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**FAST COMPUTER PROGRAM FOR NONEQUILIBRIUM
ROCKET PLUME PREDICTIONS**

R. R. Mikatarian, et al

AeroChem Research Laboratories, Incorporated.

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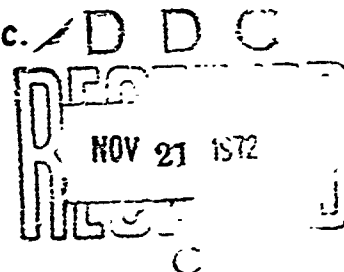
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A FAST COMPUTER PROGRAM FOR NONEQUILIBRIUM ROCKET PLUME PREDICTIONS

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FOREWORD

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ABSTRACT

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

NOMENCLATURE

a	defined by Eq. (15b)
$a_{\frac{1}{2}}$	defined by Eq. (33)
a^s	attenuation per unit length
A	constant in expression for k_r (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 i th 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 i th 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 i th species
h_{298i}	heat of formation of i th species at $T = 298 \text{ K}$
k_f	forward rate coefficient
K	eddy viscosity coefficient (see Section VI)
$\bar{K}$	eddy viscosity coefficient for Donaldson/Gray model (see Eq. (32))
K_p	equilibrium constant
Le	Lewis number (laminar or turbulent)
m_e	electron mass
$M_{\frac{1}{2}}$	Mach number at half radius, defined under Eq. (32)
N	temperature exponent in reaction rate equation (Eq. (23))
n_e	electron density
Q	arbitrary dependent variable (see Eqs. (13) - (15))

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

Greek

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

Ψ stream function
 ω signal frequency

Subscripts

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

Miscellaneous

$| |$ 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

TABLE OF CONTENTS

	<u>Page</u>
I. INTRODUCTION	1
II. GOVERNING EQUATIONS	3
A. Conservation Equations and Boundary Conditions	3
B. Transformation to Stream Function Coordinates	4
C. Finite-Difference Formulation	6
III. SOLUTION OF FINITE DIFFERENCE EQUATIONS	10
A. Integration Step Size	10
B. Edge of Mixing Layer	11
C. Halving the Mesh	11
IV. CHEMICAL REACTION RATE EQUATIONS	12
V. THERMODYNAMIC DATA	14
VI. TRANSPORT PROPERTIES	14
A. Turbulent Eddy Viscosity Models	14
B. Laminar Flow	17
VII. PLUME ELECTRICAL PROPERTIES	17
A. Electron Density	17
B. Collision Frequency	17
C. Transverse Radar Attenuation	18
D. Electrical Conductivity	18
VIII. PROGRAM OPERATION	19
A. Machine	19
B. Sense Switch Control	19
1. Sense Switch 1	19
2. Sense Switch 3	19
C. Program Optimization	19
IX. PROGRAM INPUT DATA	20

TABLE OF CONTENTS (cont'd)

	<u>Page</u>
X. PROGRAM OUTPUT	27
A. Description	27
B. Units	27
C. Card Output	29
1. Continuing Solution	29
2. Electron Density and Collision Frequency	29
XI. REFERENCES	30
APPENDIX A: A FAST COMPUTER PROGRAM FOR NONEQUILIBRIUM ROCKET PLUME PREDICTIONS - Fortran Listing	A-1
APPENDIX B: SAMPLE INPUT DATA SHEET	B-1
APPENDIX C: SAMPLE OUTPUT	C-1
APPENDIX D: COMPARISON BETWEEN MIXED IMPLICIT/EXPLICIT AND FULLY EXPLICIT FINITE DIFFERENCE SCHEMES	D-1

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I. INTRODUCTION

The need to accurately determine electromagnetic wave/plume interactions^{1,2} has motivated the development of several programs³⁻⁶ 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 others³⁻⁵ 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 scheme⁴ 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‡

*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 program² (which uses the fully explicit scheme) because the stable step size approached 10^{-10} ft, are quite easily handled by the new program. Most importantly, for the more typical case in which average step sizes range from 10^{-4} to 10^{-2} ft, the new program reduced computer run times by at least an order of magnitude. (A detailed comparison between rocket plume calculations using the original fully explicit difference scheme and the new mixed implicit/explicit scheme is given in Appendix D.)

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

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

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

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

II. GOVERNING EQUATIONS

A. Conservation Equations and Boundary Conditions

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

Global Continuity

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

Conservation of Species

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

Conservation of Momentum

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

Conservation of Energy

$$\rho c_p \left[u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial r} \right] = u \frac{dp}{dx} + \mu \left(\frac{\partial u}{\partial r} \right)^2 + \frac{1}{r} \frac{\partial}{\partial r} \left[\frac{c_p}{Pr} \mu r \frac{\partial T}{\partial r} \right] +$$

$$\mu \frac{Le}{Pr} \frac{\partial T}{\partial r} \sum_i c_{p_i} \frac{\partial F_i}{\partial r} - \sum_i \dot{w}_i h_i \quad (4)$$

State

$$\rho = \frac{pW}{RT} \quad (5)$$

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

$$\begin{aligned} x = 0: \quad u &= u(r), \quad F_1 = F_1(r), \quad T = T(r) \\ r = 0: \quad \frac{\partial u}{\partial r} &= \frac{\partial T}{\partial r} = \frac{\partial F_1}{\partial r} = 0 \\ r \rightarrow \infty: \quad u &\rightarrow u_e, \quad F_1 \rightarrow (F_1)_e, \quad T \rightarrow T_e \end{aligned} \quad (6)$$

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

$$p = c_0 + c_1 x + c_2 x^2 + c_3 x^3 \quad (7)$$

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:

$$\Psi \frac{\partial \Psi}{\partial r} = \rho u r \quad (8a)$$

$$\Psi \frac{\partial \Psi}{\partial x} = -\rho v r \quad (8b)$$

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

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

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

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

Species

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

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

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

Momentum

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

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

$$\frac{\partial u}{\partial x} = -\frac{1}{\rho u} \frac{dp}{dx} + 2\mu \frac{\partial^2 u}{\partial \psi^2} \quad (11b)$$

Energy

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

$$\frac{\mu \rho u r^2}{\psi^2} \left[\left(\frac{\partial u}{\partial \psi} \right)^2 + \frac{Le}{Pr} \frac{\partial T}{\partial \psi} \sum_i c_{p_i} \frac{\partial F_i}{\partial \psi} \right]$$

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

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

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 formulations¹³ are used:

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

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

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

$$- \frac{a_{n, m-\frac{1}{2}} [Q_{n, m} - Q_{n, m-1}]}{(\Delta \bar{y})^2}$$

where

$$a_{n, m \pm \frac{1}{2}} = \frac{a_{n, m} \pm a_{n, m \pm 1}}{2} \quad (15a)$$

and

$$a = \frac{\mu p u^2}{\Psi} \quad (15b)$$

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

Species

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

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

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

Momentum

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

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

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

Energy

$$\begin{aligned} T_{n+1,m} = & \frac{\Delta x}{(\rho c_p)_{n,m}} \left(\frac{dp}{dx} \right)_{n+1} + \frac{\Delta x}{4m(\Delta \Psi)^3} \left(\frac{a}{c_p} \right)_{n,m} (u_{n,m+1} - u_{n,m-1})^2 \\ & + \frac{\Delta x}{m(\Delta \Psi)^3 (c_p)_{n,m}} \left\{ \left(\frac{c_p}{Pr^2} \right)_{n,m+\frac{1}{2}} (T_{n,m+1} - T_{n,m}) \right. \\ & + \left(\frac{c_p}{Pr^2} \right)_{n,m-\frac{1}{2}} (T_{n,m-1} - T_{n,m}) + \frac{1}{4} \left(\frac{L_2}{Pr^2} \right)_{n,m-1} \sum_i (c_{p,i})_{n,m} \\ & \left. (F_{i,n,m+1} - F_{i,n,m-1}) [T_{n,m+1} - T_{n,m-1}] \right\} \\ & + T_{n,m} - \frac{1}{(\rho u)_{n,m}} \sum_i (h_i \dot{w}_i)_{n,m} \end{aligned} \quad (18a)$$

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

$$\begin{aligned} T_{n+1,0} = & \frac{\Delta x}{(\rho c_p)_{n,0}} \left(\frac{dp}{dx} \right)_{n+1} + \frac{4\Delta x}{(\Delta \Psi)^2} \left(\frac{\mu}{Pr} \right)_{n,0} [T_{n,1} - T_{n,0}] \\ & + T_{n,0} - \frac{1}{(\rho u)_{n,0}} \sum_i (h_i \dot{w}_i)_{n,0} \end{aligned} \quad (18b)$$

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

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

$$\begin{aligned} (F_i F_j F_k)_{n+1} &= - \underline{2(F_i F_j F_k)_n} + \underline{(F_j F_k)_n} (F_i)_{n+1} + \underline{(F_i F_k)_n} (F_j)_{n+1} \\ &\quad + \underline{(F_i F_j)_n} (F_k)_{n+1} \end{aligned} \quad (20)$$

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),

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

*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 Neuman¹⁴ 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

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

i

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

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

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,
 $\dot{w}^{(j)} = RP^{(j)} - RM^{(j)}.$ *

$$\begin{aligned}
 (1) \quad \dot{w}^{(j)} &= k_f \rho^2 F_A F_B - \frac{k_f \rho^2 F_C F_D}{K_p} \\
 (2) \quad \dot{w}^{(j)} &= \frac{k_f \rho^3 F_A F_B}{W} - \frac{k_f \rho^2 F_C}{K_p WRT} \\
 (3) \quad \dot{w}^{(j)} &= k_f \rho^2 F_A F_B - \frac{k_f \rho^3 F_C F_D F_E RT}{K_p} \\
 (4) \quad \dot{w}^{(j)} &= k_f \rho^2 F_A F_B - \frac{k_f \rho^3 F_C}{K_p RT} \\
 (5) \quad \dot{w}^{(j)} &= \frac{k_f \rho^2 F_A}{W} - \frac{k_f \rho^3 F_C F_D RT}{K_p W}
 \end{aligned}$$

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

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

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

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

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

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

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

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

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

and K_p is determined from,

$$\ln K_p = -\Delta G/RT \quad (24)$$

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} , $-\left(\frac{g_i - h_{298i}}{T}\right)$ 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 models¹⁷⁻²⁰ are incorporated into the program:

Model 1 (Ferri)¹⁷

Initial region,*

$$\mu = \rho \epsilon = \alpha 0.00137 \times |\rho_o u_o - \rho_e u_e| \quad (25a)$$

Developed region,

$$\mu = \rho \epsilon = \alpha K b_{\frac{1}{2}} |\rho_o u_o - \rho_e u_e| \quad (25b)$$

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 Schlichting,¹⁸ has been incorporated directly into the program. This can be changed by the program input data via an appropriate value for the additional constant, α , Eqs. (25-31) (Card 4, Cols. 61-70).

Model 2 (Ting/Libby)¹⁹

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

where

$$\eta^2 = 2 \int_0^r (\rho_o/\rho) r' dr' \quad (27)$$

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

Model 3

Initial region,

$$\mu = \rho \epsilon = \alpha 0.00137 \times \rho_o |u_o - u_e| \quad (28a)$$

Developed region,

$$\mu = \alpha K \bar{r}_{\frac{1}{2}} \rho_o |u_o - u_e| \quad (28b)$$

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

Model 4

Initial region,

$$\mu = \rho \epsilon = \alpha 0.00137 \times \rho_e |u_o - u_e| \quad (29a)$$

Developed region,

$$\mu = \rho \epsilon = \alpha K \bar{r}_{\frac{1}{2}} \rho_e |u_o - u_e| \quad (29b)$$

Model 5* (Ting/Libby)¹⁹

Initial region,

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

Developed region,

$$\mu = \rho \epsilon = \alpha K \bar{r}_{\frac{1}{2}} |u_o - u_e| \rho \left(\frac{p_o}{p}\right)^2 \left(\frac{r_1}{r}\right)^2 \quad (26)$$

Model 6 (Donaldson/Gray)²⁰

Initial region,

$$\mu = \rho \epsilon = \alpha \bar{K} (r_{\frac{1}{2}} - r_1) \rho |u_o - u_e|/2 \quad (31a)$$

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

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

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

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,

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

*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 Law²¹ is used to describe the viscosity as a function of temperature.

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

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

$$n_e = 0.733 (10^{22}) X_{e-} p T^{-1} \quad \text{cm}^{-3} \quad (35)$$

where p is in atm and T in degrees K.

B. Collision Frequency

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

where p is in atm, T in degrees K and Q_{ei} in cm^2 . The electron-neutral collision cross sections²² 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	$Q_{ei} \text{ cm}^2$
CO	$2.03 (10^{-23}) v_e^{\dagger} + 2.46 (10^{-16})$
CO ₂	$4.7 (10^{-23}) v_e^{-1}$
H ₂ O	$5.9 v_e^{-2}$
HCl	$1.85 v_e^{-2}$
N ₂	$3.29 (10^{-23}) v_e$
H ₂	$1.45 (10^{-23}) v_e + 8.7 (10^{-16})$
$\dagger v_e = 6.21 (10^5) T^{\frac{1}{2}} \text{ cm/sec}$	

C. Transverse Radar Attenuation

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

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

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

where r is in inches.

D. Electrical Conductivity

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

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

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

VIII. PROGRAM OPERATION

A. Machine

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

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

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

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

B. Sense Switch Control

1. Sense Switch 1 - When Sense Switch 1 is on, the current values of x , T_0 , and $n_{e,0}$ 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.

<u>Card No.</u>	<u>Columns</u>	<u>Description</u>	<u>Format</u>
1	1-72	Run identification	12A6
2	1-5	Initial number of grid points* in Ψ coordinate (26 maximum)	15
	6-16	Number of species (24 maximum)	15
	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)	15
	16-20	Number of reactions (40 maximum)	15
	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)	15

*Recommended number, 13

<u>Card No.</u>	<u>Columns</u>	<u>Description</u>	<u>Format</u>
2	26-30	RP, RM output option If 0: RP, RM for each reaction is not output 1: RP, RM for each reaction is out- out at all radial points whose temperature is greater than the kinetics cut-off temperature (Card 6, Cols. 61-70)	15
	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 solu- tion are punched 3: Both the above sets of cards are punched	
	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)*	
	41-45	Pressure option If 0: Pressure is a constant 1: Pressure is a function of axial distance	
	51-60	Signal frequencies (MHz) - 6 maximum - for which transverse attenuation calcu- lations will be made (see Section VII). Leave blank if no attenuation calculations desired	
3	1-10		E10.3

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

Card No.	Columns	Description	Format
4	1-10	Initial value of x (ft)	E10.3
	11-20	Final value of x (ft)	E10.3
	21-30	Print increment (ft)	E10.3
	31-40	Lewis number	E10.3
	41-50	Prandtl number	E10.3
	51-60	Nozzle (jet) radius (ft)	E10.3
	61-70	α , factor used to vary eddy viscosity* (see Section VI)	E10.3
5	1-10	$\Delta x_{\min}$, Minimum integration step size (ft) [†]	E10.3
	11-20	FDL, diffusion step size factor [‡]	E10.3
	21-30	c_0 (atm)	E10.3
	31-40	c_1 (atm/ft)	E10.3
	41-50	c_2 (atm/ft ²)	Pressure Coefficients (see Section II)
	51-60	c_3 (atm/ft 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	$\Delta \Psi, \left(\frac{\text{lbm}}{32.2} \text{ sec}^{-1} \right)^{\frac{1}{2}}$	E10.3
		If $\Delta \Psi = 0$ (or blank) the program computes $\Delta \Psi$ assuming velocity, temperature and species mole fractions are constant at initial station If $\Delta \Psi$ is specified, cards 7.1 to 9.13 are read next. If $\Delta \Psi$ is not specified, card 10.1 is the next card read with cards 7.1 through 9.13 being omitted	
	61-70	Kinetics cut-off temperature (kinetics are frozen at temperatures below this value*)	E10.3

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

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

*If blank or zero, 400 K is used.

