                         MAIN
           ISTEP=0                                                        MAIN
           GO TO 2000                                                     MAIN
      8000 WRITE (6,8001)                                                 MAIN
      8001 FORMAT(68H1NEGATIVE PARAMETER - NOT CORRECTED BY REPEATED HALVING  MAIN
          1OF STEP SIZE)                                                  MAIN
           IFINIS=2                                                       MAIN
           GO TO 69                                                       MAIN
      2000 CONTINUE                                                       MAIN
           CALL TICK(ISECS)                                               MAIN
           IELAPS = ISECS-ISECST                                          MAIN
           IF(IELAPS.LT.0) IELAPS = IDIFFT + ISECS                        MAIN
           IF(IELAPS.GE.ILIMIT) GO TO 6                                   MAIN
           GO TO 2                                                        MAIN
       100 FORMAT(14I5)                                                   MAIN
       102 FORMAT(8F10.4)                                                 MAIN
       111 FORMAT (7(1PE10.3))                                            MAIN
       222 FORMAT(A6,7E10.3)                                              MAIN
       333 FORMAT(12A6)                                                   MAIN
       444 FORMAT(A6,1X,A6,8X,A6,1X,A6,1X,A6,7X,I2,I1,E8.2,F4.1,F9.1)     MAIN
       555 FORMAT(7(1PE10.3))                                             MAIN
       666 FORMAT(10I5)                                                   MAIN
      1000 FORMAT(7E10.3)                                                 MAIN
      9900 FORMAT (39H1 MIXING REGION INTERSECTS AXIS AT X = 1PE15.7)     MAIN
         6 IF(IPUNCH.EQ.0.OR.IPUNCH.EQ.1) GO TO 9                         MAIN
           PUNCH333,(TITLE(I),I=1,12)                                     MAIN
           PUNCH 666,MPSI,NS,ITURB,NR,IOUT1,IOUT2,IPUNCH,ITIME,IPRESS,NT  MAIN
           PUNCH 555,FREQA(1),FREQA(2),FREQA(3),FREQA(4),FREQA(5),FREQA(6)    MAIN
```

```
      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(NPSI),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
```

```
      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),SAVSU(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),TEDG(30),IRT(40),RR(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   , MPS1   , 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 IKINET,NFREQA,ALOC,FREQA,Q0100,Q0200,Q0300,Q0400            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
```

```
      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 RALPHA(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,I2)                                     OUTPUT     114
      DO 81 I=1,MPSI                                                    OUTPUT     115
   81 WRITE (6,208)I,YOUT(I),(RALPHA(J,I),J=I1,I2),I                    OUTPUT     116
      IF(IOUT1)564,564,74                                               OUTPUT     117
   74 WRITE (6,420)                                                     OUTPUT     118
      WRITE (6,421)(AID(J),J=I1,I2)                                     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,I2),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,I2),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) XOPJ,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
```

```
          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, 6X8HMACH 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,4HPAGEI4)        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,14HHOLE 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),RI(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         WTMOLF(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(40,20)                       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,30H[illegible]     [illegible]Y VISCOSITY MO[illegible]) 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(NPSI)                                        INOUT     54
      WRITE (6,1907)U(1),U(NPSI)                                        INOUT     55
      WTMIX(1)=0.0                                                      INOUT     55
```

```
            WTMIX(MPSI)=0.0                                                     INOUT     57
            DO 1930 J=1,NS                                                      INOUT     58
            WTMIX(1)=WTMIX(1)+ALPHA(J,1)                                        INOUT     59
       1930 WTMIX(MPSI)=WTMIX(MPSI)+ALPHA(J,MPSI)                               INOUT     60
            DO 1919 J=1,NS                                                      INOUT     61
            RALPHA(J,1)=ALPHA(J,1)/WTMIX(1)                                     INOUT     62
            RALPHA(J,MPSI)=ALPHA(J,MPSI)/WTMIX(MPSI)                            INOUT     63
       1919 WRITE (6,1917)AID(J),RALPHA(J,1),RALPHA(J,MPSI)                     INOUT     64
            WRITE (6,120)                                                       INOUT     65
            DO 159 I=1,NR                                                       INOUT     66
            L=IRR(I)                                                            INOUT     67
            GO TO(131,132,133,134,135,136,137,138,139,140),L                    INOUT     68
        131 J1=IRRR(I,1)                                                        INOUT     69
            J2=IRRR(I,2)                                                        INOUT     70
            J3=IRRR(I,3)                                                        INOUT     71
            J4=IRRR(I,4)                                                        INOUT     72
            WRITE (6,121)I,AID(J1),AID(J2),AID(J3),AID(J4),(RC(I,J),J=1,3)      INOUT     73
            GO TO 159                                                           INOUT     74
        132 J1=IRRR(I,1)                                                        INOUT     75
            J2=IRRR(I,2)                                                        INOUT     76
            J3=IRRR(I,3)                                                        INOUT     77
            WRITE (6,122)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)              INOUT     78
            GO TO 159                                                           INOUT     79
        133 J1=IRRR(I,1)                                                        INOUT     80
            J2=IRRR(I,2)                                                        INOUT     81
            J3=IRRR(I,3)                                                        INOUT     82
            J4=IRRR(I,4)                                                        INOUT     83
            J5=IRRR(I,5)                                                        INOUT     84
            WRITE (6,123)I,AID(J1),AID(J2),AID(J3),AID(J4),AID(J5),(RC(I,J),J=  INOUT     85
           11,3)                                                                INOUT     86
            GO TO 159                                                           INOUT     87
        134 J1=IRRR(I,1)                                                        INOUT     88
            J2=IRRR(I,2)                                                        INOUT     89
            J3=IRRR(I,3)                                                        INOUT     90
            WRITE (6,124)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)              INOUT     91
            GO TO 159                                                           INOUT     92
        135 J1=IRRR(I,1)                                                        INOUT     93
            J2=IRRR(I,3)                                                        INOUT     94
            J3=IRRR(I,4)                                                        INOUT     95
            WRITE (6,125)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)              INOUT     96
            GO TO 159                                                           INOUT     97
        136 J1=IRRR(I,1)                                                        INOUT     98
            J2=IRRR(I,2)                                                        INOUT     99
            J3=IRRR(I,3)                                                        INOUT    100
            J4=IRRR(I,4)                                                        INOUT    101
            WRITE (6,126)I,AID(J1),AID(J2),AID(J3),AID(J4),(RC(I,J),J=1,3)      INOUT    102
            GO TO 159                                                           INOUT    103
        137 J1=IRRR(I,1)                                                        INOUT    104
            J2=IRRR(I,2)                                                        INOUT    105
            J3=IRRR(I,3)                                                        INOUT    106
            WRITE (6,127)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)              INOUT    107
            GO TO 159                                                           INOUT    108
        138 J1=IRRR(I,1)                                                        INOUT    109
            J2=IRRR(I,2)                                                        INOUT    110
            J3=IRRR(I,3)                                                        INOUT    111
```

