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GCKP84—General Chemical Kinetics Code for Gas-Phase Flow and Batch Processes Including Heat Transfer Effects

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Summary

A general chemical kinetics code for complex, homogeneous ideal-gas reactions is described. The code, GCKP84, is designed for flexibility, convenience, and speed of computation in treating a variety of reaction conditions. These conditions include (1) general reaction in a batch system or one-dimensional frictionless flow; (2) combustion in a well-stirred (highly backmixed) reactor; (3) reaction behind a shock wave; (4) ignition and combustion reactions in a batch or flowing system; and (5) nozzle expansion reactions.

The new code replaces the GCKP code developed previously and has the following new capabilities and convenience features:

(1) Heat transfer between any reacting system and its surroundings may be considered.

(2) The well-stirred-reactor model is included.

(3) A new implicit numerical integration technique is used for greatly increased speed in integrating "stiff" differential equations. Integration speed is increased by a factor of 10 to 20, compared to GCKP, while maintaining the same accuracy.

(4) The ability to use several additional types of reaction processes, including photochemical reactions, has been added.

(5) Input for combustion problems is simplified.

(6) Rocket performance parameters may be computed for any flow expansion problem.

(7) A well-stirred reactor followed by a normal flow reaction may be computed as a single case.

This report describes the theoretical equations for all problems and the numerical procedures used in their solutions. The code is described in detail, including preparation of input data, control of accuracy, sample input data, and examples of test case results.

Introduction

This report describes a new general chemical kinetics computer code that replaces the GCKP chemical kinetics program developed by Bittker and Scullin and described in reference 1. The new program provides several added capabilities including consideration of heat transfer effects. It also incorporates a greatly improved numerical integration technique that uses the latest algorithms for implicit integration of "stiff" differential equation systems.

The original GCKP computes the progress of a general complex, homogeneous, gas-phase reacting system. The system is assumed to be adiabatic and the reaction may be batch or in one-dimensional frictionless flow. Shock-tube kinetics and equilibrium combustion models are also included in the code. Any chemical system may be used if thermodynamic data for the species and the chemical reaction mechanism (including rate constants) are known.

The new code, GCKP84, has three major improvements: (1) the ability to consider nonadiabatic systems by including heat transfer terms in the fundamental equations, (2) a mathematical model of a well-stirred (highly backmixed) combustion reaction, and (3) a state-of-the-art implicit predictor-corrector numerical integration procedure (ref. 2) for systems of "stiff" differential equations, which replaces the original implicit technique described in reference 1. The integration procedure uses an algorithm that selects the largest possible step size consistent with accuracy requirements. In addition, several new convenience features have been added, including (1) the ability to use several additional types of chemical processes, including photochemical and activated species reactions; (2) simplified input for combustion problems; (3) the computation of rocket performance parameters; and (4) the ability to compute a combined well-stirred reaction followed by further flow reaction of the products in a single case.

This report describes the new chemical kinetics computer code in detail and derives all of the theoretical equations (differential and algebraic) solved. The code can be used for the following homogeneous gas-phase reaction problems:

(1) Chemical reaction in any batch system

(2) Chemical reaction in one-dimensional (no backmixing) flow with optional rocket performance parameter computation. (Either an assigned area or a pressure profile may be specified.)

(3) Well-stirred-reactor (highly backmixed) combustion

(4) Chemical reaction in one-dimensional flow behind a shock wave with boundary layer corrections

(5) Constant-pressure equilibrium reaction for batch or one-dimensional flow systems

(6) Well-stirred-reactor combustion followed by continued reaction of the products in one-dimensional flow

In all problems the system may be adiabatic or nonadiabatic. Moreover batch reactions may be either at constant volume or with an assigned-pressure profile.

Readers interested primarily in using this code should read the section General Description of Program Use for a description of all of the available options. A detailed users manual, computed test case results, and other useful user information are given in appendixes. The code is written in Fortran IV and was developed on the IBM 370. It can easily be adapted for many other systems.

Further information on the code can be obtained from the authors. (Contact COSMIC, The University of Georgia, Athens, Ga. 30602, concerning the availability of this program.)