<u>Card</u> <u>No.</u>	<u>Column</u>	<u>Description</u>	<u>Format</u>
---------------------------	---------------	--------------------	---------------

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, $r = 0$	
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 at 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_{298i} (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	$-\left(\frac{g_i - h_{298i}}{T}\right)$ (cal/mole K)	E10.3
	31-40	$h_i - h_{298i}$ (kcal/mole)	E10.3
	41-50	Second temperature point (K)	E10.3
	51-60	c_{p_i} (cal/mole-K)	E10.3
	61-70	$-\left(\frac{g_i - h_{298i}}{T}\right)$ (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 problem 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)	
12.1	36-41	Species E (or M)	A6
	42-48	Blank	
	49-50	Reaction type, 1 to 10 (see Section IV)	I2
	51	Rate coefficient type, 1 to 7 (see Section IV)	II
	52-59	A, Pre-exponential factor cm-molecule-sec units	E8.2
	60-63	N, Temperature exponent	F4.1
12.2	64-72	B, Activation energy cal/mole	F9.1
	:	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 $(u - u_e) / (u_i - u_e) = 0.95$, (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	$(\Delta x)_{\text{min}}$, ft

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

C. Card Output

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

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

XI. REFERENCES

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APPENDIX A

A FAST COMPUTER PROGRAM FOR NONEQUILIBRIUM
ROCKET PLUME PREDICTIONS

Fortran Listing

A-2

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PROGRAM          MAIN          PAGE
CNC 6600 PIN V3.0-PSIP OPTIP 09/07/79 12,56,49,

60      READ(5,100) MPSI,NS,11,URR,OH,JOY1,JOY2,IPURCH,ITIME,IPDESSH,OH
        READ(5,111) (FREQA(I), I=1,6)
        DO 113 I=1,6
        IF (FREQA(I)) 117, 114, 111
117      CONTINUE
        I=7
114      NFREQA = I-1
        MPSI=MPSI-1
        PFAC (5,1000)X,XMAX,PRNT,X17(1),SIGNA(1),RJ,XK2
        CX=0,1,RJ
        C      INPUT MINIMUM STEPSIZE LIMIT (DXMIN)
        READ(5,1000) DXMIN,FOL, PC(1),PCIP,PC(J),PC(6)
        READ (5,1000)P,T(1),TIMPSI,U(1),U(MPSI),DELPSI,TWINEY
        IF (TWINEY.EQ.0.0) TWINEY = 400.0
        C*** THE VALUE OF 30 SECONDS IS TO ALLOW FOR COMPILER TIME
        LIMIT = 60*ITIME-30
        IDIFFY = 0
        CALL TICK(TSECT)
        IF ((TSECT-60*ITIME).GT.86400) IDIFFY = 86400-TSECT
        UNIT = U(1)
        IOT77 = 2
        USUR01 = 0.0
        C      TURBULENCE MODELS
        IF (ITURB - 3) 8600,9010,9010
        8600 IF (ITURB - 1) 9010,9010,9011
        9010 USUR01 = 0.95* (U(1)-U(MPSI)) * U(MPSI)
        9011 CONTINUE
        3012 IF (DELPSI) 3011,7012,3011
        3012 READ (5,1000)(ALPHA(J,1),J=1,NS)
        85      PFAC (5,1000)(ALPHA(J,MPSI),J=1,NS)
        MMD=MPSI-2
        DO 4001 I=1,MMD
        T(I)=T(1)
        U(I)=U(1)
        90      DO 4001 J=1,NS
        ALPHA(J,I)=ALPHA(J,1)
        4002 J=1,NS
        DO 4002 J=1,NS
        ALPHA(J,MPSI)=ALPHA(J,MPSI)
        95      GO TO 3015
        3011 READ (5,1000)(T(I),I=1,MPSI)
        READ (5,1000)(U(I),I=1,MPSI)
        DO 7 I=1,MPSI
        7      READ (5,1000)(ALPHA(J,I),J=1,NS)
        100      NEW THERMO DATA INPUT IN JANNAF TABLE FORM
        3015 DO 1991 I=1,NS
        READ(5,222) ATN(1),WTMOLE(1),MF(1)
        DO 10 I=1, NS
        READ(5,102) TTR(1), CP78(1,1),GTR(1,1),HT8(1,1)
        1      ATTE(IT,1) =GTR(1,1),GTR(1,1),HT8(1,1)
        GTP(1,1) = -GTR(1,1)*TTR(1) *MF(1) *1000.
        GTH(1,1,1) = -GTR(1,1,1)*TTR(1,1) *MF(1)*1000.
        WTH(1,1) = (GTR(1,1),MF(1))*1000.
        WTH(1,1,1) = (GTH(1,1,1),MF(1))*1000.
        10      CONTINUE
        10      IF (WTMOLE(1)-1.0) 1972,1991,1991

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PROGRAM

MAIN

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1072 IECC=1
1091 CONTINUE
DO 301 J = 1,6
DO 301 I = 1,NS
IF(AID(I).EQ.XAME(J)) ISAVE(J) = 1
301 CONTINUE
DO 1992 I=1,NR
HEAD (5,444)(71D(J),J=1,5),IRR(1),IRT(1),PC(1,K),K=1,3)
DO 1993 J=1,5,
IRR(1,J)=0
DO 1993 L=1,NS
IF(71D(J)-AID(L)) 1993,1994,1993
1994 IRR(1,J)=L
1993 CONTINUE
1992 CONTINUE
DO 912 I=1,MPSI
WTV=0.0
DO 632 J=1,NS
WTVR=WTVR+ALPHA(J,1)*WTHOLE(J)
DO 633 J=1,NS
ALPHA(J,1)=ALPHA(J,1)/WTVR
612 CONTINUE
IF(DELPST) 903,3041,903
3041 DIM=0.0
DO 5001 J=1,NS
DIM=DIM+ALPHA(J,1)
XMD=MMOD-1
DELPST=SORT(P*U(1)/42.245/T(1)/DIM)*RJ/XMD
903 DO 20 I=1,29
XI=I-1
PSI(I)=XI*DELPST
XI(I)=XLE(I)
20 SIGMA(I)=SIGMA(I)
DO 90 I=NPST,29
RT(I)=T(MPSI)
I(I)=T(MPSI)
DO 90 J=1,NS
ALPHA(J,1)=ALPHA(J,MPST)
ALPHA(J,1)=ALPHA(J,MPST)
90 U(I)=U(MPST)
CALL INOUT
PPUNCH = P
P=2117.0*P
PPDX=0.0
PRESSURE OPTION, IF IPRESS=0, PRESSURE
IS CONSTANT AND = TO P, IF IPRESS = 1, COEFFICIENTS CALLED
PC(1),PC(2),PC(3),PC(4) ARE INPUT.
EQUATION USED IS P = PC(1) + PC(2)*X + PC(3)*X*X + PC(4)*X*X*X
2 IF(IPRESS) 821,822,821
821 P=(PC(1)+X*(PC(2)+X*(PC(3)+X*PC(4))))*2117.0
PPDX=PC(2)+X*(2.0*PC(3)+X*3.0*PC(4))*2117.0
PPUNCH = P/2117.0
822 DO 31 I=1,MPSI
WTHIX(I)=0.0

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PROGRAM MAIN
DO 70 J=1,NS
30 WTMIX(I)=WTMIX(I)*ALPHA(J),P
RHO(I)=P/89517.501/1(I)/WTMIX(I)
31 PHOOUT(I)=PHO(I)/1.04
DO 805 I=1,MPSI
C
FREE STREAM VELOCITY WILL BE SET TO 1.0 FPS IF ZERO IS ENTERED
U(I)=AHAX(I)*AU(I)
TFDG(I)=EMAX(I)/(I*100.00)
T4(I)=TFDG(I)*.04
XL(I)=ALOG(TFDG(I))
CPRAR(I)=0.0
HSTAT(I)=0.0
TXG(I)
CALL TKEY(ITX, ITU, ITKFY, SDT, HDT, RT)
IF (ITKEY.EQ.0) GO TO 0
DO 805 J=1,NS
CP(J,I)=0.0
H(J,I)=0.0
CALL LIPLN(ITKEY,J,CPTR,SDT,HDT,AX)
CP(J,I)=AX*45054.31
CALL LIPLN(ITKEY,J, HTR,SDT,HDT,AX)
H(J,I)=AX*45055.31
HSTAT(I)=HSTAT(I)+H(J,I)*ALPHA(J),I
R05 CPHAR(I)=CPHAR(I)+CP(J,I)*ALPHA(J),I
ETAT(I)=0.0
Y(I)=0.0
ETA(2)=DELPSI/SORT(RHO(I)*U(2))
Y(2)=DELPSI/SORT(RHO(2)*U(2))
DO 25 I=3,MPSI
ETA(I)=SORT(ETA(I-2)*.02*DELPSI*(PSI(I)/U(I)*.4*0*PSI(I-1)+U(I-1)*PSI(I-2)/U(I-2))/1.5/RHO(I))
TFMP=(Y(I-2)*.02*DELPSI*(PSI(I)/RHO(I)/U(I)*.4*0*PSI(I-1)+PHO(I-1)/U(I-1)*PSI(I-2)/RHO(I-2)/U(I-2))/1.5)
IF (TFMP.LT.0.0) CALL OUTPUT
25 Y(I)=SORT(TEMP)
C*** HAS MIXING REGION INTERSECTED X AXIS YET, YES IF 0 OR -
IF (ITURB-6) 8010,8011,8010
8010 IF (U(I)-USUR01) 9000,9000,9001
C
MODEL 6 COMMON CALCULATIONS
8011 Q1=U(I)*U(MPSI)/2.0
DO 8012 I=2,MPSI
IF (Q01-U(I))*Q01-U(I-1)) 8013,8013,8012
8012 CONTINUE
8013 Q02=(Q01-U(I-1))/U(I-1))
Q0100=Y(I-1),Y(I)-Y(I-1)*Q02
Q030=1-I(I-1),I(I)-I(I-1)*Q02
Q03=CPHAR(I-1)*(CPHAR(I)-CPHAR(I-1))*Q02
Q04=1.0/(WTMIX(I-1)*WTMIX(I)-WTMIX(I-1))*Q02
Q05=89517.501/Q04
Q06=Q03/INCL3-Q05
Q07=SORT(1006*Q05*Q030)
Q0300=Q01/Q07
Q08=(ABS(U(I)-U(MPSI)))/2.0
IF (Q0300-1.2) 8014,8014,8015
8014 Q0400=(.0468*Q0300*(Q0300*(-.0460))+.0250*(Q0300*Q0300))*AK2

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PROGRAM MAIN

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GO TO 8016
R015 Q0200 = .0248*KK2
R016 IF (U(1)-USUB01)*U(1)-U(MPS1)) R020,R020,0.000
R020 IF (USUB01-9000.0) R021,R021,0.900
R021 USUB01 = 10000.0
WRITE (6,9900) X
GO TO 8900
MODEL 6 BEFORE MIXING ZONE REACHES AXIS
C 8900 Q09 = 0.95* (U(1)-U(MPS1)) * U(MPS1)
DO R021 = 2,MPS1
IF ((Q09-U(1))*(Q09-U(1))) R004,R004,0.000
R002 CONTINUE
R004 Q0200 = Y(1)-Y(1-1)*(Q09-U(1-1))/U(1)-U(1-1))
Q010 = Q0400*Q08*(Q0100-Q0200)
DO R010 = 1,MPS1
R010 XW(1) = Q010*RHO(1)
GO TO 98
MODEL 6 AFTER MIXING ZONE REACHES AXIS
C 9000 Q011 = Q0400*Q0100*Q05
DO R010 = 1,MPS1
R010 XW(1) = Q011*RHO(1)
Q0200 = 0.0
GO TO 98
9000 I077 = 9
USUB01 = 0.0
WRITE (6,9900) X
9001 LL = ITURB + I077
FOOD VISCOSITY MODEL5
GO TO (51,59,666,78,8667,8668,9003,91,99,65,70,26,30,70),LL
MODEL 1 BEFORE MIXING ZONE REACHES AXIS
R0666 XW(1) = 0.06137*(X+1.0E-05)*ABS(RHO(1))*U(1)-RHO(MPS1)*U(MPS1)
GO TO 37
MODEL 3 BEFORE MIXING ZONE REACHES AXIS
R0667 XW(1) = 0.00137*(X+1.0E-05)*RHO(1)*ANS(U(1))-U(MPS1)
GO TO 37
MODEL 4 BEFORE MIXING ZONE REACHES AXIS
R0668 XW(1) = 0.00137*(X+1.0E-05)*RHO(MPS1)*ANS(U(1))-U(MPS1)
GO TO 37
91 DO 92 I=1,MPS1
92 MODEL 0 LAMINAR FLOW
GO TO 98
45 DUM=.5*(RHO(1)*U(1)+RHO(MPS1)*U(MPS1))
DO 52 J=1,MPS1
I=MPS1-J+1
IF (RHO(1)*U(1)-DUM) 52,52,51
52 CONTINUE
MODEL 1 AFTER MIXING ZONE REACHES AXIS
C 51 ZCY(1) = (Y(1)-Y(1-1))*(RHO(1)*U(1)-DUM)/(RHO(1)*U(1)-RHO(MPS1)*U(MPS1))
XW(1) = XK2*Z*ABS(RHO(1)*U(1)-RHO(MPS1)*U(MPS1))*0.025
GO TO 37
99 DO 39 I=1,MPS1
39 XW(1) = XK2*0.025
GO TO 98