```
      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)                                                      INCUT     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-ML-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
```

```
SUBROUTINE  INOUT                                      CDC 6600 FTN V3.0-P312 OPT=2  08/07/72  12.54.49.       PAGE      4

              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
 170               RETURN                                                            INOUT     171
                   END                                                               INOUT     172
```

```
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)
                     CALL SECOND(TIME)                                                    TICK       2
                     JJJJ=TIME                                                            TICK       3
                     RETURN                                                               TICK       4
                     END                                                                  TICK       5
                                                                                          TICK       6
```

```
      SUBROUTINE SLOP(X.A.N)                                            SLOP       2
C     THIS PROGRAM FINDS THE SOLUTIONS TO A SET OF N SIMULTANEOUS LINEAR SLOP       3
C     EQUATIONS BY USING THE GAUSS-GORDAN REDUCTION ALGORITHM WITH THE  SLOP       4
C      DIAGONAL PIVOT STRATEGY                                          SLOP       5
      DIMENSION A(25.25).X(25)                                          SLOP       6
      DO 9 K=1.N                                                        SLOP       7
      IF (ABS(A(K.K)) .GT. 1.E-10) GO TO 5                              SLOP       8
      WRITE (6.101)                                                     SLOP       9
      GO TO 99                                                          SLOP      10
    5 KP1= K+1                                                          SLOP      11
      DO 6 J= KP1. N                                                    SLOP      12
    6 A(K.J)= A(K.J)/A(K.K)                                             SLOP      13
      X(K)= X(K)/A(K.K)                                                 SLOP      14
      A(K.K)= 1.0                                                       SLOP      15
      DO 9 I=1.N                                                        SLOP      16
      IF (I.EQ.K .OR. A(I.K).EQ.0.) GO TO 9                             SLOP      17
      DO 8 J=KP1.N                                                      SLOP      18
    8 A(I.J)= A(I.J)- A(I.K)*A(K.J)                                     SLOP      19
      X(I)= X(I)- A(I.K)*X(K)                                           SLOP      20
      A(I.K)=0.                                                         SLOP      21
    9 CONTINUE                                                          SLOP      22
   99 CONTINUE                                                          SLOP      23
  101 FORMAT( * ERROR--- SMALL PIVOT *)                                 SLOP      24
      RETURN                                                            SLOP      25
      END                                                               SLOP      26
```

```
SUBROUTINE  TKEY                            CDC 6600 FTN V3.0-P312 OPT=2  08/07/72  12.54.49.       PAGE       1
                 SUBROUTINE TKEY(T,TTB,ITKEY,SDT,HDT,NT)                                TKEY        2
                 DIMENSION TTB(30)                                                      TKEY        3
                 NT1=NT-1                                                               TKEY        4
                 DO 10 IT=1,NT1                                                         TKEY        5
                 DT= TTB(IT+1)-TTB(IT)                                                  TKEY        6
                 SDT=(T-TTB(IT))/DT                                                     TKEY        7
                 HDT=(TTB(  IT+1)-T) /DT                                                TKEY        8
                 IF ((SDT*HDT).GE.0.0) GO TO 11                                         TKEY        9
              10 CONTINUE                                                               TKEY       10
                 WRITE(6,100) T,I                                                       TKEY       11
                 ITKEY=0                                                                TKEY       12
             100 FORMAT(1H , *   TEMPERATURE OUT OF RANGE *, E14.5,I5)                  TKEY       13
                 RETURN                                                                 TKEY       14
              11 ITKEY=IT                                                               TKEY       15
                 RETURN                                                                 TKEY       16
                 END                                                                    TKEY       17
```

```
SUBROUTINE  LIPLN                                    CDC 6600 FTN V3.0-P312 OPT=2  08/07/72  12.54.49.      PAGE      1
                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
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 } CARD TYPES 7, 8 AND 9 OMITTED
9 }
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									