Symbols

General

A	flow cross-sectional area
$A_1,\ldots,A_7$	thermodynamic coefficients in eqs. (98) to (101)
$\mathbf{A}$	species production function, defined by eq. (47), sec^{-1}
$\mathbf{A}^*$	$\mathbf{A}/V$
$\mathbf{B}$	enthalpy production function, defined by eq. (48), sec^{-1}
$\mathbf{B}^*$	$\mathbf{B}/V$
b	internal combustion engine cylinder diameter (bore) used in eq. (32), length units
C_0,C_1,C_2,C_3	coefficients in eq. (77) for assigned variable
c_p	heat capacity of gas mixture at constant composition, defined by eq. (46), energy/(mass-deg)
D	diameter of cylindrical tube cross section (eq. (30)), length units
$\mathbf{D},\mathbf{D}_v$	enthalpy loss functions, defined by eqs. (49) and (59), sec^{-1}
$\mathbf{D}_v^*$	$\mathbf{D}/V$
f	internal combustion engine speed used in eq. (32a), rpm
f/o	fuel-oxidant mass ratio of unburned combustible mixture
$\mathfrak{H}$	heat transfer coefficient (eqs. (26) and (30)), heat units/(length^2-sec-deg)
h	static enthalpy of gas mixture per unit mass, energy/mass
h_T	total enthalpy per unit mass of flowing mixture (eq. (54)), energy/mass
L_m	characteristic shock-tube reaction length for boundary layer correction of eq. (97), length units
L_w	perimeter of flow cross section used in eq. (26), length units
l	total number of chemical reactions
l_s	internal combustion engine cylinder length (stroke) used in eq. (32), length units
M	general collisional third-body species
M_w	mixture molecular weight, g/mole
$\mathfrak{M}$	mixture Mach number, defined by eq. (60)
$\mathfrak{M}_s$	shock Mach number
m	total mixture mass for batch reaction, mass units
$\dot{m}$	mixture mass flow rate, mass/sec
N	number of reacting species in mixture, not including inerts
NS	total number of species in reacting mixture, including inerts
n	number of iteration steps
O/F	oxidant-fuel mole ratio
$(O/F)_s$	stoichiometric oxidant-fuel mole ratio of unburned combustible mixture
p	static pressure, force/area or atm
$\dot{Q}$	positive heat loss rate from reacting system, heat units/sec (eqs. (38) and (76)) or heat units/(length-sec) (eq. (55))
q	independent variable, either t or x (eq. (77)); heat absorbed per unit mass (eqs. (35) and (37))

R	universal gas constant, energy/(mole-K)
s	entropy per unit mass of mixture, defined by eq. (102), energy/(mass-deg)
T	gas mixture temperature, K or °R
T_f	film temperature for heat transfer computations, K
T_w	wall temperature, K
T_0	reference temperature for enthalpy computations, K
t	time, sec
u	total internal energy per unit mass of mixture, energy/mass
V	linear flow velocity, length/time
V_{ass}	assigned variable (eq. (77)), either pressure or area
V_s	shock velocity (eqs. (78) to (80)), length/time
v	volume of well-stirred reactor, volume units
X_H	total energy exchange rate, defined by eq. (103)
x	distance, length units
Z	density, ρ, if $q=t$; or mass flux, ρV, if $q=x$
γ	specific heat ratio, defined by eq. (45)
η	exponent in shock-tube boundary layer correction of eq. (97)
κ	thermal conductivity of gas mixture, heat units/(deg-length-sec)
μ	gas mixture viscosity, g/(cm-sec)
ρ	gas mixture density, mass/volume
τ	average residence time in a well-stirred reactor, defined by eq. (74), sec
φ	equivalence ratio of unburned combustible mixture, defined by eq. (14)
Ω	internal combustion engine cranking velocity used in eq. (32), rad/sec

Subscripted Thermochemical Symbols

In general, subscript i refers to a species and j to a chemical reaction. In the appendixes other subscripts may sometimes be used to avoid confusion, but their meaning should be clear.