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280      7R RD=(U(1)+U(MPSI))/2.0
          DO 47 I=2,MPSI
            IF ((RD-U(I))* (RD-U(I-1))) 48,4R,47
          47 CONTINUE
          4R RHALVE=ETA(I-1)*(ETA(I)-ETA(I-1))* (RD-U(I-1))/(U(I)-U(I-1))
          DUMY=XK2*RHALVE*ABS(U(I)-U(MPSI))*0.025
          XHU(I)=DUMY*RHU(I)
          DO 79 I=2,MPSI
            C      MODEL 2 BEFORE MIXING ZONE REACHES AXIS
          285      79 XHU(I)=DUMY*(RHU(I)*ETA(I)/Y(I))*2/RHO(I)
              GO TO 98
          C      MODEL 2 AFTER MIXING ZONE REACHES AXIS
          290      26 RD=(U(1)+U(MPSI))/2.0
              DO 27 I=2,MPSI
                IF ((RD-U(I))* (RD-U(I-1))) 28,2R,27
              27 CONTINUE
              2R RHALVE=Y(I-1)*(Y(I)-Y(I-1))* (RD-U(I-1))/(U(I)-U(I-1))
              C      MODEL 3 AFTER MIXING ZONE REACHES AXIS
          295      XHU(I)=XK2*RHALVE*RHU(I)*ABS(U(I)-U(MPSI))*0.025
              DO 29 I=1,MPSI
                29 XHU(I)=XHU(I)
              GO TO 98
          300      33 RD=(U(1)+U(MPSI))/2.0
              DO 34 I=2,MPSI
                IF ((RD-U(I))* (RD-U(I-1))) 35,35,34
              34 CONTINUE
              35 RHALVE=Y(I-1)*(Y(I)-Y(I-1))* (RD-U(I-1))/(U(I)-U(I-1))
              C      MODEL 4 AFTER MIXING ZONE REACHES AXIS
          305      XHU(I)=XK2*RHALVE*RHU(I)*ABS(U(I)-U(MPSI))*0.025
              DO 36 I=1,MPSI
                36 XHU(I)=XHU(I)
              GO TO 98
          C      MODEL 5 BEFORE MIXING ZONE REACHES AXIS
          310      9003 XHU(1) = 0.00137*(5+1.0E-05)*ABS(UNIT-I(MPSI))*RHU(1)
              DO 9004 I = 2,MPSI
                XHU(I)=0.00137*(5+1.0E-05)*ABS(UNIT-U(MPSI))* (RHU(I))*2/RHO(I)
          315      9004 CONTINUE
              9R A(1)=0.0
              C      CALCULATE A
              43 A(I)=XHU(I)*RHU(I)*U(I)*Y(I)*Y(I)/PSI(I)
              DO 899 L=1,MPSI
                8RT=1.986*TL
                800TT=800T(T(L))
                TX=T(L)
                CALL TKEY(TX ,TTR,ITKEY,SDT,HDT,NT)
                IF (ITKEY.FO.0) GO TO 9
              320      DO 855 I=1,NS
                  G(I)=0.0
                  WP(I)=0.0
                  WM(I)=0.0
                  OX(I,L)=0.0
              325      DO 872 J=1,NS
                  CM(I,J,L)=0.0
              330      872 CALL LIPLN(ITKEY,I, G1R,SDT,HDT,AX)

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

PROGRAM MAIN

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707 CONTINUE
  CRP=RATE*RHOUT(L)*RHOUT(L)*WTMIX(L)*AV
  RP(I,L)=CRP*RHOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)
  RM(I,L)=CRP*ALPHA(J3,L)/(E*RT(I))
  DO 774 J=1,3
    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)
    CM(IROW,J5,L)= CM(IROW,J5,L) *SIGN*RM(I,L)/ALPHA(J5,L)
    OX(IROW,L)= OX(IROW,L) + SIGN*(RP(I,L))
    GO TO 868
  774 J1=IRRR(I,1)
  868 J1=IRRR(I,1)
  J2=IRRR(I,2)
  J3=IRRR(I,3)
  J4=IRRR(I,4)
  J5=IRRR(I,5)
  E = (G(J1)+G(J2)+G(J3)+G(J4)+G(J5))/RRT
  IF (ABS(E).LT.80.0) GO TO 708
  IF (E.LT.0.0) E=EXP(-80.0)
  IF (E.GT.0.0) E = EXP(80.0)
  GO TO 709
  708 E = EXP(E)
  709 CONTINUE
  CRP=RATE*RHOUT(L)*RHOUT(L)
  RM(I,L)=CRP*ALPHA(J1,L)*ALPHA(J2,L)
  RM(I,L)=CRP*ALPHA(J3,L)*ALPHA(J4,L)*ALPHA(J5,L)*RHOUT(L)*RT(L)/E
  DO 775 J=1, 5
    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)
    CM(IROW,J5,L)= CM(IROW,J5,L) *SIGN*RM(I,L)/ALPHA(J5,L)
    OX(IROW,L)= OX(IROW,L) + SIGN*(RP(I,L)-2.*RM(I,L))
    GO TO 861
  775 J1=IRRR(I,1)
  861 J1=IRRR(I,1)
  J2=IRRR(I,2)
  J3=IRRR(I,3)
  CRP=RATE*RHOUT(L)
  RM(I,L)=CRP*RHOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)
  RM(I,L)=0.0
  DO 776 J=1, 3
    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)
    OX(IROW,L)= OX(IROW,L) + SIGN* RP(I,L)
    GO TO 868
  776 J1=IRRR(I,1)
  868 J1=IRRR(I,1)
  J2=25

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EX5=XLE(I)*A(I)/SIGMA(I)
EX6=.5*(EX5*XLE(I+1)*A(I+1)/SIGMA(I+1))
EX7=.5*(EX5*XLE(I-1)*A(I-1)/SIGMA(I-1))
EX8=CPBAR(I)*A(I)/SIGMA(I)
EX9=.5*(EX8*CPBAR(I+1)*A(I+1)/SIGMA(I+1))
EX10=.5*(EX8*CPBAR(I-1)*A(I-1)/SIGMA(I-1))
EX14=EX4*EX5/4.0
C
- INTEGRATE ENERGY EQUATION
RT(I)=(U(I+1)-U(I-1))*2*A(I)/EX2/4.0+DX*DPDX/RHO(I)/CPBAR(I)+T(I)
1*(EX5*EX14)*T(I+1)*(EX10-EX14)+7(I-1)-(EX9*EX10)*T(I))/EX2-EX3*DX
2/CPBAR(I)
RHOIX=DX/(RHOOUT(I)*U(I))
C
- INTEGRATE SPECIES EQUATIONS
DO 41 J=1,NS
DO 41 J=1,NS
41 OX(J) = (EX6*(ALPHA(J,I+1)-ALPHA(J,I-1))*EX7*(ALPHA(J,I+1)-ALPHA(J,I-1))-ALPHA(J,I))/EX1+ALPHA(J,I)+ OX(J,I)*RHOIX
DO 781 M=1,NS
DO 781 M=1,NS
CMI(M,N)=CM(M,N)*RHOIX
IF (M.EQ.N) CMI(M,N)=CMI(M,N)+1.0
781 CONTINUE
CALL SLDP(OX1,CMI,NS)
785 FORMAT (1H, 215)
DO 782 J=1, NS
782 RALPHA(J,I)= OX1(J)
101 CONTINUE
786 WRITE(6,786) DX,X
FORMAT(1H, 1P2E12.5)
EX1=4.0*XMU(1)*DX/DELPSI/DELPSI
RHOIX=DX/(RHOOUT(1)*U(1))
C
COMPUTE U AT CENTER LINE
RUI(1)=EX3*(U(2)-U(1))+U(1)-DX*DPDX/RHO(1)/U(1)
FX4=0.0
DO 200 J=1,NS
DO 200 J=1,NS
EX4=EX4+H(J,I)*WDOT(J,I)
RALPHA(J,MPSI)=ALPHA(J,MPSI)
200 OX1(J) =EX3*XLF(1)*(ALPHA(J,2)-ALPHA(J,I))/SIGMA(I)+ALPHA(J,I)
1+ OX(J,I)*RHOIX
DO 783 M=1,NS
DO 783 M=1,NS
CMI(M,N)=CM(M,N,1)*RHOIX
IF (M.EQ.N) CMI(M,N)=CMI(M,N)+1.0
783 CONTINUE
CALL SLDP(OX1,CMI,NS)
DO 784 J=1, NS
C
COMPUTE SPECIES AT CENTER LINE
784 RALPHA(J,I)= OX1(J)
C
CALCULATE TEMP. AT CENTER LINE
PT(I)=EX3*(T(2)-T(1))/SIGMA(I)+T(1)+DX*DPDX/RHO(1)/CPBAR(1)
1-EX4*DX/CPBAR(1)
PT(MPSI)=T(MPSI)
IF (EDGE) 230,231,230
C
COMPUTE TEMP. AND U AT EDGE
270 RUI(MPSI)=U(MPSI)+DX*DPDX/RHO(MPSI)/U(MPSI)
PT(MPSI)=T(MPSI)+DX*DPDX/RHO(MPSI)/CPBAR(MPSI)

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PROGRAM MAIN

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665      DC 210 I=MPSI,29
          RU(I)=RU(MPSI)
          U(I)=U(MPSI)
          PT(I)=PT(MPSI)
          210 T(I)=RT(MPSI)
          231 CONTINUE
          1 IFNIS=1
          921 SAVEEX=X
          940 CONTINUE
          941 CONTINUE
          MINT = 13
          MHALF = 25
          NTEST=MPSI-1
          DO 967 I=1,NTEST
            CHECK NEGATIVE MOLE FRACTION
          965 DO 967 J=1,NS
            IF (RALPHA(J,I)) 995,967,967
          967 CONTINUE
          X=X+DX
          PCNT=PCNT+DX
          DX=XD
          DO 925 I=1,29
            DO 926 J=1,NS
          926 ALPHA(J,I)=RALPHA(J,I)
            T(I)=RT(I)
          925 U(I)=RU(I)
          GO TO 999
          995 IF (DX.LT.DXMIN) GO TO 8000
          981 DX=SAVEDX/2.0
          X=SAVEX
          DO 985 I=1,29
            DO 982 J=1,NS
          982 ALPHA(J,I)=SAVEAL(J,I)
            T(I)=SAVET(I)
          985 U(I)=SAVEU(I)
          GO TO 2
          C
          IF MPSI.GE.26,MPSI IS HALVED
          999 IF (MPSI-MHALF) 1001,1500,1500
          1001 IF (ABS(U(MPSI)-U(MPSI-1))) 1011,1011,1004
          1011 IF (ABS(T(MPSI)-T(MPSI-1))) 1002,1002,1004
          1002 CONTINUE
          GO TO 2000
          1004 MPSI=MPSI-1
          MPSI=MPSI-1
          DO 1101 I=MPSI,29
            SAVEU(I)=U(MPSI)
            PT(I)=U(MPSI)
            U(I)=U(MPSI)
            SAVET(I)=T(MPSI)

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PROGRAM MAIN

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720      T(I)=T(NPSI)
          PT(I)=T(NPSI)
          DO 1102 J=1,NS
              SAVEA(J,I)=ALPHA(J,NPSI)
              ALPHA(J,I)=ALPHA(J,NPSI)
1102      RALPHA(J,I)=ALPHA(J,NPSI)
1101      CONTINUE
          GO TO 2000
1500      IFINIS=0
          ORLPSI=DELPSI*DFLPSI
          DO 1600 I=1,MINIT
              DO 1650 J=1,NS
                  ALPHA(J,I)=ALPHA(J,2*I-1)
1650      T(I)=T(2*I-1)
          T(I)=T(I-1)
1600      U(I)=U(2*I-1)
          MPSI=MINIT
          NPSI=MPSI-1
          DO 1700 I=MINIT,29
              DO 1750 J=1,NS
                  ALPHA(J,I)=ALPHA(J,NPSI)
1750      RALPHA(J,I)=ALPHA(J,NPSI)
          T(I)=T(NPSI)
          U(I)=U(NPSI)
          RT(I)=T(NPSI)
1700      RU(I)=U(NPSI)
          DO 1800 I=2,29
1800      PSI(I)=PSI(I-1)*DELPSI
          ITER=0
          ISTEP=0
          GO TO 2000
8000      WRITE (6,R001)
8001      FORMAT(68HNEGATIVE PARAMETER - NOT CORRECTED BY REPEATED HALVING
              10F,STEP SIZE)
          IFINIS=2
          GO TO 69
2000      CONTINUE
          CALL TICK(ISECS)
          IELAPS = ISECS-ISECST
          IF (IELAPS.LT.0) IELAPS = IDIFFT + ISECS
          IF (IELAPS.GE.ILIMIT) GO TO 6
          GO TO 2
100      FORMAT(14I5)
102      FORMAT(8F10.4)
111      FORMAT (7(1PE10.3))
222      FORMAT (A6,7E10.3)
333      FORMAT(12A6)
444      FORMAT(A6,1X,A6,8X,A6,1X,A6,7X,12,11,E8,2,F4,1,F9,1)
555      FORMAT(7(1PE10.3))
666      FORMAT(10I5)
1000      FORMAT(7E10.3)
9900      FORMAT (39H1 MIXING REGION INTERSECTS AXIS AT X = 1PE15.7)
          IF (IPUNCH.EQ.0.OR.IPUNCH.EQ.7) GO TO 9
          PUNCH333,(TITLE(I),I=1,12)
          PUNCH 666,MPSI,NS,ITURQ,NR,IOUT1,IOUT2,IPUNCH,ITIME,IPRESS,NT
          PUNCH 555,FREQA(1),FREQA(2),FREQA(3),FREQA(4),FREQA(5),FREQA(6)

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PROGRAM MAIN

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PUNCH 555,X,XHAX,PNT,XLE(1),SIGNA(1),RJ,XK2
PUNCH 555,DXMIN,FIL,PC(1),PC(2),PC(3),PC(4)
PUNCH 555,PPUNCH,T(1),TIMPSI,U(1),UINPSI,DELPSI,TKINET
PUNCH 555,T(1),I=1,MPSI)
PUNCH 555,U(1),I=1,MPSI)
ON H I = 1,MPSI
PUNCH 555,(ALPHA(J,I),J=1,NS)
R CONTINUE
9 CONTINUE
END
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SUBROUTINE OUTPUT

CNC 6600 FTM V3.0-P312 OPT=2 08/07/77 12.54.49.