IBM

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.
```

B-4

IBM

FORTRAN Coding Form

FORTRAN STATEMENT

```
12.12 H     +HCL        =CL    +H2                     15 8.8E-11         -4622.
12.13 HCL   +ØH         =H2Ø   +CL                     15 7.2E-12         -3250.
12.14 ØH    +CL         =HCL   +Ø                      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                      INNER MIXING                 MACH NUMBER              MIXING RATE
    RADIUS/R                   ZONE RADIUS/R               AT HALF RADIUS             COEFFICIENT
   1.199084E+00                 1.019909E+00                1.775436E+00               2.480000E-02

 PT      Y/R      VELOCITY    TEMPERATURE     DENSITY       MACH NO.      ENTHALPY      VISCOSITY     ELECTRON          PSI        PT
                  FEET/SEC         K           GM/CC                       CAL/GM       LB/FT/SEC   DENSITY(1/ML)
  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
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X=  0.         FEET              SAMPLE TEST CASE (8/7/72)                                              PAGE   1
                                          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  4.96081E-06  5.36470E-07  8.14646E-02  2.85125E-01   1
 2   .10000  3.27844E-08  5.36470E-03  5.04680E-02  4.96081E-06  5.36470E-07  8.14646E-02  2.85125E-01   2
 3   .20000  3.27844E-08  5.36470E-03  5.04680E-02  4.96081E-06  5.36470E-07  8.14646E-02  2.85125E-01   3
 4   .30000  3.27844E-08  5.36470E-03  5.04680E-02  4.96081E-06  5.36470E-07  8.14646E-02  2.85125E-01   4
 5   .40000  3.27844E-08  5.36470E-03  5.04680E-02  4.96081E-06  5.36470E-07  8.14646E-02  2.85125E-01   5
 6   .50000  3.27844E-08  5.36470E-03  5.04680E-02  4.96081E-06  5.36470E-07  8.14646E-02  2.85125E-01   6
 7   .60000  3.27844E-08  5.36470E-03  5.04680E-02  4.96081E-06  5.36470E-07  8.14646E-02  2.85125E-01   7
 8   .70000  3.27844E-08  5.36470E-03  5.04680E-02  4.96081E-06  5.36470E-07  8.14646E-02  2.85125E-01   8
 9   .80000  3.27844E-08  5.36470E-03  5.04680E-02  4.96081E-06  5.36470E-07  8.14646E-02  2.85125E-01   9
10   .90000  3.27844E-08  5.36470E-03  5.04680E-02  4.96081E-06  5.36470E-07  8.14646E-02  2.85125E-01  10
11  1.00000  3.27844E-08  5.36470E-03  5.04680E-02  4.96081E-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
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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  2.35445E-01  1.76033E-01  2.68235E-03  5.16600E-07  1.29142E-08  6.06012E-05  1.19212E-03   1
 2   .10000  2.35445E-01  1.76033E-01  2.68235E-03  5.16600E-07  1.29142E-08  6.06012E-05  1.19212E-03   2
 3   .20000  2.35445E-01  1.76033E-01  2.68235E-03  5.16600E-07  1.29142E-08  6.06012E-05  1.19212E-03   3
 4   .30000  2.35445E-01  1.76033E-01  2.68235E-03  5.16600E-07  1.29142E-08  6.06012E-05  1.19212E-03   4
 5   .40000  2.35445E-01  1.76033E-01  2.68235E-03  5.16600E-07  1.29142E-08  6.06012E-05  1.19212E-03   5
 6   .50000  2.35445E-01  1.76033E-01  2.68235E-03  5.16600E-07  1.29142E-08  6.06012E-05  1.19212E-03   6
 7   .60000  2.35445E-01  1.76033E-01  2.68235E-03  5.16600E-07  1.29142E-08  6.06012E-05  1.19212E-03   7
 8   .70000  2.35445E-01  1.76033E-01  2.68235E-03  5.16600E-07  1.29142E-08  6.06012E-05  1.19212E-03   8
 9   .80000  2.35445E-01  1.76033E-01  2.68235E-03  5.16600E-07  1.29142E-08  6.06012E-05  1.19212E-03   9
10   .90000  2.35445E-01  1.76033E-01  2.68235E-03  5.16600E-07  1.29142E-08  6.06012E-05  1.19212E-03  10
11  1.00000  2.35445E-01  1.76033E-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
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                FEET            SAMPLE TEST CASE (8/7/72)                                          PAGE  1

                                          MOLE FRACTIONS

PT    X/H     O2            AL2O3         N2
 1   0.00000  1.19212E-04   3.40757E-02   1.27162E-01  0.         0.         0.         0.          1
 2    .10000  1.19212E-04   3.40757E-02   1.27162E-01  0.         0.         0.         0.          2
 3    .20000  1.19212E-04   3.40757E-02   1.27162E-01  0.         0.         0.         0.          3
 4    .30000  1.19212E-04   3.40757E-02   1.27162E-01  0.         0.         0.         0.          4
 5    .40000  1.19212E-04   3.40757E-02   1.27162E-01  0.         0.         0.         0.          5
 6    .50000  1.19212E-04   3.40757E-02   1.27162E-01  0.         0.         0.         0.          6
 7    .60000  1.19212E-04   3.40757E-02   1.27162E-01  0.         0.         0.         0.          7
 8    .70000  1.19212E-04   3.40757E-02   1.27162E-01  0.         0.         0.         0.          8
 9    .80000  1.19212E-04   3.40757E-02   1.27162E-01  0.         0.         0.         0.          9
10    .90000  1.19212E-04   3.40757E-02   1.27162E-01  0.         0.         0.         0.         10
11   1.00000  1.19212E-04   3.40757E-02   1.27162E-01  0.         0.         0.         0.         11
12   [illegible]  2.10000E-01   0.                      7.90000E-01  0.         0.         0.         0.         12
13   [illegible]  2.10000E-01   0.                      7.90000E-01  0.         0.         0.         0.         13