A_j	preexponential factor in reaction rate-constant equations (eqs. (3) and (4)), cgs units for all code input unit options
$(C_p)_i$	molar heat capacity of species i, energy/(mole-deg)
c_j	constant in exponential factor of special rate-constant equation (eq. (4)), K^{-1}
E_j	activation energy in standard rate-constant equation (eq. (3)), cal/mole for all code input unit options
F_j	equilibration factor for reaction j, defined by eq. (13)
G_i	Gibbs free energy of species i, energy/mole
H_i	static enthalpy of species i, energy/mole
K_j	forward-direction equilibrium constant for reaction j, cgs units
k_j	forward-direction reaction rate constant for reaction j, cgs units
k_{-j}	reverse-direction reaction rate constant for reaction j (eq. (5)), cgs units
M_j	third-body collisional efficiency factor of reaction j, defined by eq. (A14)
m_{ij}	relative collisional efficiency of species i in reaction j, defined by eq. (A15)
n_j	temperature exponent in rate-constant equations (eqs. (3) and (4))
R_j	forward-direction rate of reaction j, moles/(volume-sec)
R_{-j}	reverse-direction rate of reaction j, moles/(volume-sec)
$(R_{net})_j$	$R_j - R_{-j}$, moles/(volume-sec)
S_i	molar entropy of species i, energy/(mole-deg)
$S_1, S_2, \ldots, S_N$	symbols for species names in general reaction (eq. (2)) and in eqs. (A1), (A11), and (A23)
W_i	net production rate of species i, moles/(volume-sec)
$X_{H,j}$	net energy conversion rate of reaction j, defined by eq. (9), (energy-volume)/(mass²-sec)

X_j	net reaction conversion rate of reaction j, defined by equation (7), (mole-volume)/(mass^2-sec)
ν_{ij}, ν'_{ij}	forward- and reverse-direction stoichiometric coefficients for species i in reaction j (eq. (2) and appendix A)
σ_i	concentration of species i, moles/mass of mixture
ω_{ij}	net rate of production of species i in reaction j, moles/(volume-sec)

Chemical and Fluid Dynamic Equations

Species Production Rates and Chemical Reaction Equations

Species production rates.—The total molar species formation rate W_i per unit volume for species i in any reactive system is computed from

$$W_i = \sum_{j=1}^{I} \omega_{ij} \tag{1}$$

where I is the number of reactions occurring and ω_{ij} is the rate of formation of species i by reaction j in moles per unit volume per second. The j^{th} chemical reaction is written in the general form

$$\sum_{j=1}^{NS} \nu_{ij} S_i \underset{k_{-j}}{\overset{k_j}{=}} \sum_{j=1}^{NS} \nu'_{ij} S_i \tag{2}$$

Because NS is the total number of species, reacting plus inert, this form includes third-body collisional reactions. Here S_i represents species i and ν_{ij} and ν'_{ij} are the forward and reverse stoichiometric coefficients of S_i in reaction j. The k_j and k_{-j} are the forward and reverse rate constants for the reaction. Each k_j is a function of temperature usually given by the modified Arrhenius expression

$$k_j = A_j T^{n_j} e^{-E_j/RT} \tag{3}$$

The temperature dependence for some rate constants is given in the form

$$k_j = A_j T^{n_j} e^{c_j T} \tag{4}$$

The GCKP84 code allows either type of expression to be used. Most reactions are considered to be reversible and the reverse-direction rate constant k_{-j} is calculated from k_j and the equilibrium constant K_j (in concentration units) by the law of microscopic reversibility:

$$k_{-j} = \frac{k_j}{K_j} \tag{5}$$

Equation (1) for W_i can be rewritten

$$W_i = \sum_{j=1}^{I} \omega_{ij} = \sum_{j=1}^{I} (\nu'_{ij} - \nu_{ij})(R_j - R_{-j}) \tag{6}$$

where R_j and R_{-j} are the forward and reverse molar rates of reaction j as given by the law of mass action. We shall now define a net reaction conversion rate X_j for each reaction as

$$X_j = \frac{(R_j - R_{-j})}{\rho^2} \tag{7}$$

Then the net formation rate for any species W_i can be written

$$W_i = \rho^2 \sum_{j=1}^{I} (\nu'_{ij} - \nu_{ij}) X_j \tag{8}$$

For convenience in the computation and for ease of comparison of net reaction rates, X_j is used instead of $R_j - R_{-j}$ since X_j values are of larger magnitude than the net molar rates. In problems where heat release is an important consideration, we have previously defined the net energy conversion rate (ref. 1) for reaction j as

$$X_{Hj} = X_j (\Delta H_{298})_j \tag{9}$$

Here $(\Delta H_{298})_j$ is the molar heat of reaction at 298 K for reaction j in the forward direction. The temperature 298 K is the standard reference temperature used for most thermodynamic computations. General formulas for X_j and its derivatives are given in appendix A.