PAGE

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SUBROUTINE OUTPUT
  DIMENSION A(30),RHO(30),Y(30),T(30),PSI(30),RT(30),SUM(30),AR(25),
  JHSTAT(30),H(25,30),ALPHA(25,30),RALPHA(25,30),CP(25,30),SIGMA(30),
  5 WMQ(F(25),CPRAP(30),C(25,9),AID(25),ETA(30),RATIO(30),
  3PU(30),U(30),TIT(12),XLE(30),XMU(30),
  4RC(40,3),IRRP(40,5),WP(25),WM(25),WMQ(25,30),SAVEU(30),
  5 IRR(40,5),ERED(30),SAVEA(25,30),
  6 ECC(30),HOUT(30),YOUT(30),RHOUT(30),XHUOUT(30),XLT(30),
  7T4(30),TFDG(30),IRTI(40),REL(40,30),RM(40,30),
  10 DIMENSION ISAVE(4),FREDA(6),ALOC(50,4),ATT(6),YATT(50)
  COMMON A , RHO , Y , T , PSI , RT ,
  COMMON SUM , AR , HSTAT , H , ALPHA , RALPHA ,
  COMMON CP , SIGMA , WMQ , WMOLE , CPRAP , C ,
  COMMON AID , ETA , RATIO , RU , U , TITLE ,
  15 COMMON XLE , XHU , XG , WMIX , XDOT ,
  COMMON SAVEU , SAVED , WM , PC , RC , XMAX ,
  COMMON PRNT , DXMIN , DX , FDL , DELPSI , RJ ,
  COMMON XK2 , P , ZID , FREQ , ECC , DPDX ,
  COMMON YOUT , HOUT , RHOUT , IRRP , IRR , IFINIS ,
  20 COMMON IPAGE , MPSI , BY , NS , NR , IEDGE ,
  COMMON ITURB , IPRESS , MPSI , ITES , ITFR , IECC ,
  COMMON IPT , XHUOUT , XLT , T4 , TFDG , IOUT ,
  COMMON IOUT1 , IOUT2 , RP , RM , ISAVE , IPUNCH ,
  25 COMMON TRINET,NFREDA,ALOC,FREDA,00100,00200,00300,00400
  DATA ZC02/6HC0 /
  DATA ZC02/6HC0 /
  DATA ZH20/6HR20 /
  RTG=1.0E30
  DO 5 I=1, NS
  IF (AID(I),EQ,ZC0 ) IC0=1
  IF (AID(I),EQ,ZC02) IC02=1
  IF (AID(I),EQ,ZH20)...IR20=1
  30
  5 CONTINUE
  IF (IECC) 531,539,531
  531 DO 532 I=1,MPSI
  532 ECC(I)=RHO(I)*ALPHA(IECC,I)*3.108E23
  539 DO 10 I=1,MPSI
  YOUT(I)=Y(I)/PJ
  XHUOUT(I)=XHU(I)*32.174
  HOUT(I)=HSTAT(I)/45055.31
  SUM(I)=0.0
  DO 10 J=1,NS
  40 SUM(I)=SUM(I)+ALPHA(J,I)*WMOLE(J)
  UD=.05*U(I)+.95*U(MPSI)
  DO 43 I=2,MPSI
  IF ((U(I)-UD)*(U(I-1)-UD)) 84,84,83
  43 CONTINUE
  83 V0=Y(I)-Y(I-1)*(UD-U(I-1))/(U(I)-U(I-1))+Y(I-1)
  84 V0=Y(I)-Y(I-1)*(UD-U(I-1))/(U(I)-U(I-1))+Y(I-1)
  50 IC=.05*V(I)+.95*V(MPSI)
  DO 45 I=2,MPSI
  IF ((I(I)-T0)*(I(I-1)-T0)) 86,86,85
  45 CONTINUE
  85 IC=V(I)-Y(I-1)*(T(I)-T(I-1))/(T(I)-T(I-1))+Y(I-1)
  86 IC=V(I)-Y(I-1)*(T(I)-T(I-1))/(T(I)-T(I-1))+Y(I-1)
  55 TP=TR/RJ
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VP=VR/PJ
DO 87 J=1,NS
  AR(J)=0.0
  AD=.05*ALPHA(J,1)*.95*ALPHA(J,MPSI)
  IF (ALPHA(J,MPSI)) 91,92,93
91  DO 88 I=1,MPSI
    IF (ALPHA(J,I)-AD) 88,88,89
88  CONTINUE
89  AR(J)=Y(I-1)*Y(I-1)*(AD-ALPHA(J,I-1))/(ALPHA(J,I)-ALPHA(J,I-1))
  AR(J)=AR(J)/RJ
  GO TO 87
92  DO 93 I=1,MPSI
    IF (ALPHA(J,I)-AD) 94,93,93
93  CONTINUE
94  GO TO 89
87  CONTINUE
PCNT=0.0
IPAGE=IPAGE+1
WRITE (6,201)X,(TITLE(I),I=1,12),IPAGE
WRITE (6,102)
XOPJ=X/RJ
POUT=P/2117.0
POUT=POUT/2117.0
WRITE(6,103) XOPJ,DX,POUT
IF (ITURB-6) 8600,8500,8600
8500 WRITE (6,8555)
    Q0101=00100/RJ
    Q0201=00200/RJ
    WRITE (6,8556) Q0101,Q0201,Q0300,Q0400
8556 FORMAT(1H0.8X,4HHALF,21X,12HINFR MIXING,17X,11HMACH NUMBER,16X,11
    *MIXING RATE/7X,10HRADIUS/R *16X,15HZONE RADIUS/P *14X,14HAT HAL
    *F RADIUS,14X,11HCOEFFICIENT)
855A FORMAT (4X,1PE14.6,1P3E28.6)
8600 WRITE (6,107)
    DO 73 I=1,MPSI
      SS1= 89517.501*WTHIX(I)
      SS2= CPBAR(I)/(CPBAR(I)-SS1)
      SS=SQRT(SS2*SS1)*T(I)
      XMACH= U(I)/SS
      IF (IECC) 71,72,71
71  WRITE (6,207)I,YOUT(I),U(I),T(I),RHQOUT(I),XMACH, HOUT(I), XMUOUT(
      11)-ECC(I),PSI(I),I
      GO TO 73
72  WRITE (6,307)I,YOUT(I),U(I),T(I),RHQOUT(I),XMACH, HOUT(I), XMUOUT(
      11) *PSI(I),I
73  CONTINUE
    DO 581 I=1,MPSI
      DO 581 J=1,NS
581  RALPHA(J,I)=ALPHA(J,I)/WTHIX(I)
      IPRT=(NS+6)/7
      DO 564 KK=1,IPRT
        II=1+(KK-1)*7
        IP=7*(KK-1)*7

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SUBROUTINE OUTPUT

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      FT3 = 1.0/FT(1)
      FT4 = 1/(1.00.75)
      SUMS = 0.0
      DO 603 IDX = 1,6
      IF (ISAVE(IDX).EQ.0) GO TO 603
      K = ISAVE(IDX)
      TERM = ALPHA(K,1)
      GO TO (604,605,606,607,608,614),IDX
      604 Q = (1.29E-17)*FT2 + 2.46E-16
      GO TO 609
      605 Q = (0.758E-13)*FT1
      GO TO 609
      606 Q = (1.53E-11)*FT3
      GO TO 609
      607 Q = (9.0E-18)*FT2 + 8.9E-16
      GO TO 609
      608 Q = 3.29E-23*6.21E5*FT2
      GO TO 609
      614 Q = 1.85*(6.21)**(-2)*(1.0E-10)*FT3
      609 SUMS = SUMS + Q*TERM
      601 CONTINUE
      XNEU = (4.57E27)*SUMS*POUT*FT1
      ECON = 0.07157* ECC(1)/XNEU
      IF (NFREQA) 1000, 1001, 1000
      1000 CATT = 1.17
      GO 1003 J = 1,NFREQA
      ALOC1 = 1. + (6.283*6.283*FREQA(J)*FREQA(J)*1.0E12/(XNEU*XNEU))
      1003 ALOC(I,J) = CATT*ECC(I)/XNEU*ALOC1
      GO TO 1008
      1001 WRITE(6,610) I, YOUT(I),XNEU,ECON
      GO TO 1010
      1008 WRITE(6,610) I, YOUT(I),XNEU,ECON*(ALOC(I,J),J=1,NFREQA)
      1010 IF (IPUNCH.EQ.0.OR.IPUNCH.EQ.2) GO TO 602
      RPT = YOUT(I)
      PPCO = ALPHA(IC0,1)*POUT
      ECCO2 = ALPHA(IC02,1)*POUT
      PPH20 = ALPHA(IP20,1)*POUT
      WRITE(7,780) RPT,ECC(I),XNEU,T(I),PPCO,PPCO2,PPH20
      602 CONTINUE
      IF (NFREQA) 1009, 1015, 1009
      1009 DO 1004 J = 1, NFREQA
      DO 1005 I = 1, NPST
      1005 YATT(I) = 24.0*PJ*ALOC(I,J)
      CALL GRATE(ATT(J),YATT,YOUT,NPST)
      1004 CONTINUE
      1004 WRITE (6,1014) (ATT(J),J=1,NFREQA)
      1015 CONTINUE
      102 FORMAT(1H0,8X,3HX/P,
      1FFET,4X,10HPRESS(ATM)).
      103 FORMAT(4X,10PE16.6)
      107 FORMAT(4H0 PT,5X,3HY/R, 6X,9HVELOCITY,4X,11HTEMPERATURE,5X,7HDENSI
      1TY, 6X,8HMAC NO., 8X,8HENTHALPY,5X,9HVIScosity,5X,*ELECTRON*
      12X,3HPSI,6X,2HPT )
      109 FORMAT(3H0PT,3X,5H Y/R, 7(3X,46,4X),1X,3H PT)
      201 FORMAT(1H1,//////3H X=1PE15,7,5H FEET,8X,12A6,8X,4HPAGE16)

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SUBROUTINE OUTPUT

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207 FORMAT(14,F10.4,1PE14.6,14)
208 FORMAT(13,F9.5,1PE13.5,13)
209 FORMAT(1H,/,40X,REACTION_RATES,(NOLE/HL*SEC),/)/
210 FORMAT(14,F10.4,1PE14.6,14X,14)
211 FORMAT(1H0,44X,14HOLE FRACTIONS)
212 FORMAT(1H0,35X,36HNET RATE OF PRODUCTION (N-DOT/RH0*U))
213 FORMAT(3H0PT,8X,7(13X,A6,4X),1X,3H,PT)
214 FORMAT(13,9X,1PE13.5,13)
215 FORMAT(1H0,2HPL,4X,3HPL,8X,5(8HREACTION,13,11X),2HPT)
216 FORMAT(19X,5(2HPP, 9X,2HPP,10X))
217 FORMAT(13,1X,1PE13.5,14)
218 FORMAT(18X,8HFEET/SEC,3X,DENSITY(11/ML),*
219 1X,9HLB/FT/SEC,3X,DENSITY(11/ML),*
220 1X,9HLB/FT/SEC,3X,DENSITY(11/ML),*
221 1X,9HLB/FT/SEC,3X,DENSITY(11/ML),*
222 1X,9HLB/FT/SEC,3X,DENSITY(11/ML),*
223 1X,9HLB/FT/SEC,3X,DENSITY(11/ML),*
224 1X,9HLB/FT/SEC,3X,DENSITY(11/ML),*
225 1X,9HLB/FT/SEC,3X,DENSITY(11/ML),*
226 1X,9HLB/FT/SEC,3X,DENSITY(11/ML),*
227 1X,9HLB/FT/SEC,3X,DENSITY(11/ML),*
228 1X,9HLB/FT/SEC,3X,DENSITY(11/ML),*
229 1X,9HLB/FT/SEC,3X,DENSITY(11/ML),*
230 1X,9HLB/FT/SEC,3X,DENSITY(11/ML),*
231 1X,9HLB/FT/SEC,3X,DENSITY(11/ML),*
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248 1X,9HLB/FT/SEC,3X,DENSITY(11/ML),*
249 1X,9HLB/FT/SEC,3X,DENSITY(11/ML),*
250 1X,9HLB/FT/SEC,3X,DENSITY(11/ML),*
251 1X,9HLB/FT/SEC,3X,DENSITY(11/ML),*

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SUBROUTINE INOUT

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115      J4=IRRR(1,4)
      J5=IRRR(1,5)
      WRITE (6,128)I,AID(J1),AID(J2),AID(J3),AID(J4),AID(J5),(RC(I,J),J=
116      11,3)
      GO TO 159
130      J1=IRRR(1,1)
      J2=IRRR(1,2)
      J3=IRRR(1,3)
      WRITE (6,129)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)
120      GO TO 159
140      J1=IRRR(1,1)
      J2=IRRR(1,2)
      J3=IRRR(1,3)
      WRITE (6,130)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)
125      159 CONTINUE
120      FORMAT(1H0,19X,26HREACTIONS REING CONSIDERED,6X,19HKA=EXP(B/RT)/
121      11=N,7X,1HA,8X,1HN,9X,1HR,7X,*(MOLECULEF-ML-SEC UNITS),*)
121      FORMAT(19,9X,A6,2H, *A6,8X,2H= *A6,2H, *A6,18X,1PE9,3,2X,0PF4,1,2X
122      1,F10,1)
122      FORMAT(19,9X,A6,2H, *A6,3H, *M,5X,2H= *A6,3H, *M,23X,1PE9,3,2X,0PF4,
123      1,1,2X,F10,1)
123      FORMAT(19,9X,A6,2H, *A6,8X,2H= *A6,2H, *A6,10X,1PE9,3,2X,0
124      1PF4,1,2X,F10,1)
124      FORMAT(19,9X,A6,2H, *A6,8X,2H= *A6,26X,1PE9,3,2X,0PF4,1,2X,F10,1)
125      FORMAT(19,9X,A6,3H, *M,13X,2H= *A6,2H, *A6,3H, *M,15X,1PE9,3,2X,0PF4
126      1,1,2X,F10,1)
126      FORMAT(19,9X,A6,2H, *A6,8X,2H= *A6,2H, *A6,18X,1PE9,3,2X,0PF4,1,2X
127      1,F10,1,3X,16HONE WAY REACTION)
127      FORMAT(19,9X,A6,2H, *A6,3H, *M,5X,2H= *A6,3H, *M,23X,1PE9,3,2X,0PF4,
128      1,1,2X,F10,1,3X,16HONE WAY REACTION)
128      FORMAT(19,9X,A6,2H, *A6,8X,2H= *A6,2H, *A6,10X,1PE9,3,2X,0
129      1PF4,1,2X,F10,1,3X,16HONE WAY REACTION)
129      FORMAT(19,9X,A6,2H, *A6,8X,2H= *A6,26X,1PE9,3,2X,0PF4,1,2X,F10,1,3
130      1X,16HONE WAY REACTION)
130      FORMAT(19,9X,A6,3H, *M,13X,2H= *A6,2H, *A6,3H, *M,15X,1PE9,3,2X,0PF4
131      1,1,2X,F10,1,3X,16HONE WAY REACTION)
131      FORMAT(1H1,37X,46HAEROCHEM RESEARCH LABORATORIES PRINCETON N.J.)
132      FORMAT(25X,*)A FAST COMPUTER PROGRAM FOR NONEQUILIBRIUM ROCKET PLUM
133      1E PREDICTIONS)
133      FORMAT(1H0,24X,12A6)
134      FORMAT(1H0,22X,19HPRESSURE(INITIAL) =1PE15,7,12H ATMOSPHERES)
135      FORMAT(1H0,22X,20HPRESSURE(CONSTANT) =1PE15,7,12H ATMOSPHERES)
136      FORMAT(123X,24HTEMPERATURE( DEG. KELVIN),3X,1PE15,7,4X,1PE15,7)
137      FORMAT(23X,24HVELOCITY (FEET/SECOND),3X,1PE15,7,4X,1PE15,7)
138      FORMAT(1H0,22X,14HNOZZLE RADIUS=1PE15,7,5H FEET)
139      FORMAT(1,0,22X,23HEWIC NUMBER(CONSTANT)=1PE15,7,5X,25HPRANDTL NUM
140      1BER(CONSTANT)=1PF15,7)
141      FORMAT(1H0,54X,3HJET,16X,4HEDGE)
142      FORMAT(23X,13HMOLE FRACTION,3X,A6,5X,1PE15,7,4X,1PE15,7)
143      FORMAT(1H0,22X,40HMINAP VISCOSITY MODEL (SUTHERLANDS LAW))
144      FORMAT(1H0,22X,29HCONSTANT VISCOSITY MODEL MU=1PE15,7)
145      FORMAT(1H0,22X,27HFERRI VISCOSITY MODEL K=1PE15,7)
146      FORMAT(1H0,22X,31HTING-LIBBY VISCOSITY MODEL K=1PF15,7)
147      FORMAT(1H0,22X,14HX INITIAL (FEET)=1PE15,7,12X,14HX FINAL (FEET)=1PE
148      115,7)

```

SUBROUTINE INOUT

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

PAGE