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

PT            O2            AL2O3         N2                                                       PT
 1           -2.56912E-06   0.            0.           0.         0.         0.         0.          1
 2           -2.56912E-06   0.            0.           0.         0.         0.         0.          2
 3           -2.56912E-06   0.            0.           0.         0.         0.         0.          3
 4           -2.56912E-06   0.            0.           0.         0.         0.         0.          4
 5           -2.56912E-06   0.            0.           0.         0.         0.         0.          5
 6           -2.56912E-06   0.            0.           0.         0.         0.         0.          6
 7           -2.56912E-06   0.            0.           0.         0.         0.         0.          7
 8           -2.56912E-06   0.            0.           0.         0.         0.         0.          8
 9           -2.56912E-06   0.            0.           0.         0.         0.         0.          9
10           -2.56912E-06   0.            0.           0.         0.         0.         0.         10
11           -2.56912E-06   0.            0.           0.         0.         0.         0.         11
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XM  0.            FEET              SAMPLE TEST CASE (8/7/72)                                                  PAGE   1

                                        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.            5.9858E-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/R          REACTION  6               REACTION  7               REACTION  8               REACTION  9               REACTION 10          PT
                    RP          RM            RP          RM            RP          RM            RP          RM            RP          RM
 1  0.            1.0711E-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
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X= 0.        FEET              SAMPLE TEST CASE (8/7/72)                                              PAGE   1

                                            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
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                   COLLISION    ELECTRICAL       UNIT ATTENUATION (DB/IN)
                   FREQUENCY   CONDUCTIVITY
 PT       Y/A       (1/SEC)      (MHO/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   7.7762E+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
1.27584E-01 7.08394E-01
1.00442E-01 8.35977E-01
9.88467E-02 9.36419E-01
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X= 1.0353036E+00 FEET           SAMPLE TEST CASE (8/7/72)                                                                   PAGE   2

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

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

 PT      Y/R      VELOCITY      TEMPERATURE      DENSITY       MACH NO.       ENTHALPY      VISCOSITY      ELECTRON          PSI        PT
                  FEET/SEC          K             GM/CC                        CAL/GM       LB/FT/SEC    DENSITY(1/ML)
  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   4.425511E+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   2.729697E-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   5.149061E-01  -9.124333E+01   1.872640E-02   1.356855E+09   1.511199E-01  13
 14    1.7194   3.504702E+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
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X=  1.0353036E+00 FEET              SAMPLE TEST CASE (8/7/72)                                                PAGE   2

                                                   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    .04968   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    .44942   1.57035E-07  5.09133E-03  5.07663E-02  5.83368E-06  5.39173E-07  8.18515E-02  2.84457E-01   6
 7    .54932   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   2.99167E-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  2.00126E-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  7.81955E-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   2.13956   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   3.29216   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  4.21406E-07 -2.28665E-11  8.93334E-11  5.84642E-06 -5.74383E-06   4
 5            -6.51064E-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 -1.46273E-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  7.77680E-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            -1.32601E-06  8.85255E-05 -1.88459E-05  1.32608E-06 -6.69097E-11 -5.19879E-05  3.83775E-05  13
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X=  1.0353036E+00 FEET              SAMPLE TEST CASE (8/7/72)                                          PAGE   2

                                              MOLE FRACTIONS

PT    Y/R      CO           CO2          CL           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  2.35124E-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   .80070  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          CL           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          -5.83808E-06  5.83808E-06 -4.16952E-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  9.01292E-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
```

```
X= 1.03540386E+00 FEET            SAMPLE TEST CASE (8/7/72)