Equilibration factor.—For any chemical reaction it is often important to know how far it is from its equilibrium condition at any time. We can derive a simple equilibration factor to determine this from the net rate expression for reaction j:

$$(R_{net})_j = R_j - R_{-j} \tag{10}$$

The factor $(R_{net})_j$ will be positive or negative depending on the magnitudes of R_j and R_{-j}. If R_j is greater than R_{-j}, we divide by R_j to get

$$\frac{(R_{net})_j}{R_j} = 1 - \frac{R_{-j}}{R_j} \tag{11}$$

If the reaction is far from equilibrium, R_j is much larger than R_{-j} and the right side of equation (11) is a positive number very close to 1. If the reaction is near equilibrium, $R_j \cong R_{-j}$ and the right side of equation (11) is a positive number close to 0. Therefore the ratio $(R_{net})_j/R_j$ varies between 0 and 1 for the extreme situations of equilibrium ($R_j = R_{-j}$) and irreversibility ($R_{-j} = 0$). Likewise, if R_{-j} is greater than R_j, we divide by R_{-j} to get

$$\frac{(R_{net})_j}{R_{-j}} = \frac{R_j}{R_{-j}} - 1 \tag{12}$$

and the ratio $(R_{net})_j/R_{-j}$ varies between 0 and -1 for the extreme conditions of equilibrium ($R_j = R_{-j}$) and irreversibility ($R_j = 0$). The two ratios on the left sides of equations (11) and (12) can be combined into a single equilibration factor F_j as

$$F_j = \left| \frac{(R_{net})_j}{(R_{pos})_j} \right| \tag{13}$$

where $(R_{pos})_j$ is the larger of R_j and R_{-j} and $0 \le F_j \le 1$. The equilibration factor is very useful in determining the effect of a single reaction on the entire complex process.

Types of Chemical Reactions

The GCKP84 code allows the consideration of many different types of chemical reaction. In addition, any reaction may be made either reversible or irreversible, at the user's option. Any reaction of the general type

$$\nu_1 S_1 + \nu_2 S_2 \rightleftharpoons \nu_3 S_3 + \nu_4 S_4$$

may be used. The stoichiometric coefficients ν_i may be any single-digit positive integer or a two- or three-digit decimal with one decimal place, if desired. Either species S_1 or S_4 or both may be omitted or replaced by the general third-body collision partner M. The following types of reaction may therefore be considered:

$$aA + bB \rightleftharpoons dD + eE \tag{I}$$

$$bB \rightleftharpoons dD + eE \tag{II}$$

$$aA + bB \rightleftharpoons dD \tag{III}$$

$$bB \rightleftharpoons dD \tag{IV}$$

$$M + bB \rightleftharpoons dD + eE + M \tag{V}$$

$$M + bB \rightleftharpoons dD + M \tag{VI}$$

$$M + aA + bB \rightleftharpoons dD + M \tag{VII}$$

Therefore any collisional process, including spontaneous activation and deactivation of excited species, may be considered. In addition, photochemical reactions of the type

$$h\nu + bB \rightarrow dD + eE \tag{VIII}$$

may also be used. This reaction is an irreversible decomposition.

Input for Hydrocarbon Combustion Problems

In the original general chemical kinetics code, gas composition was required to be in either mole or mass fractions in the input data. The new program allows gas composition to be given initially as either equivalence ratio φ or mass fuel-oxidant ratio f/o for combustion in an oxidant containing oxygen, nitrogen, argon, and carbon dioxide in any proportion. A "standard air" oxidant has been built into the program. The user may change this, however, in the input data. The standard dry air composition used is given in table I. The molecular weight of this standard air is 28.9644.