```

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

```

170

SUBROUTINE GRATE

```

SUBROUTINE GRATE(ANSWER,Y,X,N)
DIMENSION X(30),Y(50)
SUM = 0.0
INTER = N-1
I1 = 1
I2 = 2
DO 1 I = 1,INTER
SUM = SUM + (X(I2)-X(I1))*Y(I2)+Y(I1))
I1 = I1 + 1
I2 = I2 + 1
1 CONTINUE
ANSWER = 0.5*SUM
RETURN
END

```

CDC 6600 FTN V3.0-P312 OP1=2 08/07/72 12.54.49.

PAGE 1

GRATE
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SUBROUTINE TICK

SUBROUTINE TICK(JJJJ)
CALL SECONDTIMEF
JJJ=TIME
RETURN
END

CDC 6600 FTU VJ.6-P312 OPT=2

08/07/72

12.54.49.

PAGE

1

TICK
TICK
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TICK

SUBROUTINE SLOP

```

      C      SUBROUTINE SLOP(X,A,N)
      C      THIS PROGRAM FINDS THE SOLUTIONS TO A SET OF N SIMULTANEOUS LINEAR
      C      EQUATIONS BY USING THE GAUSS-JORDAN REDUCTION ALGORITHM WITH THE
      C      DIAGONAL PIVOT STRATEGY
      C      DIMENSION A(25,25),X(25)
      C      DO 9 K=1,N
      C      IF (ABS(A(K,K)) .GT. 1.E-10) GO TO 5
      C      WRITE (6,101)
      C      GO TO 99
      C      5 KPI= K+1
      C      DO 6 J= KPI, N
      C      A(K,J)= A(K,J)/A(K,K)
      C      X(K)= X(K)/A(K,K)
      C      A(K,K)= 1.0
      C      DO 9 J=1,N
      C      IF (1.E0.K .OR. A(I,K).EQ.0.) GO TO 9
      C      DO 8 J=KPI,N
      C      A(I,J)= A(I,J)- A(I,K)*A(K,J)
      C      X(I)= X(I)- A(I,K)*X(K)
      C      A(I,K)=0.
      C      9 CONTINUE
      C      99 CONTINUE
      C      101 FORMAT( * ERROR--- SMALL PIVOT *)
      C      RETURN
      C      END

```

SURROUTINE TKFY

CDC 6600 F1N V3.0-P312 OPT=2 08/07/72 12.54.49.

PAGE

1

SURROUTINE TKFY(IT,ITB,ITKEY,SOT,HOT,NT)

DIMENSION ITB(30)

NTI=NT-1

DO 10 IT=1,NTI

OT= ITB(IT+1)-ITR(IT)

SOT=(1-ITB(IT))/OT

HOT=(ITB(IT+1)-1) /OT

IF ((SOT*HOT).GE.0.0) GO TO 11

10 CONTINUE

WRITE(6,100) T,I

ITKPY=0

100 FORMAT(1H , * TEMPERATURE OUT OF RANGE *,E14.5,15)

RETURN

11 ITKEY=IT

RETURN

END

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SUBROUTINE LIPLN

CDC 6606 FIN V3.0-P312 01-1-2 08/07/72 12.56.49.

PAGE

1

SUBROUTINE LIPLN (ITKEY,I,ATR,SDI,MOT,AX)
DIMENSION ATR(25,30)
AX= ATR(I,ITKEY)*MOT+ ATR(I,ITKEY,I)*SDI
RETURN
END

LIPLN 2
LIPLN 3
LIPLN 4
LIPLN 5
LIPLN 6

5

APPENDIX B

SAMPLE INPUT DATA SHEET

FOUO: All Coding Form

A FAST COMPUTER PROGRAM FOR NONEQUILIBRIUM ROCKET PLUME PREDICTIONS

CARD	SAMPLE TEST CASE										TABLET										
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
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1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
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1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
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IBM

FORTHAN Coding Form

THERMODYNAMIC DATA CARDS IN THE FOLLOWING ORDER: K, H, HCL, KCL, K ⁺ , H ₂ , H ₂ O, CO, CO ₂ , CL ₂ , CL ⁻ , F ⁻ , O, OH, O ₂ , Al ₂ O 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	2 ND SPECIES (H)								
11.2.1	18 TH SPECIES (N ₂)								
11.1.12									

IBM

CHEMICAL REACTION CARDS:

12.1 KCL	+ H	= K	+ HCL	15 3.0E-11	4072.
12.2 ϕ	+ ϕ	+ M	= ϕ Z	22 1.0E-29	1.0
12.3 H	+ H	+ M	= H Z	22 1.0E-29	1.0
12.4 ϕ	+ H	+ M	= ϕ H	22 1.0E-29	1.0
12.5 H	+ ϕ H	+ M	= H Z ϕ	22 1.0E-28	1.0
12.6 C ψ	+ ϕ	+ M	= C ϕ Z	26 5.0E-29	1.0 -4000.
12.7 ϕ H	+ ϕ H		= H Z ϕ	15 1.0E-11	-1000.
12.8 ϕ H	+ H Z		= H Z ϕ	15 4.0E-11	-5500.
12.9 ϕ	+ H Z		= ϕ H	15 3.0E-11	-8200.
12.10 H	+ ϕ Z		= ϕ H	15 3.0E-10	-16500.
12.11 C ϕ	+ ϕ H		= C ϕ Z	15 5.0E-13	-600.

IBM

FORTRAN Coding Form

B-4

FORTRAN STATEMENT

1212 H	+HCL	=CL	+H2	15 8.0E-11	-4622.
1213 HCL	+ΦH	=H2Φ	+CL	15 7.2E-12	-3250.
1214 ΦH	+CL	=HCL	+Φ	15 3.0E-11	-5000.
1215 H	+CL	=HCL	+M	22 3.0E-29	
1216 K+	+E-	=K	+M	27 2.0E-22	1.5
1217 K+	+CL-	=K	+CL	14 1.0E-08	0.5
1218 CL	+E-	=CL-	+M	21 3.0E-30	
1219 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 (R7772)

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 H	3.2784627E-08	0.
MOLE FRACTION HCL	5.3647026E-03	0.
MOLE FRACTION HCL	5.0467965E-02	0.
MOLE FRACTION K	5.9608140E-04	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(P/RT)/T**N			A			N			B			(MOLECULE-ML-SEC UNITS)		
	K	H	M	K	H	M	K	H	M	K	H	M	K	H	M	K	H	M
1	KCl	+	H	=	K	+	HCL	3.000E-11	-0.0	4072.0	-0.0							
2	O	+	O	=	O2	+		1.000E-29	1.0	-0.0								
3	H	+	H	=	H2	+		1.000E-29	1.0	-0.0								
4	O	+	H	=	OH	+		1.000E-29	1.0	-0.0								
5	H	+	OH	=	H2O	+		1.000E-29	1.0	-0.0								
6	CO	+	O	=	CO2	+		1.000E-29	1.0	-0.0								
7	OH	+	H2	=	H2O	+		1.000E-11	-0.0	-4000.0	-0.0							
8	OH	+	H2	=	H2O	+		1.000E-11	-0.0	-1000.0	-0.0							
9	O	+	H2	=	H2O	+		1.000E-11	-0.0	-5500.0	-0.0							
10	H	+	OH	=	H2O	+		1.000E-11	-0.0	-6200.0	-0.0							
11	CO	+	OH	=	CO2	+		1.000E-11	-0.0	-16500.0	-0.0							
12	HCl	+	OH	=	H2O	+		1.000E-11	-0.0	-4622.0	-0.0							
13	HCl	+	OH	=	H2O	+		1.000E-11	-0.0	-3250.0	-0.0							
14	OH	+	Cl	=	OHCl	+		1.000E-11	-0.0	-5000.0	-0.0							
15	H	+	Cl	=	HCl	+		1.000E-11	-0.0	-0.0	-0.0							
16	K+	+	F-	=	KF	+		1.000E-11	-0.0	-0.0	-0.0							
17	K+	+	Cl-	=	KCl	+		1.000E-11	-0.0	-0.0	-0.0							
18	Cl	+	F-	=	ClF	+		1.000E-11	-0.0	-0.0	-0.0							
19	Cl	+	Cl-	=	Cl2	+		1.000E-11	-0.0	-6210.0	-0.0							

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SAMPLE TEST CASE (8/7/72)

FFFT

X= 0.

DELTA X FEET
2.500000E-02

PRESS(ATM)
1.000000E-01

INNER MIXING
ZONE RADIUS/R
1.019904E+00

HALF
RADIUS/P
1.19904E+00

X/R
0.

MIXING RATE
COEFFICIENT
2.480000E-02

MACH NUMBER
AT HALF RADIUS
1.775436E+00

TEMPERATURE
K

VELOCITY
FEET/SEC

Y/R

PT

PT	Y/R	VELOCITY FEET/SEC	TEMPERATURE K	DENSITY G/CC	MACH NO.	ENTHALPY CAL/GM	VISCOSITY LB/FT/SEC	ELECTRON DENSITY(1/ML)	PSI	PT
1	0.0000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	0.	1
2	.1000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	1.259332E-02	2
3	.2000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	2.518665E-02	3
4	.3000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	3.777997E-02	4
5	.4000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	5.037330E-02	5
6	.5000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	6.296662E-02	6
7	.6000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	7.559994E-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

SAMPLE TEST CASE (U/777)

MOL FRACTIONS

PT	Y/R	K	FEET	H	HCL	HCL	K ₂	H ₂	H ₂ O	PT
1	0.0000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	1
2	.10000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	2
3	.20000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	3
4	.30000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	4
5	.40000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	5
6	.50000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	6
7	.60000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	7
8	.70000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	8
9	.80000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	9
10	.90000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	10
11	1.00000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	11
12	1.20000	0.		0.	0.	0.	0.	0.	0.	12
13	2.28737	0.		0.	0.	0.	0.	0.	0.	13

NET RATE OF PRODUCTION (W-00T/PHOEU)

PT	Y/R	K	FEET	H	HCL	HCL	K ₂	H ₂	H ₂ O	PT
1	0.0000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	1
2	.10000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	2
3	.20000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	3
4	.30000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	4
5	.40000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	5
6	.50000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	6
7	.60000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	7
8	.70000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	8
9	.80000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	9
10	.90000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	10
11	1.00000	3.27844E-04		9.76470E-03	5.04480E-02	5.04480E-02	5.36470E-07	8.14646E-02	2.85125E-01	11
12	1.20000	0.		0.	0.	0.	0.	0.	0.	12
13	2.28737	0.		0.	0.	0.	0.	0.	0.	13

SAMPLE TEST CASE (8/7/72)

FFET

X= U.

MOLE FRACTIONS

PT	Y/R	CO	CO2	CI	CL	E	O	OH	PT
1	0.0000	2.35445E-01	1.76033E-01	2.48235E-03	5.16600E-07	1.29142E-08	0.06012E-05	1.19212E-03	1
2	.10000	2.35445E-01	1.76033E-01	2.48235E-03	5.16600E-07	1.29142E-08	0.06012E-05	1.19212E-03	2
3	.20000	2.35445E-01	1.76033E-01	2.48235E-03	5.16600E-07	1.29142E-08	0.06012E-05	1.19212E-03	3
4	.30000	2.35445E-01	1.76033E-01	2.48235E-03	5.16600E-07	1.29142E-08	0.06012E-05	1.19212E-03	4
5	.40000	2.35445E-01	1.76033E-01	2.48235E-03	5.16600E-07	1.29142E-08	0.06012E-05	1.19212E-03	5
6	.50000	2.35445E-01	1.76033E-01	2.48235E-03	5.16600E-07	1.29142E-08	0.06012E-05	1.19212E-03	6
7	.60000	2.35445E-01	1.76033E-01	2.48235E-03	5.16600E-07	1.29142E-08	0.06012E-05	1.19212E-03	7
8	.70000	2.35445E-01	1.76033E-01	2.48235E-03	5.16600E-07	1.29142E-08	0.06012E-05	1.19212E-03	8
9	.80000	2.35445E-01	1.76033E-01	2.48235E-03	5.16600E-07	1.29142E-08	0.06012E-05	1.19212E-03	9
10	.90000	2.35445E-01	1.76033E-01	2.48235E-03	5.16600E-07	1.29142E-08	0.06012E-05	1.19212E-03	10
11	1.00000	0.	0.	0.	0.	0.	0.	0.	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 (M-DOT/RHO*U)