                                      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  3.73759E-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  6.88949E-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           1.36616E-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
```

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                                            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  4.9884E-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 5.6874E-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 9.8998E-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 5.2026E-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  4.9884E-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 1.4764E-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-05 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 1.1555E-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
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** 1.0353036E+00 FEET             SAMPLE TEST CASE (8/7/72)                                              PAGE  2

                                      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.           3.8821E-05  3.8059E-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  4.9884E-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   3.8872E-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  6.2900E-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   1.8844E-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              REACTION 17              REACTION 18              REACTION 19              REACTION 20          PT
                     RP          RM           RP          RM           RP          RM           RP          RM           RP          RM
  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  4.9884E-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  1.4073E-11  3.6666E-11  9.3970E-12  5.5627E-13  2.4399E-10  2.2662E-10  0.          0.           8
  9  8.0070E-01   2.0047E-12  3.2526E-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  4.1516E-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
```

```
                     COLLISION     ELECTRICAL       UNIT ATTENUATION (DB/IN)
                     FREQUENCY    CONDUCTIVITY
PT          Y/R       (1/SEC)       (MHO/IN)

                      SIG. FREQ. (MEGACYC)= 9.7500E+02


 1        0.000    3.6895E+10   1.0241E-02   3.3930E-02
 2         .100    3.6895E+10   1.0241E-02   3.3930E-02
 3         .200    3.6895E+10   1.0241E-02   3.3930E-02
 4         .300    3.6895E+10   1.0241E-02   3.3930E-02
 5         .400    3.6895E+10   1.0241E-02   3.3931E-02
 6         .499    3.6895E+10   1.0251E-02   3.3962E-02
 7           .     3.6480E+10   1.0393E-02   3.4424E-02
 8         .699    3.3928E+10   1.1588E-02   3.8240E-02
 9         .801    3.1486E+10   1.7335E-02   5.6254E-02
10         .907    2.9045E+10   3.2465E-02   9.7411E-02
11        1.031    2.5943E+10   4.9231E-02   1.2159E-01
12        1.145    2.3502E+10   2.5773E-02   5.4470E-02
13        1.419    2.0940E+10   4.6375E-03   7.4316E-03
14        1.719    1.6228E+10   4.0595E-03   4.3819E-03
15        2.14     1.0744E+10   2.5026E-03   1.2209E-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
```

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 → 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 → 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 → KCl + H identically 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 $K + HCl \rightarrow KCl + H$ 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

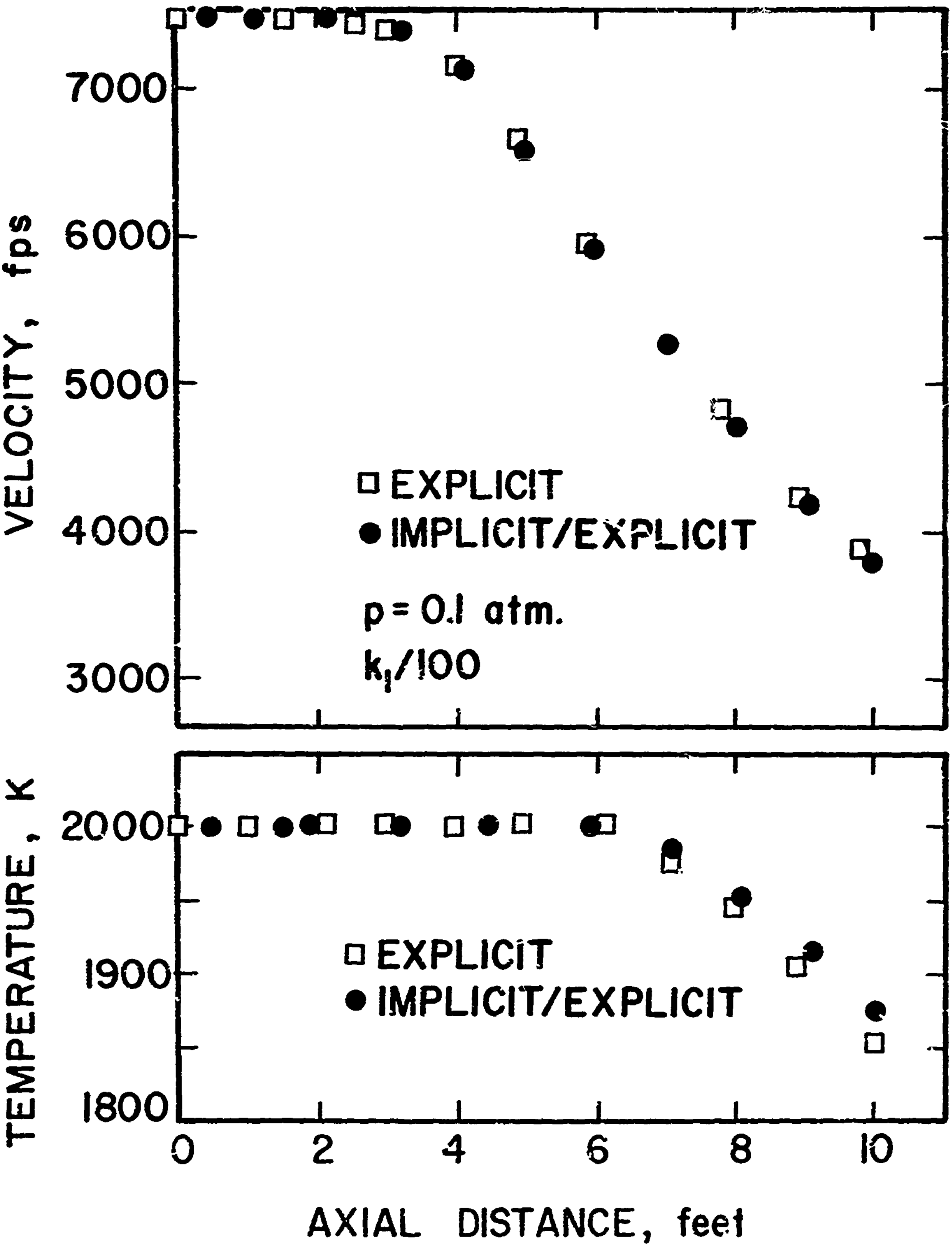

FIG. D1 COMPARISONS BETWEEN CENTERLINE DISTRIBUTIONS OF VELOCITY AND TEMPERATURE COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$r_j = 0.25$ ft