To obtain the relations between species mole fractions and φ, we start with the stoichiometric reaction for the oxidation of the general fuel $C_mH_nO_p$:

$$C_mH_nO_p + \left(\frac{4m+n-2p}{4}\right)O_2 \rightarrow \frac{n}{2}H_2O + mCO_2 \tag{IX}$$

This stoichiometry is valid for any fuel having $(4m+n) > 2p$.

Next, we let x_i be the mole fraction of species i and use subscript f for the fuel. The equivalence ratio is defined as

$$\varphi = \frac{(O/F)_s}{O/F} \tag{14}$$

where O/F is the actual molar oxidant-fuel ratio of the mixture and $(O/F)_s$ is the stoichiometric value.

TABLE I. - STANDARD DRY AIR COMPOSITION

[Molecular weight, 28.9644.]

Species	Mole fraction	Mass fraction
N_2	0.78088	0.75524
O_2	.20950	.23145
Ar	.00932	.01285
CO_2	.00030	.00046

From reaction (1X) we can immediately write

$$(O/F)_s = \frac{1}{y_{O_2}}\left(\frac{4m+n-2p}{4}\right) \tag{15}$$

$$O/F = \frac{x_{O_2}}{x_f y_{O_2}} \tag{16}$$

where y_{O_2} is the mole fraction of oxygen in the oxidant and is 0.2095 for the "standard air."

Substituting equations (15) and (16) into (14) and rearranging give

$$\frac{x_f}{x_{O_2}} = \frac{4\varphi}{4m+n-2p} \tag{17}$$

We now use the following relations:

$$x_f + x_{O_2} + x_{N_2} + x_{Ar} + x_{CO_2} = 1 \tag{18}$$

$$x_{N_2} = r_1 x_{O_2} \tag{19}$$

$$x_{Ar} = r_2 x_{O_2} \tag{20}$$

$$x_{CO_2} = r_3 x_{O_2} \tag{21}$$

where r_1, r_2, and r_3 are, of course, known, to obtain from equation (17):

$$x_{O_2} = \frac{4m+n-2p}{4\varphi + (1+r_1+r_2+r_3)(4m+n-2p)} \tag{22}$$

Equations (17) and (19) to (22) allow the computation of all mole fractions from the value of φ and the given fuel and oxidant stoichiometry.

To compute the gas composition from a specified fuel-oxidant mass ratio f/o, we use the relations:

$$O/F = \frac{M_f}{M_{ox}(f/o)} \tag{23}$$

and

$$(O/F)_s = \frac{4m+n-2p}{4y_{O_2}} \tag{24}$$

When f/o is specified, equations (23) and (24) are used to compute φ from its definition, and mole fractions are then computed from the equations just derived.

Heat Transfer

In general the heat transfer rate between a reacting system and its surroundings is a function of the reacting gas and ambient temperatures, as well as flow rate and geometry. It is most likely that exact heat exchange rates will not be known when GCKP84 is used to model an experimental reacting system. Therefore the main usefulness of GCKP84 will be in determining the effect of various assumed heat exchange rates. We have used the idea of Pratt (ref. 3) and assumed that the most useful way of expressing the heat loss is in the form of a polynomial function of the reaction temperature T. Therefore the standard option for specifying heat transfer rate $\dot{Q}$ for flow or batch reactions is to give values of coefficients a_0, a_1, and a_2 in the formula

$$\dot{Q} = a_0 + a_1 T + a_2 T^2 \tag{25}$$

In this expression $\dot{Q}$ is expressed as heat units per second for a batch or well-stirred-reactor problem and heat units per length-second for a one-dimensional flow problem. Note that $\dot{Q}$ can be made negative to simulate a heat source for an ignition problem.