PT	CO	CO2	CI	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

MOLECULAR FRACTIONS

[illegible]

DATE OF PRODUCTION (W-DOT/PHOU)

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300 301 302 303 304 305 306 307 308 309 310 311 312 313 314 315 316 317 318 319 320 321 322 323 324 325 326 327 328 329 330 331 332 333 334 335 336 337 338 339 340 341 342 343 344 345 346 347 348 349 350 351 352 353 354 355 356 357 358 359 360 361 362 363 364 365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 408 409 410 411 412 413 414 415 416 417 418 419 420 421 422 423 424 425 426 427 428 429 430 431 432 433 434 435 436 437 438 439 440 441 442 443 444 445 446 447 448 449 450 451 452 453 454 455 456 457 458 459 460 461 462 463 464 465 466 467 468 469 470 471 472 473 474 475 476 477 478 479 480 481 482 483 484 485 486 487 488 489 490 491 492 493 494 495 496 497 498 499 500 501 502 503 504 505 506 507 508 509 510 511 512 513 514 515 516 517 518 519 520 521 522 523 524 525 526 527 528 529 530 531 532 533 534 535 536 537 538 539 540 541 542 543 544 545 546 547 548 549 550 551 552 553 554 555 556 557 558 559 560 561 562 563 564 565 566 567 568 569 570 571 572 573 574 575 576 577 578 579 580 581 582 583 584 585 586 587 588 589 590 591 592 593 594 595 596 597 598 599 600 601 602 603 604 605 606 607 608 609 610 611 612 613 614 615 616 617 618 619 620 621 622 623 624 625 626 627 628 629 630 631 632 633 634 635 636 637 638 639 640 641 642 643 644 645 646 647 648 649 650 651 652 653 654 655 656 657 658 659 660 661 662 663 664 665 666 667 668 669 670 671 672 673 674 675 676 677 678 679 680 681 682 683 684 685 686 687 688 689 690 691 692 693 694 695 696 697 698 699 700 701 702 703 704 705 706 707 708 709 710 711 712 713 714 715 716 717 718 719 720 721 722 723 724 725 726 727 728 729 730 731 732 733 734 735 736 737 738 739 740 741 742 743 744 745 746 747 748 749 750 751 752 753 754 755 756 757 758 759 760 761 762 763 764 765 766 767 768 769 770 771 772 773 774 775 776 777 778 779 780 781 782 783 784 785 786 787 788 789 790 791 792 793 794 795 796 797 798 799 800 801 802 803 804 805 806 807 808 809 810 811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829 830 831 832 833 834 835 836 837 838 839 840 841 842 843 844 845 846 847 848 849 850 851 852 853 854 855 856 857 858 859 860 861 862 863 864 865 866 867 868 869 870 871 872 873 874 875 876 877 878 879 880 881 882 883 884 885 886 887 888 889 890 891 892 893 894 895 896 897 898 899 900 901 902 903 904 905 906 907 908 909 910 911 912 913 914 915 916 917 918 919 920 921 922 923 924 925 926 927 928 929 930 931 932 933 934 935 936 937 938 939 940 941 942 943 944 945 946 947 948 949 950 951 952 953 954 955 956 957 958 959 960 961 962 963 964 965 966 967 968 969 970 971 972 973 974 975 976 977 978 979 980 981 982 983 984 985 986 987 988 989 990 991 992 993 994 995 996 997 998 999 1000 1001 1002 1003 1004 1005 1006 1007 1008 1009 1010 1011 1012 1013 1014 1015 1016 1017 1018 1019 1020 1021 1022 1023 1024 1025 1026 1027 1028 1029 1030 1031 1032 1033 1034 1035 1036 1037 1038 1039 104

X B " FEET

SAMPLE TEST CASE (B/7/7P)

PAGE 1

REACTION RATES (MOLE/ML-SEC)

WT	Y/W	REACTION 1 RP	RM	REACTION 2 RP	RM	REACTION 3 RP	RM	REACTION 4 RP	RM	REACTION 5 RP	RM	PT
1	1.0000F-01	5.9454F-07	1.1564E-07	1.5003F-12	2.1300E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	1
2	1.0000F-01	5.9454F-07	1.1564E-07	1.5003F-12	2.1300E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	2
3	1.0000F-01	5.9454F-07	1.1564E-07	1.5003F-12	2.1300E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	3
4	1.0000F-01	5.9454F-07	1.1564E-07	1.5003F-12	2.1300E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	4
5	1.0000F-01	5.9454F-07	1.1564E-07	1.5003F-12	2.1300E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	5
6	1.0000F-01	5.9454F-07	1.1564E-07	1.5003F-12	2.1300E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	6
7	1.0000F-01	5.9454F-07	1.1564E-07	1.5003F-12	2.1300E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	7
8	1.0000F-01	5.9454F-07	1.1564E-07	1.5003F-12	2.1300E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	8
9	1.0000F-01	5.9454F-07	1.1564E-07	1.5003F-12	2.1300E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	9
10	1.0000F-01	5.9454F-07	1.1564E-07	1.5003F-12	2.1300E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	10
11	1.0000F-01	5.9454F-07	1.1564E-07	1.5003F-12	2.1300E-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)

WT	Y/W	REACTION 6 RP	RM	REACTION 7 RP	RM	REACTION 8 RP	RM	REACTION 9 RP	RM	REACTION 10 RP	RM	PT
1	1.0000F-01	1.0711E-08	1.1404E-09	2.4730F-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	1
2	1.0000F-01	1.0711E-08	1.1404E-09	2.4730F-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	2
3	1.0000F-01	1.0711E-08	1.1404E-09	2.4730F-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	3
4	1.0000F-01	1.0711E-08	1.1404E-09	2.4730F-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	4
5	1.0000F-01	1.0711E-08	1.1404E-09	2.4730F-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	5
6	1.0000F-01	1.0711E-08	1.1404E-09	2.4730F-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	6
7	1.0000F-01	1.0711E-08	1.1404E-09	2.4730F-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	7
8	1.0000F-01	1.0711E-08	1.1404E-09	2.4730F-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	8
9	1.0000F-01	1.0711E-08	1.1404E-09	2.4730F-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	9
10	1.0000F-01	1.0711E-08	1.1404E-09	2.4730F-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	10
11	1.0000F-01	1.0711E-08	1.1404E-09	2.4730F-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	11

REACTION RATES (MOLE/ML-SEC)

PT	Y/M	REACTION 11 RM	REACTION 12 RM	REACTION 13 RM	REACTION 14 RM	REACTION 15 RM	PT
1	1.0000F-01	2.7000E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	1
2	1.0000F-01	2.7000E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	2
3	1.0000F-01	2.7000E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	3
4	1.0000F-01	2.7000E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	4
5	1.0000F-01	2.7000E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	5
6	1.0000F-01	2.7000E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6
7	1.0000F-01	2.7000E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	7
8	1.0000F-01	2.7000E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	8
9	1.0000F-01	2.7000E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	9
10	1.0000F-01	2.7000E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	10
11	1.0000F-00	2.7000E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	11

REACTION RATES (MOLE/ML-SEC)

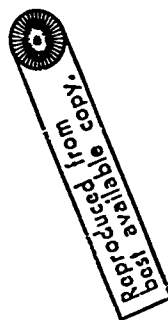
PT	Y/M	REACTION 16 RM	REACTION 17 RM	REACTION 18 RM	REACTION 19 RM	REACTION 20 RM	PT
1	1.0000F-01	1.2714E-13	6.3496E-12	5.9077E-13	2.2084E-10	2.1994E-10	1
2	1.0000F-01	1.2714E-13	6.3496E-12	5.9077E-13	2.2084E-10	2.1994E-10	2
3	1.0000F-01	1.2714E-13	6.3496E-12	5.9077E-13	2.2084E-10	2.1994E-10	3
4	1.0000F-01	1.2714E-13	6.3496E-12	5.9077E-13	2.2084E-10	2.1994E-10	4
5	1.0000F-01	1.2714E-13	6.3496E-12	5.9077E-13	2.2084E-10	2.1994E-10	5
6	1.0000F-01	1.2714E-13	6.3496E-12	5.9077E-13	2.2084E-10	2.1994E-10	6
7	1.0000F-01	1.2714E-13	6.3496E-12	5.9077E-13	2.2084E-10	2.1994E-10	7
8	1.0000F-01	1.2714E-13	6.3496E-12	5.9077E-13	2.2084E-10	2.1994E-10	8
9	1.0000F-01	1.2714E-13	6.3496E-12	5.9077E-13	2.2084E-10	2.1994E-10	9
10	1.0000F-01	1.2714E-13	6.3496E-12	5.9077E-13	2.2084E-10	2.1994E-10	10
11	1.0000F-00	1.2714E-13	6.3496E-12	5.9077E-13	2.2084E-10	2.1994E-10	11

PT	Y%	CURR. IN FREQUENCY (1/SEC)	ELECTRICAL CONDUCTIVITY (MMH./IN)	UNIT ATTENUATION (DB/IN)
		SIGMA, FREQ. (MEGACYC) = 0.750MF+00		
1	0.000	7.6402E+10	1.1017E-02	7.6402E-02
2	.100	7.6402E+10	1.1017E-02	7.6402E-02
3	.200	7.6402E+10	1.1017E-02	7.6402E-02
4	.300	7.6402E+10	1.1017E-02	7.6402E-02
5	.400	7.6402E+10	1.1017E-02	7.6402E-02
6	.500	7.6402E+10	1.1017E-02	7.6402E-02
7	.600	7.6402E+10	1.1017E-02	7.6402E-02
8	.700	7.6402E+10	1.1017E-02	7.6402E-02
9	.800	7.6402E+10	1.1017E-02	7.6402E-02
10	.900	7.6402E+10	1.1017E-02	7.6402E-02
11	1.000	7.6402E+10	1.1017E-02	7.6402E-02
12	1.398	7.6402E+00	0.	0.

TRANSMISSION

ATTENUATION (DB) = 2.6130E-01

2.50000E-02 0.
 1.90000E-01 2.50000E-02
 2.27500E-01 2.15000E-01
 1.77170E-01 4.2630E-01
 8.45850E-02 4.2630E-01
 1.77170E-01 5.7120E-01
 1.27500E-01 7.0030E-01
 1.00400E-01 8.5597E-01
 9.8447E-02 9.76410E-01



SAMPLE TEST CASE (8/7/72)

X# 1.0353036E+00 FEET

X/R 0.0000 PRESS(A7M)
4.141214E+00 0.488472E-02 1.000000E-01

HALF RADIUS/R
1.094830E+00
INNER MIXING
ZONE RADIUS/R
8.188491E-01

MACH NUMBER
AT HALF RADIUS
1.509756E+00

MIXING RATE
COEFFICIENT
2.440000E-02

PT	Y/R	VELOCITY FEET/SEC	TEMPERATURE K	DENSITY G/CC	MACH NO.	ENTHALPY CAL/GM	VISCOSITY LB/FT/SEC	ELECTRON DENSITY (1/ML)	PST	PT
1	0.0000	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419232E+09	0.	1
2	0.0999	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419308E+09	1.259332E-02	2
3	0.1998	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419308E+09	2.518665E-02	3