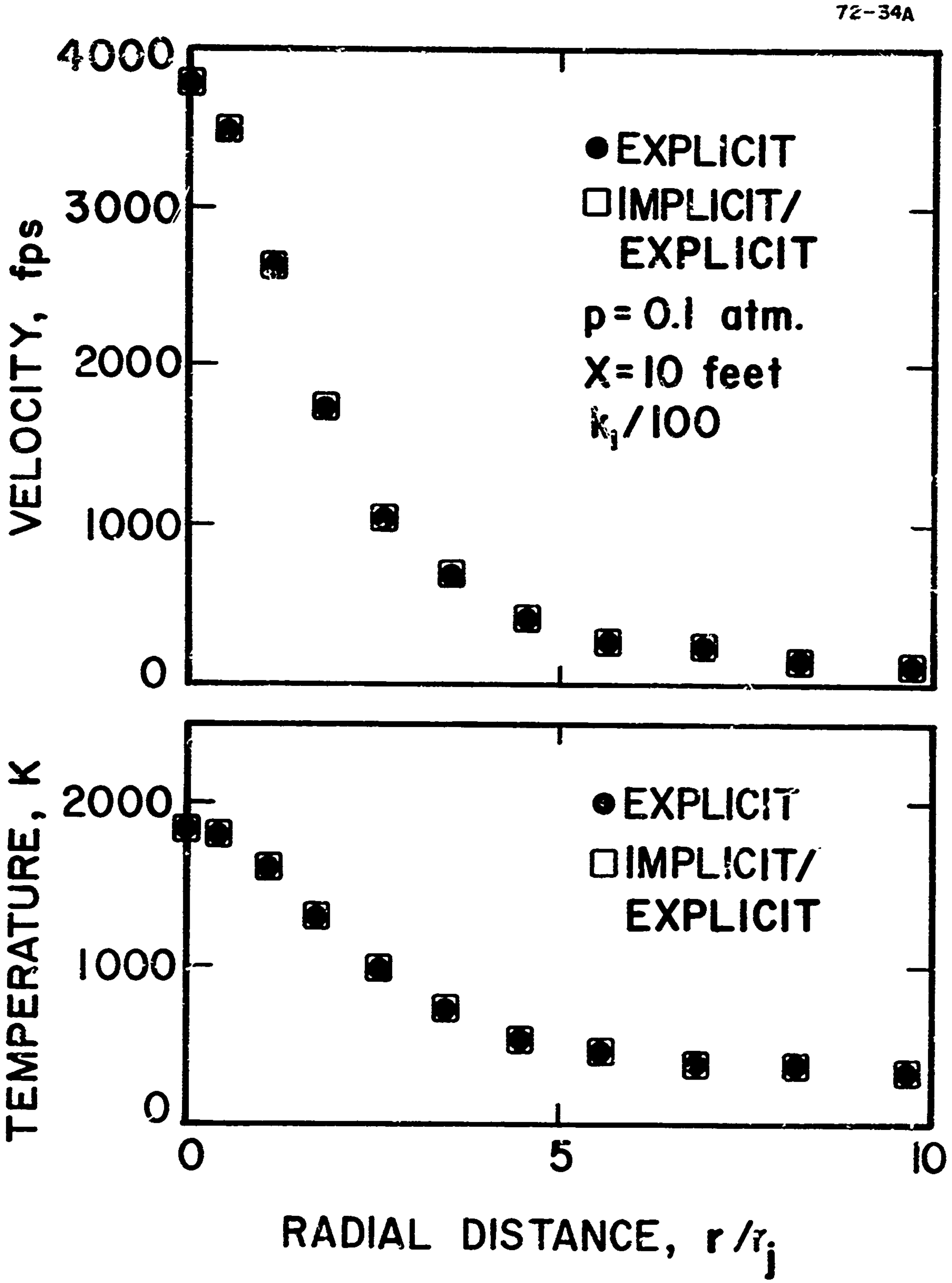

FIG. D2 COMPARISONS BETWEEN RADIAL DISTRIBUTIONS OF VELOCITY AND TEMPERATURE COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$r_j = 0.25$ ft