For one-dimensional flow $\dot{Q}$ can be computed by using the heat transfer coefficient $\mathcal{H}$ and the ambient or wall temperature T_w from the expression

$$\dot{Q} = \mathcal{H} L_w (T - T_w) \tag{26}$$

where

$\mathcal{H}$ heat transfer coefficient, heat units/(length^2-sec-deg)

L_w perimeter of flow cross section

We shall derive a formula for $\dot{Q}$ in cylindrical tube flow and give a useful correlation for computing $\mathcal{H}$. This information is incorporated as an option for heat transfer computation in GCKP84. For a cylindrical tube $A = \pi D^2/4$, so that

$$L_w = \pi D = 2\sqrt{\pi A}$$

where A is the flow cross-sectional area, which is either assigned or computed at each step of the integration. Using this L_w expression in equation (26) and dividing by $\dot{m}$ give

$$\frac{\dot{Q}}{\dot{m}} = \frac{2\sqrt{\pi A}\,\mathcal{H}(T - T_w)}{\dot{m}} \tag{27}$$

For a flowing system $\mathcal{H}$ changes with conditions. There are many correlations that can be used to estimate $\mathcal{H}$. One of the most useful for turbulent flow is

$$\frac{\mathcal{H}D}{\kappa} = 0.023\,\mathrm{Re}^{0.8}\mathrm{Pr}^{0.4} \tag{28}$$

In this formula Re and Pr are the Reynolds and Prandtl numbers given by

$$\mathrm{Re} = \frac{DV\rho}{\mu} \tag{29a}$$

and

$$\mathrm{Pr} = \frac{c_p\mu}{\kappa} \tag{29b}$$

where μ is the mixture viscosity and κ is its thermal conductivity. These two properties are evaluated at the "film" temperature

$$T_f = \frac{T + T_w}{2}$$

The correlation of equation (28) is valid for tubes with a length-diameter ratio greater than 60, for Pr values from 0.7 to 100 and Re values greater than 10 000.

A modification of the correlation given in equation (28) can be used to compute Q/m for one special batch reaction application. This is the assigned-pressure, variable-volume reaction in the cylinder of an internal combustion or Otto-cycle engine. We assume the cylinder has diameter b (bore) and length l_s (stroke) and that heat is lost only through the curved cylindrical surface. If we assume that the length of the cylinder varies with time from 0 to l_s, it can be shown that

$$\frac{\dot{Q}}{m} = \frac{\mathcal{H}(T - T_w)}{b\rho} \tag{30}$$

To compute $\mathcal{H}$, we use the correlation of equation (28), with D replaced by b (ref. 2)

$$\frac{\mathcal{H}b}{\kappa} = 0.023\,\mathrm{Re}^{0.8}\mathrm{Pr}^{0.4} \tag{31}$$

The Prandtl number is computed in the same way as for a flowing system, but the Reynolds number is now given by

$$\mathrm{Re} = \frac{bl_s\Omega\rho}{\pi\mu} \tag{32a}$$

In this formula Ω is the cranking angular velocity in radians per second and is calculated from the engine speed f, in revolutions per minute, by

$$\Omega = \frac{\pi f}{30} \tag{32b}$$

The use of these formulas for an Otto-cycle computation is included as an option in the GCKP84 code.

Differential Equations for Batch Reaction

The general differential equations for complex chemical reactions will first be derived for a batch reaction. The gas mixture is assumed to be homogeneous and viscosity effects are neglected. All species and energy variables are written for unit mass of mixture. If σ_i is the number of moles of species i per unit mass at time t, the molar rate of change of species i in mass m of gas is

$$\frac{d}{dt}(\sigma_i m) = W_i\left(\frac{m}{\rho}\right) \tag{33}$$

where W_i is the molar formation rate per unit volume given by equation (1) and ρ is the gas mixture density. Differentiating for assumed constant mass gives the species differential equations for the N reacting species

$$\frac{d\sigma_i}{dt} = \frac{W_i}{\rho} \qquad i = 1,2,\ldots,N \tag{34}$$

To obtain the temperature differential equation, we start with the first law of thermodynamics for a unit mass of gas:

$$du + p\,dv = dq \tag{35}$$

where

- u internal energy per unit mass
- v specific volume
- q heat absorbed per unit mass

Using the relation

$$h = u + pv \tag{36}$$

between enthalpy and internal energy and replacing v by the reciprocal of density give

$$dh - \frac{dp}{\rho} = dq \tag{37}$$

We differentiate with respect to time and replace q by $-Q$, where Q is the positive heat lost from mass m of gas. The resulting enthalpy differential equation is

$$\frac{dh}{dt} - \frac{1}{\rho}\frac{dp}{dt} = -\frac{1}{m}\frac{dQ}{dt} = -\frac{\dot{Q}}{m} \tag{38}$$

This equation can now be transformed into a temperature differential equation for two different situations.