4	0.2997	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419308E+09	3.779979E-02	4
5	0.3995	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419308E+09	5.037330E-02	5
6	0.4994	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419308E+09	6.266664E-02	6
7	0.5993	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419308E+09	7.555994E-02	7
8	0.6992	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419308E+09	8.815327E-02	8
9	0.7991	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419308E+09	1.007466E-01	9
10	0.8990	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419308E+09	1.133399E-01	10
11	0.9989	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419308E+09	1.259332E-01	11
12	1.0988	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419308E+09	1.385266E-01	12
13	1.1987	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419308E+09	1.511199E-01	13
14	1.2986	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419308E+09	1.637132E-01	14
15	1.3985	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419308E+09	1.763065E-01	15
16	1.4984	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419308E+09	1.888999E-01	16
17	1.5983	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419308E+09	2.014932E-01	17
18	1.6982	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419308E+09	2.140865E-01	18
19	1.7981	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907385E-03	4.419308E+09	2.266798E-01	19

X# 1.0353016E+00 FFF

SAMPLE TEST CASE (8/7/77)

PAGE 2

MOL FRACTIONS

PT	Y/H	K	H	HCL	KCL	K*	H2	H2O	PT
1	0.0000	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	1
2	0.0498	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	2
3	0.1497	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	3
4	0.2496	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	4
5	0.3495	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	5
6	0.4494	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	6
7	0.5493	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	7
8	0.6492	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	8
9	0.7491	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	9
10	0.8490	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	10
11	0.9489	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	11
12	1.0488	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	12
13	1.1487	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	13
14	1.2486	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	14
15	1.3485	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	15
16	1.4484	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	16
17	1.5483	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	17
18	1.6482	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	18
19	1.7481	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39184E-07	8.14652E-02	2.84461E-01	19

NET RATE OF PRODUCTION (W-DOT/RHOFU)

PT	K	H	HCL	KCL	K*	H2	H2O	PT
1	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	1
2	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	2
3	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	3
4	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	4
5	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	5
6	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	6
7	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	7
8	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	8
9	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	9
10	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	10
11	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	11
12	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	12
13	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	13
14	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	14
15	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	15
16	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	16
17	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	17
18	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	18
19	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	19



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SAMPLE TEST CASE (B/7/72)

1.035010E+00 FEET

MOLE FRACTIONS

PT	Y/R	CO	CO2	CI	CL	E-	O	OH	PT
1	0.0000	2.35311E-01	1.76973E-01	2.37974E-03	5.20233E-07	1.19973E-08	7.89347E-05	1.70718E-03	1
2	0.0998	2.35311E-01	1.76973E-01	2.37974E-03	5.20233E-07	1.19973E-08	7.89347E-05	1.70718E-03	2
3	0.1497	2.35311E-01	1.76973E-01	2.37974E-03	5.20233E-07	1.19973E-08	7.89347E-05	1.70718E-03	3
4	0.2485	2.35311E-01	1.76973E-01	2.37974E-03	5.20233E-07	1.19973E-08	7.89347E-05	1.70718E-03	4
5	0.3953	2.35311E-01	1.76973E-01	2.37974E-03	5.20233E-07	1.19973E-08	7.89347E-05	1.70718E-03	5
6	0.4952	2.35299E-01	1.76967E-01	2.37964E-03	5.20233E-07	1.20085E-08	7.92055E-05	1.70949E-03	6
7	0.5982	2.35124E-01	1.76895E-01	2.42473E-03	5.17488E-07	1.21720E-08	8.30479E-05	1.74256E-03	7
8	0.6941	2.33509E-01	1.76322E-01	2.78895E-03	5.17400E-07	1.35410E-08	1.19987E-04	2.03246E-03	8
9	0.9070	2.25104E-01	1.73470E-01	4.44909E-03	5.06121E-07	1.59862E-08	4.33977E-04	3.63397E-03	9
10	0.9726	1.95704E-01	1.63158E-01	9.62337E-03	4.73545E-07	3.52964E-08	2.74125E-03	8.84767E-03	10
11	0.3100	1.24695E-01	1.70421E-01	1.75220E-02	7.80943E-07	4.41914E-08	9.70302E-03	1.28187E-02	11
12	0.19452	5.93039E-02	6.41834E-02	9.78882E-03	1.79322E-07	1.68830E-08	7.78412E-03	3.25615E-03	12
13	0.14188	2.29510E-02	2.22697E-02	3.15918E-03	6.20097E-08	1.56597E-09	1.08184E-03	1.52159E-04	13
14	0.171845	7.76035E-03	6.76917E-03	6.97186E-04	1.87894E-08	5.64541E-10	2.70944E-04	1.11768E-04	14
15	0.13854	2.04985E-03	1.45776E-03	1.06450E-04	4.64453E-09	1.72677E-10	5.03626E-05	3.67502E-05	15
16	0.68327	6.01088E-04	7.10788E-04	1.18801E-05	8.89377E-10	2.50529E-11	3.95033E-06	4.26322E-06	16
17	0.24214	0.12012E-04	0.43519E-05	1.01155E-06	1.34655E-10	3.22056E-12	9.24337E-08	3.17798E-07	17
18	0.76375	0.	0.	0.	0.	0.	0.	0.	18
19	0.5210	0.	0.	0.	0.	0.	0.	0.	19

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

PT	Y/R	CO	CO2	CI	CL	E-	O	OH	PT
1	-5.43544E-04	-5.43544E-04	5.43544E-04	-4.21406E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	1
2	-5.43544E-04	-5.43544E-04	5.43544E-04	-4.21406E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	2
3	-5.43544E-04	-5.43544E-04	5.43544E-04	-4.21406E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	3
4	-5.43544E-04	-5.43544E-04	5.43544E-04	-4.21406E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	4
5	-5.43544E-04	-5.43544E-04	5.43544E-04	-4.21406E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	5
6	-5.43544E-04	-5.43544E-04	5.43544E-04	-4.21406E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	6
7	-5.43544E-04	-5.43544E-04	5.43544E-04	-4.21406E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	7
8	-5.43544E-04	-5.43544E-04	5.43544E-04	-4.21406E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	8
9	-5.43544E-04	-5.43544E-04	5.43544E-04	-4.21406E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	9
10	-5.43544E-04	-5.43544E-04	5.43544E-04	-4.21406E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	10
11	-5.43544E-04	-5.43544E-04	5.43544E-04	-4.21406E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	11
12	-5.43544E-04	-5.43544E-04	5.43544E-04	-4.21406E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	12
13	-5.43544E-04	-5.43544E-04	5.43544E-04	-4.21406E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	13

1.0354034E+00 FSTT

SAMPLE TEST CASE (R/7/72)

MOLF FRACTIONS

PT	Y/R	OP	AI 203	N2	MOLF FRACTIONS				
1	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
2	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
3	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
4	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
5	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
6	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
7	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
8	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
9	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
10	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
11	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
12	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
13	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
14	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
15	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
16	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
17	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
18	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
19	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.

NET RATE OF PRODUCTION (W-DOT/RHSCU)

PT	Y/R	OP	AI 203	N2	NET RATE OF PRODUCTION (W-DOT/RHSCU)				
1	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
2	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
3	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
4	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
5	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
6	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
7	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