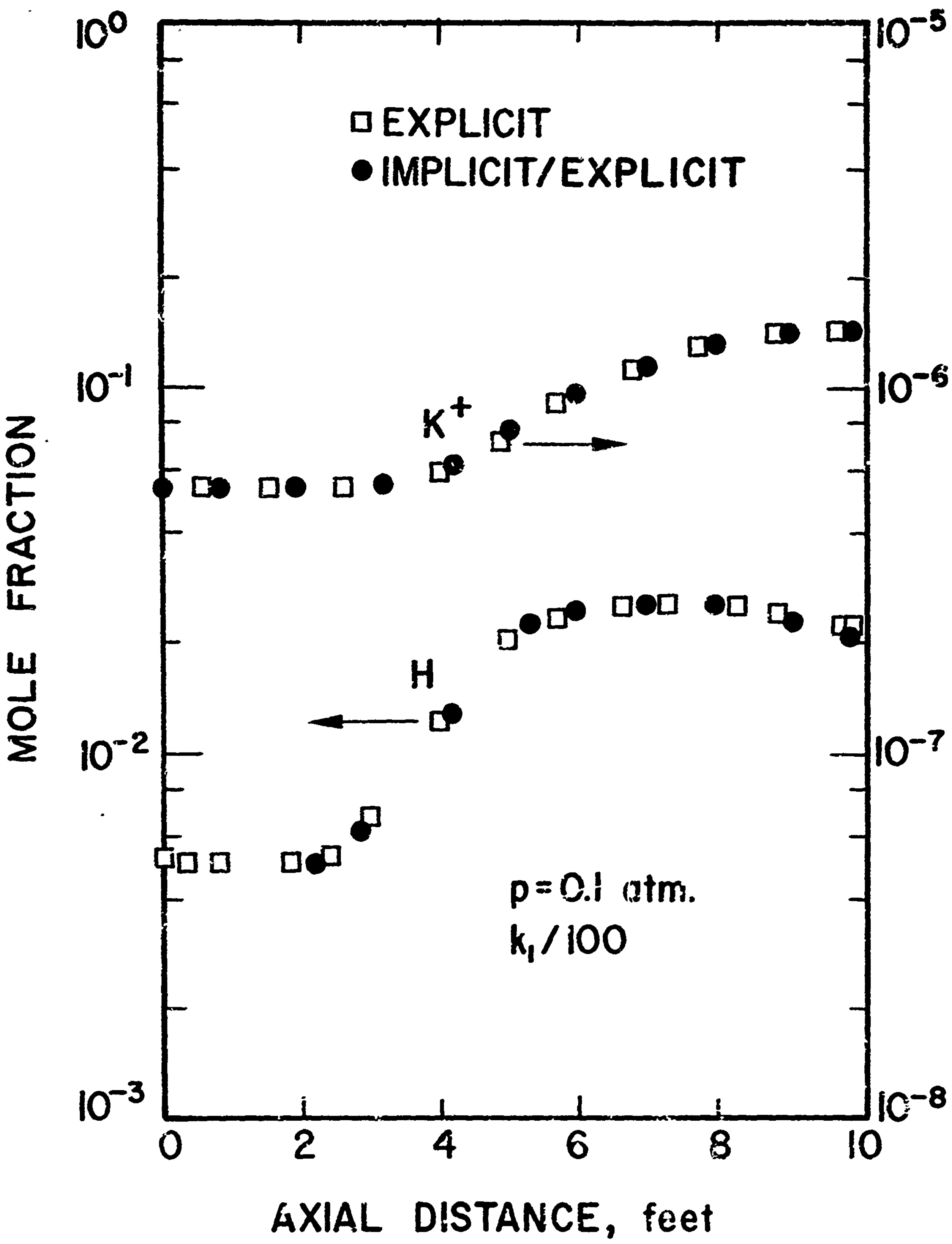

FIG. D3 COMPARISONS BETWEEN CENTERLINE DISTRIBUTIONS OF X_{K^+} AND X_H COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$r_j = 0.25$ ft