Variable-volume reaction.—For this situation the pressure-versus-time profile is assigned and the dependent variables are T, ρ, and the σ_i's. The following formulas, given in reference 1, are used here: the specific enthalpy is

$$h = \sum_{i=1}^{NS} \sigma_i H_i \tag{39}$$

where H_i is the molar enthalpy of species i given by

$$H_i = H_f(T_0) + \int_{T_0}^{T} (C_p)_i dT \tag{40}$$

The mixture molecular weight is

$$M_w = \frac{1}{\sum_{i=1}^{NS} \sigma_i} \tag{41}$$

and the ideal equation of state is assumed:

$$p = \frac{\rho R T}{M_w} \tag{42}$$

We combine equation (38) with the logarithmically differentiated form of equation (42) and with equations (34), (39), and (41) to give the temperature equation

$$\frac{dT}{dt} = T\left(\frac{\gamma - 1}{\gamma}\frac{1}{p}\frac{dp}{dt} - \mathbf{B} - \mathbf{D}\right) \tag{43}$$

Equation (43) can then be combined with the logarithmically differentiated equation (42) to give the density equation

$$\frac{d\rho}{dt} = \rho\left(\frac{1}{\gamma p}\frac{dp}{dt} - \mathbf{A} + \mathbf{D}\right) \tag{44}$$

We have used the following definitions to obtain the final forms shown:

$$\gamma = \frac{c_p}{c_p - \frac{R}{M_w}} \tag{45}$$

$$c_p = \sum_{i=1}^{NS} \sigma_i (C_p)_i \tag{46}$$

$$\mathbf{A} = \frac{RT}{p}\sum_{i=1}^{N} W_i - \mathbf{B} \tag{47}$$

$$\mathbf{B} = \frac{1}{p}\left(\frac{\gamma - 1}{\gamma}\right)\sum_{i=1}^{N} h_i W_i \tag{48}$$

$$\mathbf{D} = \frac{M_w}{RT}\frac{\dot{Q}}{m}\left(\frac{\gamma - 1}{\gamma}\right) \tag{49}$$

where **A** can be described as a species production function and **B** is an enthalpy production function. The term **D** is an enthalpy loss function. All three have units of seconds^{-1}. The quantity c_p is the specific heat of the mixture at constant composition, and γ is the specific heat ratio at constant composition.

Equations (34), (43), and (44) are a system of $N+2$ equations in σ_i ($i = 1, 2, \ldots, N$), T, and ρ.

Constant-volume reaction.—For this situation the dependent variables in the differential equation system are the σ_i's and T, since ρ is a constant. The temperature differential equation is obtained by combining equation (38) with equation (42), differentiated with constant density. Using the definitions of equations (39), (41), and (45) to (49) gives the temperature differential equation

$$\frac{dT}{dt} = T[(\gamma - 1)\mathbf{A} - \mathbf{B} - \gamma\mathbf{D}] \tag{50}$$

This equation is solved with the species equations (eqs. (34)) and p is determined from the ideal-gas law.

Differential Equations for General One-Dimensional Flow Reactions

These equations can be derived for two different situations. Either we may assign an area profile for the flow and let the pressure profile be determined by the ideal-gas law, or we may assign a desired pressure profile and let

the area profile be determined by mass continuity. In either case we now have $N+2$ variables, the N species concentrations plus ρ, T, and velocity V. We assume, as before, a homogeneous, frictionless gas in one-dimensional flow with linear velocity V and constant mass flow rate $\dot{m}$. Global mass continuity is then represented by the equation

$$\frac{d}{dt}(\rho A V) = \frac{d\dot{m}}{dt} = 0 \tag{51}$$

where A is the flow cross-sectional area at any point. The individual species continuity equations are now written as

$$\frac{d}{dt}(\sigma_i \dot{m}) = W_i A V \tag{52}$$

Performing the indicated differentiation and using equation (51) give the species equations (eqs. (34)) already obtained for batch reaction. We need only derive new differential equations for V, ρ, and T. These are obtained from the momentum and energy conservation equations (see, e.g., the book by Penner, ref. 3).