8	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
9	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
10	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
11	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
12	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
13	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
14	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
15	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
16	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
17	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
18	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.
19	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	0.

1.0353036E+00 FEET

SAMPLE TEST CASE (8/7/72)

PAGE 2

REACTION RATES (MOLE/ML-SEC)

PT	Y/R	REACTION 1 RP	REACTION 2 RP	REACTION 3 RP	REACTION 4 RP	REACTION 5 RP	RM	PT
1	0.9884E-02	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	3.6013E-08	1
2	1.0077E-01	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	3.6013E-08	2
3	2.9965E-01	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	3.6013E-08	3
4	3.0083E-01	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	3.6013E-08	4
5	4.9942E-01	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	3.6013E-08	5
6	5.9972E-01	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	3.6013E-08	6
7	6.9941E-01	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	3.6013E-08	7
8	7.9941E-01	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	3.6013E-08	8
9	8.9941E-01	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	3.6013E-08	9
10	9.9941E-01	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	3.6013E-08	10
11	1.0710E-00	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	3.6013E-08	11
12	1.1945E-00	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	3.6013E-08	12
13	1.4184E-00	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	5.5927E-07	3.6013E-08	13

REACTION RATES (MOLE/ML-SEC)

PT	Y/R	REACTION 6 RP	REACTION 7 RP	REACTION 8 RP	REACTION 9 RP	REACTION 10 RP	RM	PT
1	0.9884E-02	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	6.3167E-07	1
2	1.0077E-01	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	6.3167E-07	2
3	2.9965E-01	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	6.3167E-07	3
4	3.0083E-01	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	6.3167E-07	4
5	4.9942E-01	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	6.3167E-07	5
6	5.9972E-01	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	6.3167E-07	6
7	6.9941E-01	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	6.3167E-07	7
8	7.9941E-01	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	6.3167E-07	8
9	8.9941E-01	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	6.3167E-07	9
10	9.9941E-01	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	6.3167E-07	10
11	1.0710E-00	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	6.3167E-07	11
12	1.1945E-00	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	6.3167E-07	12
13	1.4184E-00	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	5.0921E-06	6.3167E-07	13

SF 1.0353076E+00 FEET

SAMPLE TEST CASE (8/7/72)

PAGE 2

REACTION RATES (MOLE/ML-SEC)

PT	Y/H	REACTION 11 RP	REACTION 12 RP	REACTION 13 RP	REACTION 14 RP	REACTION 15 RP	PT
1	0.9984F-02	3.4821F-05	3.4059E-05	1.5915E-03	6.1800E-05	6.1926E-05	1
2	0.9984F-02	3.4821F-05	3.4059E-05	1.5915E-03	6.1800E-05	6.1926E-05	2
3	1.0077F-01	1.4821F-05	3.4059E-05	1.5915E-03	6.1800E-05	6.1926E-05	3
4	0.9984F-01	3.4821F-05	3.4059E-05	1.5915E-03	6.1800E-05	6.1926E-05	4
5	0.9984F-01	3.4821F-05	3.4059E-05	1.5915E-03	6.1800E-05	6.1926E-05	5
6	0.9984F-01	3.4821F-05	3.4059E-05	1.5915E-03	6.1800E-05	6.1926E-05	6
7	0.9984F-01	3.4821F-05	3.4059E-05	1.5915E-03	6.1800E-05	6.1926E-05	7
8	0.9984F-01	3.4821F-05	3.4059E-05	1.5915E-03	6.1800E-05	6.1926E-05	8
9	0.9984F-01	3.4821F-05	3.4059E-05	1.5915E-03	6.1800E-05	6.1926E-05	9
10	0.9984F-01	3.4821F-05	3.4059E-05	1.5915E-03	6.1800E-05	6.1926E-05	10
11	0.9984F-01	3.4821F-05	3.4059E-05	1.5915E-03	6.1800E-05	6.1926E-05	11
12	0.9984F-01	3.4821F-05	3.4059E-05	1.5915E-03	6.1800E-05	6.1926E-05	12
13	0.9984F-01	3.4821F-05	3.4059E-05	1.5915E-03	6.1800E-05	6.1926E-05	13

REACTION RATES (MOLE/ML-SEC)

PT	Y/H	REACTION 16 RP	REACTION 17 RP	REACTION 18 RP	REACTION 19 RP	REACTION 20 RP	PT
1	0.9984F-02	1.2014F-12	1.4212F-11	2.6851E-11	7.0894E-12	5.6732E-13	1
2	0.9984F-02	1.2014F-12	1.4212F-11	2.6851E-11	7.0894E-12	5.6732E-13	2
3	1.0077F-01	1.2014F-12	1.4212F-11	2.6851E-11	7.0894E-12	5.6732E-13	3
4	0.9984F-01	1.2014F-12	1.4212F-11	2.6851E-11	7.0894E-12	5.6732E-13	4
5	0.9984F-01	1.2014F-12	1.4212F-11	2.6851E-11	7.0894E-12	5.6732E-13	5
6	0.9984F-01	1.2014F-12	1.4212F-11	2.6851E-11	7.0894E-12	5.6732E-13	6
7	0.9984F-01	1.2014F-12	1.4212F-11	2.6851E-11	7.0894E-12	5.6732E-13	7
8	0.9984F-01	1.2014F-12	1.4212F-11	2.6851E-11	7.0894E-12	5.6732E-13	8
9	0.9984F-01	1.2014F-12	1.4212F-11	2.6851E-11	7.0894E-12	5.6732E-13	9
10	0.9984F-01	1.2014F-12	1.4212F-11	2.6851E-11	7.0894E-12	5.6732E-13	10
11	0.9984F-01	1.2014F-12	1.4212F-11	2.6851E-11	7.0894E-12	5.6732E-13	11
12	0.9984F-01	1.2014F-12	1.4212F-11	2.6851E-11	7.0894E-12	5.6732E-13	12
13	0.9984F-01	1.2014F-12	1.4212F-11	2.6851E-11	7.0894E-12	5.6732E-13	13

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UNIT ATTENUATION (dB/IN)

CONDUCTION
ELECTRICAL
EFFICIENCY
(1/SEC)
CONDUCTIVITY
(MMO/IN)

PT

V/W

SIG. FREQ. (MEGACYC) = 0.7500E+02

1	0.000	3.000E+10	1.0241E-02	3.3930E-02
2	.100	3.000E+10	1.0241E-02	3.3930E-02
3	.200	3.000E+10	1.0241E-02	3.3930E-02
4	.300	3.000E+10	1.0241E-02	3.3930E-02
5	.400	3.000E+10	1.0241E-02	3.3930E-02
6	.449	3.000E+10	1.0251E-02	3.3930E-02
7	.499	3.000E+10	1.0309E-02	3.3930E-02
8	.549	3.000E+10	1.1500E-02	3.3930E-02
9	.600	3.000E+10	1.7334E-02	3.3930E-02
10	.650	3.000E+10	3.2465E-02	3.3930E-02
11	.700	3.000E+10	4.9231E-02	3.3930E-02
12	.750	3.000E+10	2.5773E-02	3.3930E-02
13	.800	3.000E+10	4.6375E-02	3.3930E-02
14	.850	3.000E+10	4.0505E-02	3.3930E-02
15	.900	3.000E+10	2.5026E-02	3.3930E-02
16	.950	3.000E+10	5.2965E-02	3.3930E-02
17	1.000	3.000E+10	7.5163E-02	3.3930E-02
18	1.050	3.000E+10	0.	3.3930E-02

TRANSMISSION

ATTENUATION (DB) = 4.5217E-01

A.77202E-02 1.03530E+00
A.74182E-02 1.11003E+00

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APPENDIX D

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

APPENDIX D

Comparisons between rocket exhaust plume calculations obtained using the present program (mixed implicit/explicit scheme) and the original AeroChem program⁶ (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 $k_i/100$ means that the rate coefficients for $K + HCl \rightarrow KCl + H$ (which is very near equilibrium, even at a pressure of 0.1 atm) was arbitrarily reduced by a factor of 100. This was necessary in order to run the original (explicit) AeroChem program⁶ without excessive computer time. Figures D1-D4 show that the two schemes do, in fact, give identical results and we are therefore confident that the new program properly calculates exhaust plume properties.

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

Table D-I shows a comparison between computer run times for the present and original programs for a typical solid propellant plume at sea level and at 50 kft. For this case, the original AeroChem program cannot be used (in a practical sense) to compute plume properties--primarily because the reaction $K + HCl \rightarrow KCl + H$ is very nearly in equilibrium--resulting in stable integration step sizes of less than about 10^{-8} ft. Thus we record an (essentially) infinite computer run time in Table D-I. However this case can be run using a modified version of the original AeroChem program⁶ which keeps the reaction $K + HCl \rightarrow KCl + H$ 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-1

CDC 6600 COMPUTER RUN TIME, MINUTES10 ft plume; $r_j = 0.25$ ft

	<u>Sea Level</u>	<u>50 kft</u>
Original AeroChem (Explicit) Program ⁶	∞	∞
Original AeroChem (Explicit-modified to put Program ⁶ $K + HCl \rightleftharpoons KCl + H$ 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

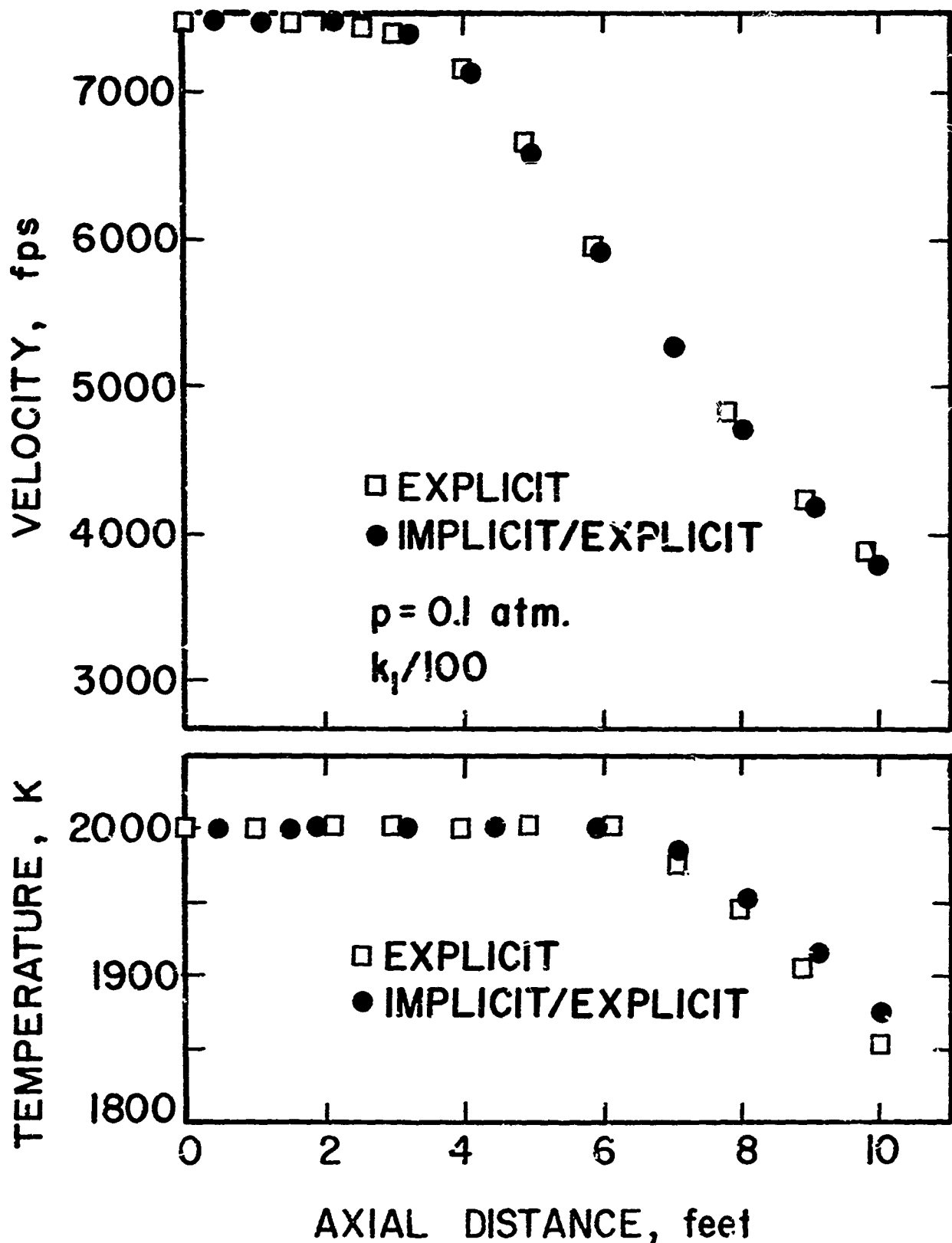


FIG. D1 COMPARISONS BETWEEN CENTERLINE DISTRIBUTIONS OF VELOCITY AND TEMPERATURE COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$$r_j = 0.25 \text{ ft}$$

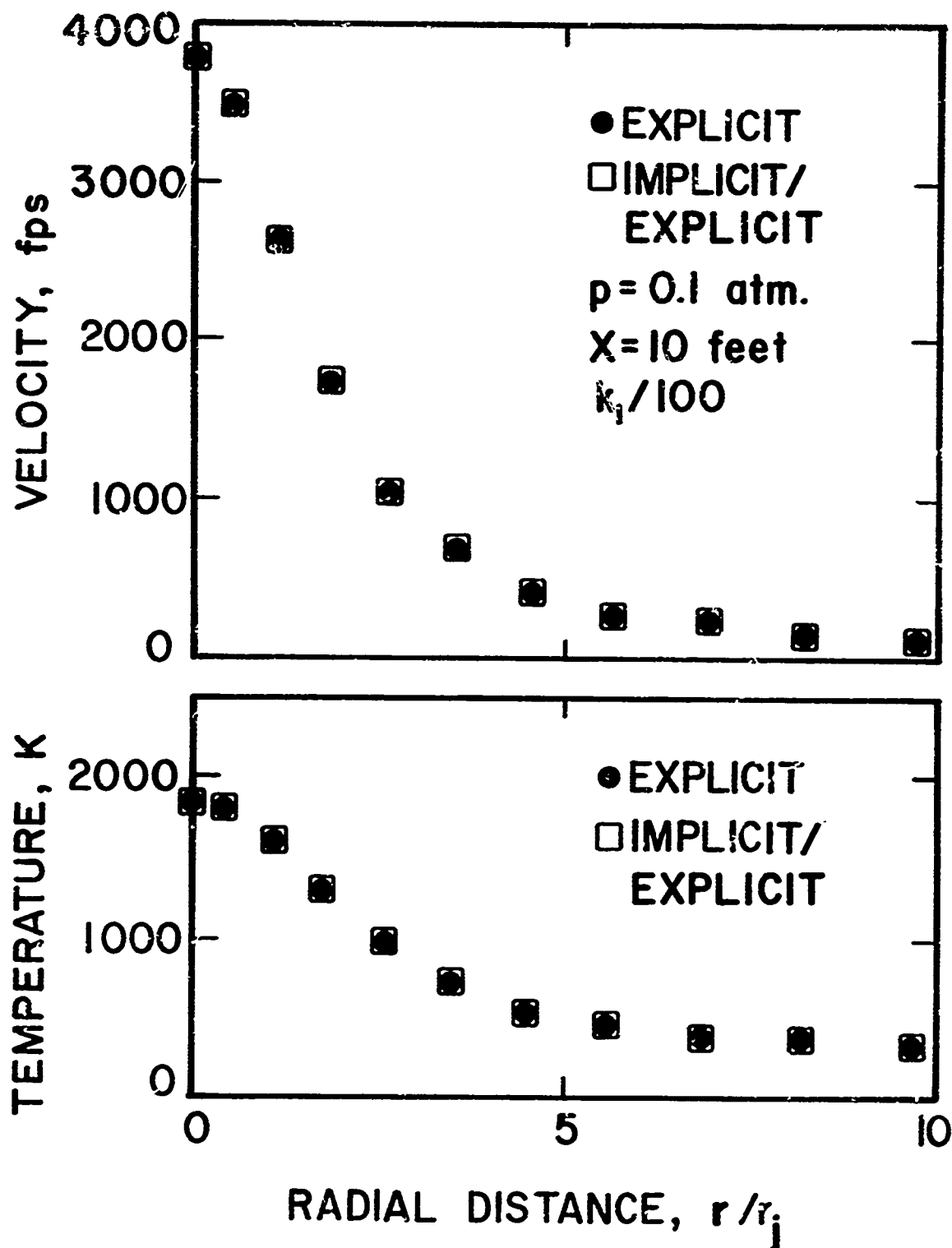


FIG. D2 COMPARISONS BETWEEN RADIAL DISTRIBUTIONS OF VELOCITY AND TEMPERATURE COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$$r_j = 0.25 \text{ ft}$$

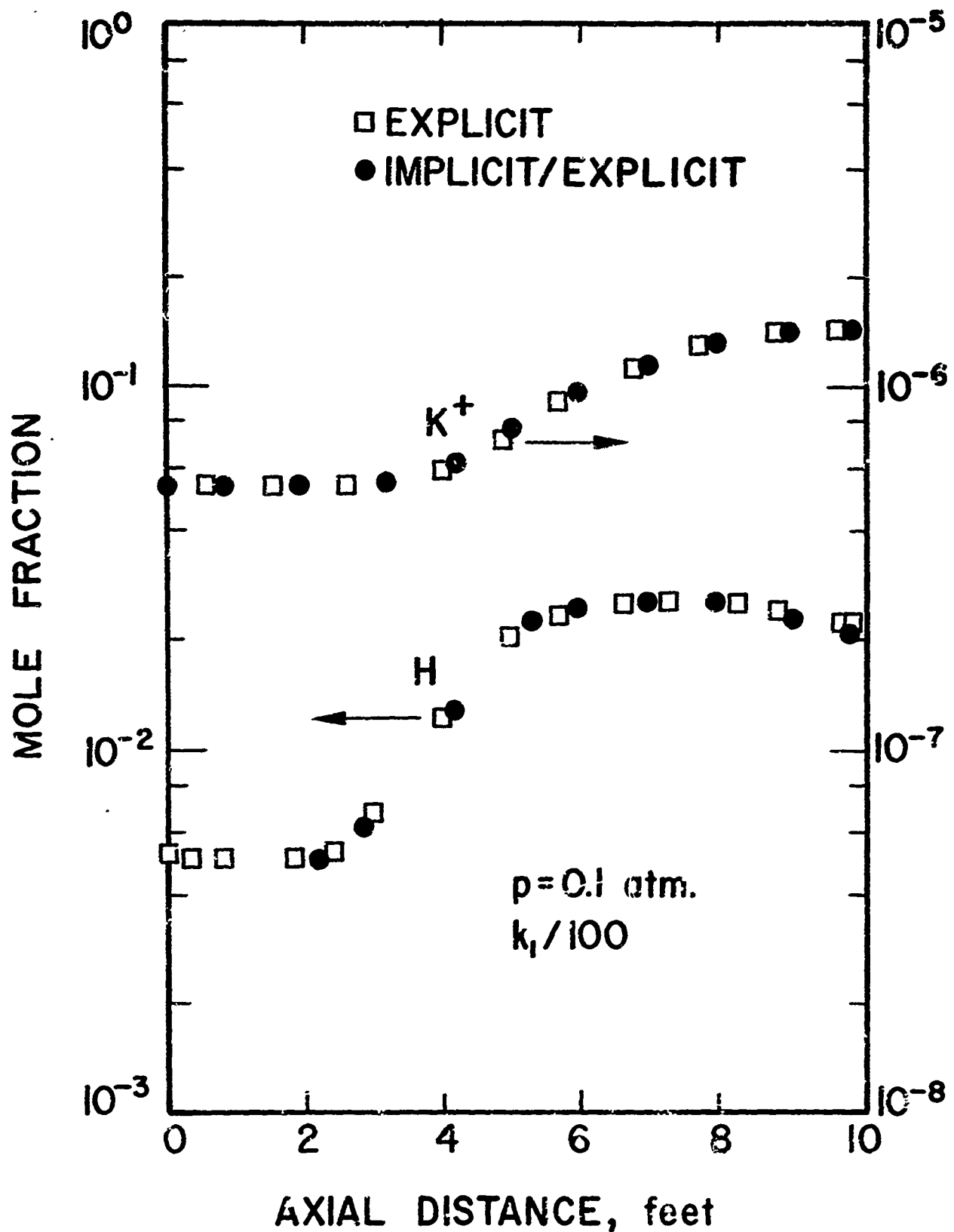


FIG. D3 COMPARISONS BETWEEN CENTERLINE DISTRIBUTIONS OF X_{K^+} AND X_H COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$$r_j = 0.25 \text{ ft}$$

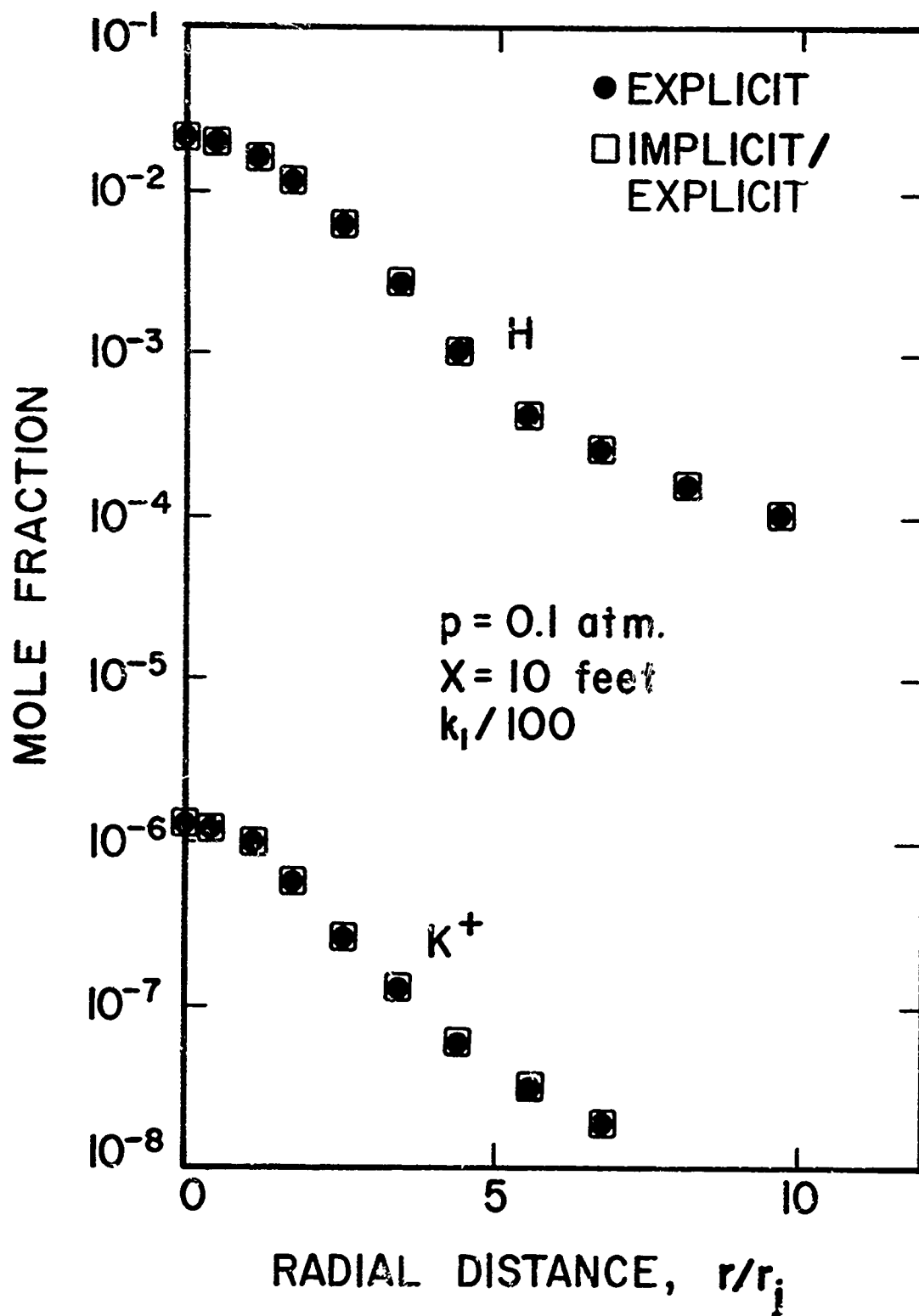


FIG. D4 COMPARISONS BETWEEN RADIAL DISTRIBUTIONS OF X_{K^+} AND X_H COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$$r_j = 0.25 \text{ ft}$$

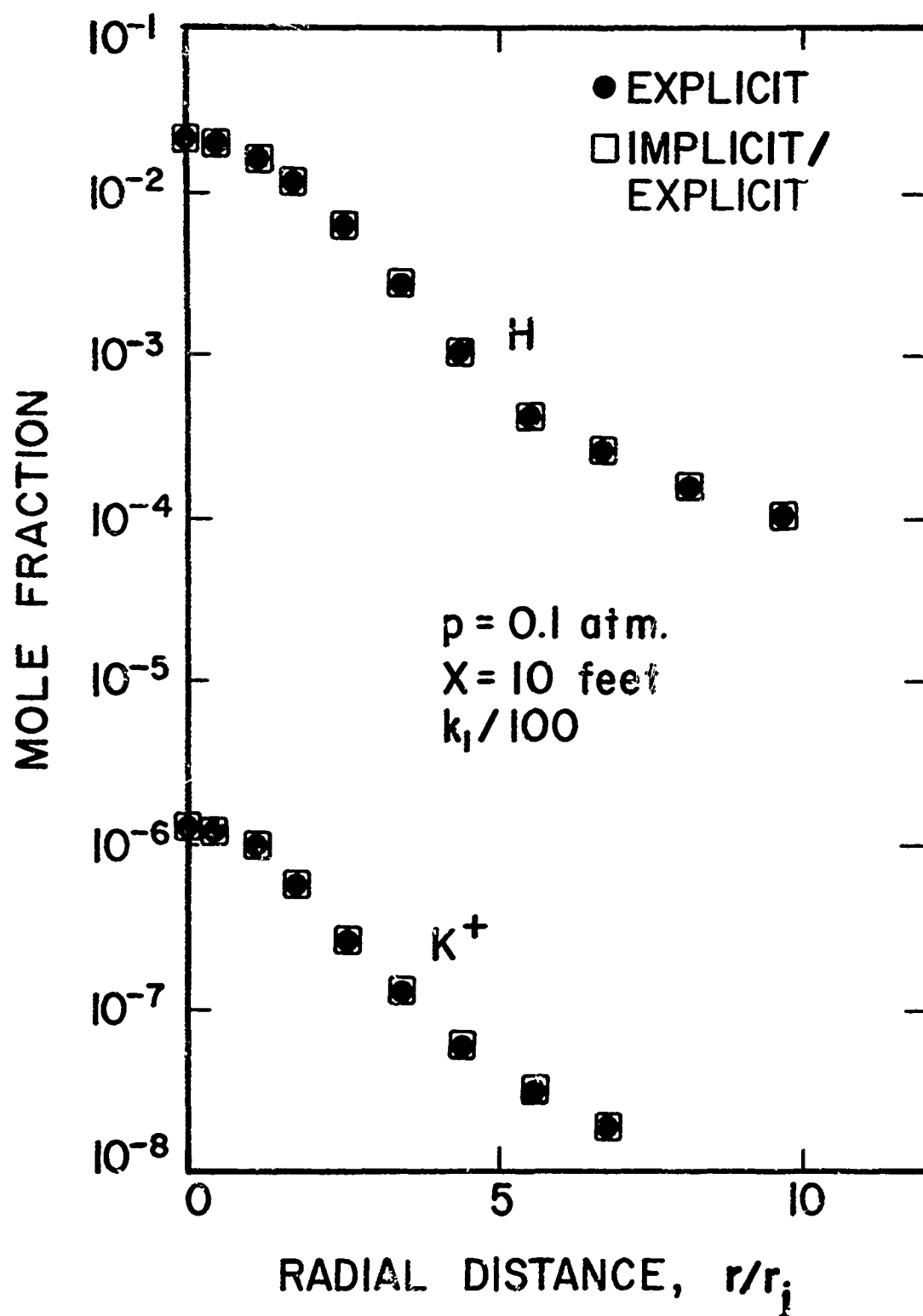


FIG. D4 COMPARISONS BETWEEN RADIAL DISTRIBUTIONS OF X_{K^+} AND X_H COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$$r_j = 0.25 \text{ ft}$$