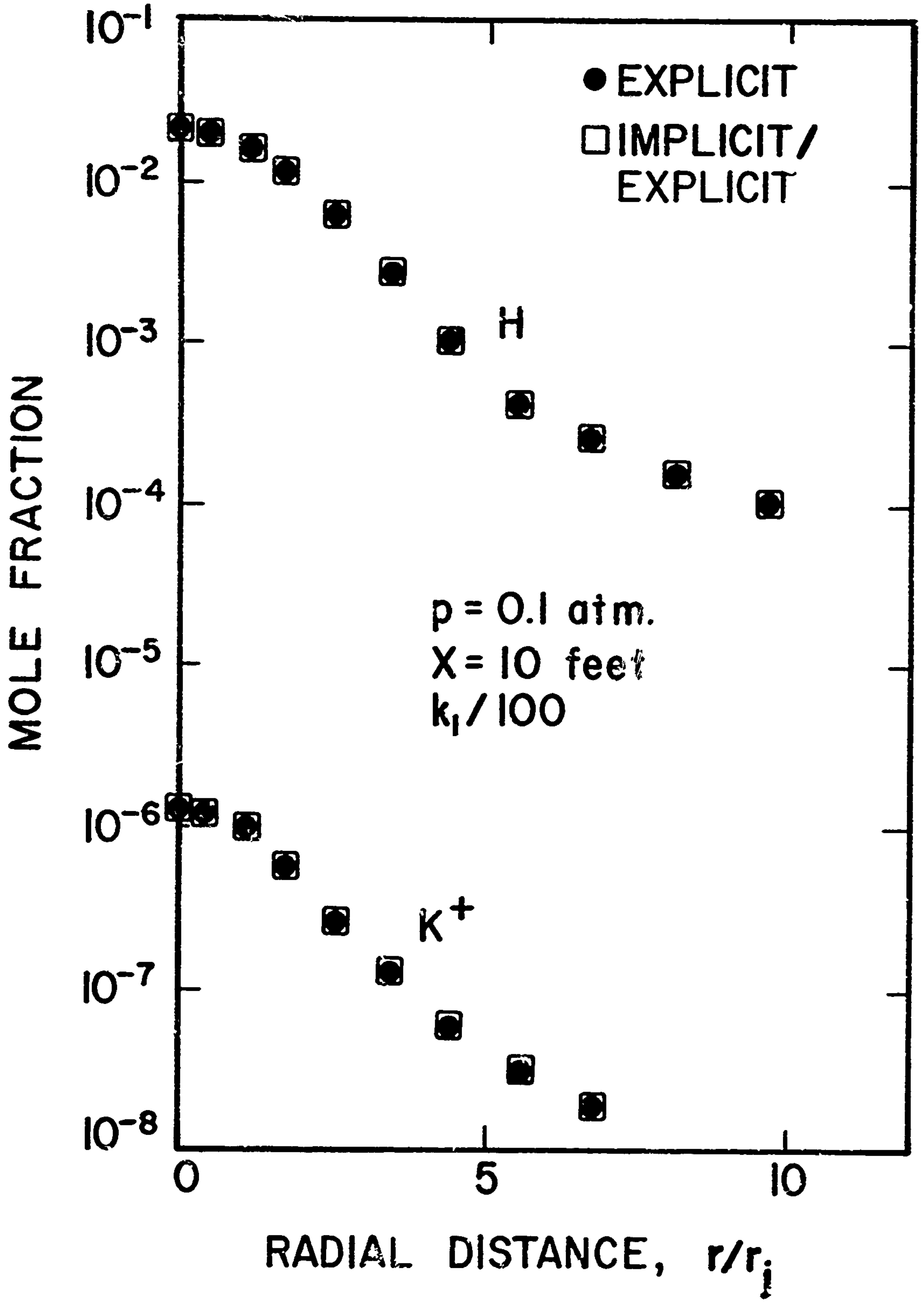

FIG. D4 COMPARISONS BETWEEN RADIAL DISTRIBUTIONS OF X_{K^+} AND X_H COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$r_j = 0.25$ ft

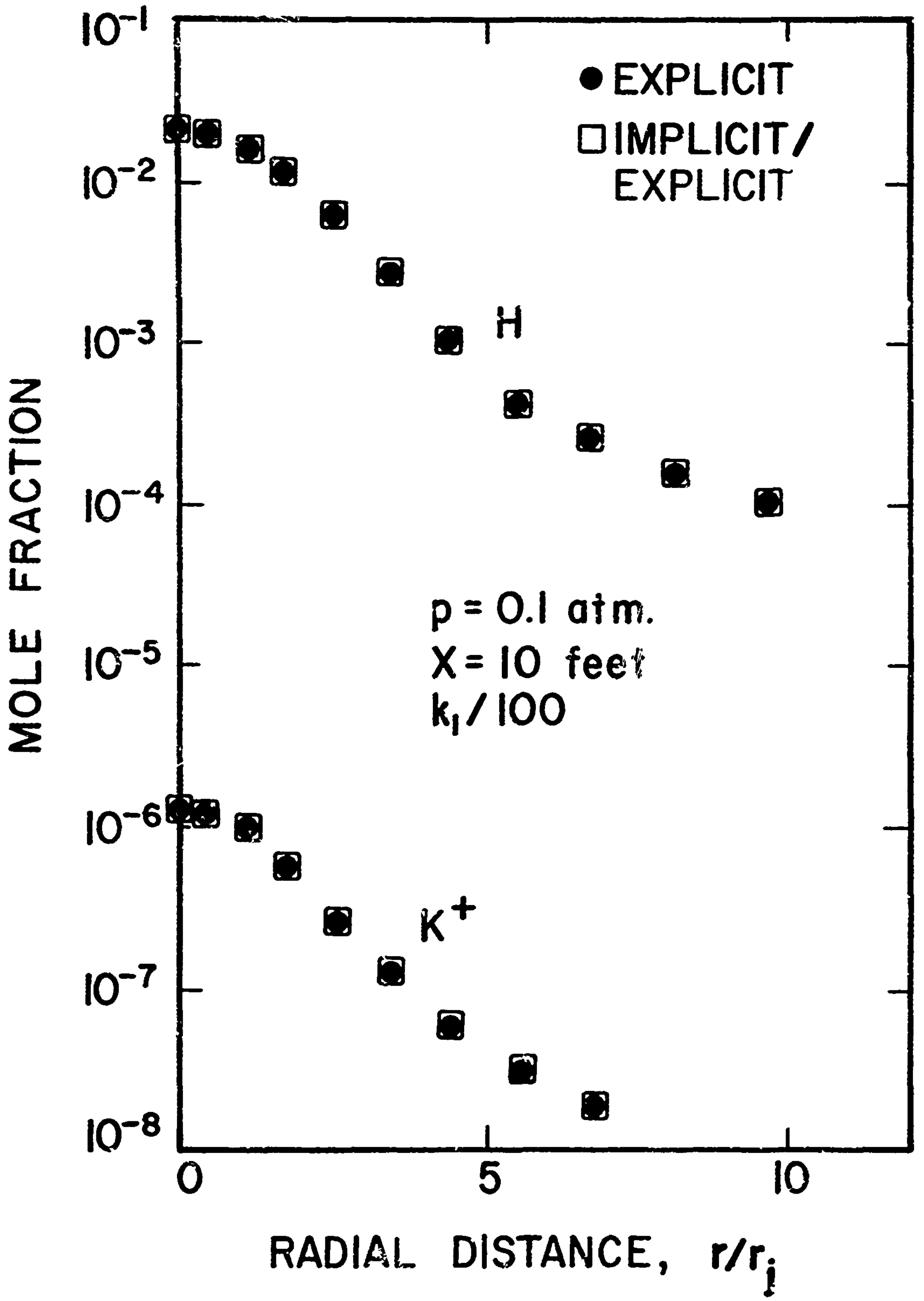

FIG. D4 COMPARISONS BETWEEN RADIAL DISTRIBUTIONS OF X_{K^+} AND X_H COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$r_j = 0.25$ ft