$$\rho \frac{dV}{dt} + \frac{1}{V}\frac{dp}{dt} = 0 \tag{53}$$

and, from the definition of total enthalpy,

$$h + \frac{V^2}{2} = h_T \tag{54}$$

where h_T is the total enthalpy of the flowing gas per unit mass. Equation (54) is differentiated with respect to time by using

$$\frac{dh_T}{dt} = \frac{dh_T}{dx}\frac{dx}{dt} = -\left(\frac{\dot{Q}}{\dot{m}}\right)V$$

where $\dot{Q}$ is now defined as the (positive) instantaneous heat loss rate per unit length of flow (heat units lost per unit length and time). The resulting enthalpy differential equation is

$$\frac{dh}{dt} + V\frac{dV}{dt} + \frac{\dot{Q}V}{\dot{m}} = 0 \tag{55}$$

Note that if $\dot{Q}$ is negative, heat flows into the reacting system. The dependence of $\dot{Q}$ on temperature, mass flow rate, and flow geometry has been discussed in a previous section.

Assigned area profile.—For this situation we use the logarithmically differentiated form of the ideal-gas law (eq. (42)) to eliminate dp/dt from equation (53). Then, by using the definitions of h, M_w, γ, **A**, and **B** along with equation (51), we obtain the following differential equations:

$$\frac{dV}{dt} = \frac{V}{\mathfrak{M}^2 - 1}\left(\frac{1}{A}\frac{dA}{dt} - \mathbf{A} + \mathbf{D}_v\right) \tag{56}$$

$$\frac{d\rho}{dt} = -\rho\left[\frac{\mathfrak{M}^2}{\mathfrak{M}^2 - 1}\left(\frac{1}{A}\frac{dA}{dt} - \mathbf{A} + \mathbf{D}_v\right) + \mathbf{A} - \mathbf{D}_v\right] \tag{57}$$

$$\frac{dT}{dt} = -T\left[\frac{(\gamma-1)\mathfrak{M}^2}{\mathfrak{M}^2 - 1}\left(\frac{1}{A}\frac{dA}{dt} - \mathbf{A} + \mathbf{D}_v\right) + \mathbf{B} + \mathbf{D}_v\right] \tag{58}$$

In these equations the flow heat loss function $\mathbf{D}_v$ is defined by

$$\mathbf{D}_v = \frac{VM_w}{RT}\frac{\dot{Q}}{\dot{m}}\left(\frac{\gamma-1}{\gamma}\right) \tag{59}$$

and the Mach number $\mathfrak{M}$ is defined by

$$\mathfrak{M}^2 = \frac{V^2 M_w}{\gamma RT} \tag{60}$$

Equations (34) and (56) to (58) constitute a system of $N+3$ equations in the $N+3$ unknowns V, ρ, T, and the σ_i's.

The reacting gas can also be described by equations that use distance x as the independent variable. The relationship $dZ/dx = (1/V)\,dZ/dt$ is used to rewrite equations (34) and (56) to (58), where Z represents any of the dependent variables V, ρ, T, or the σ_i's. The distance equations are

$$\frac{d\sigma_i}{dx} = \frac{W_i}{\rho V} \qquad i = 1,2,\ldots,N \tag{61}$$

$$\frac{dV}{dx} = \frac{V}{\mathfrak{M}^2 - 1}\left(\frac{1}{A}\frac{dA}{dx} - \mathbf{A}^* + \mathbf{D}_v^*\right) \tag{62}$$

$$\frac{d\rho}{dx} = -\rho\left[\frac{\mathfrak{M}^2}{(\mathfrak{M}^2-1)}\left(\frac{1}{A}\frac{dA}{dx} - \mathbf{A}^* + \mathbf{D}_v^*\right) + \mathbf{A}^* - \mathbf{D}_v^*\right] \tag{63}$$

$$\frac{dT}{dx} = -T\left[\frac{(\gamma-1)\mathfrak{M}^2}{\mathfrak{M}^2-1}\left(\frac{1}{A}\frac{dA}{dx} - \mathbf{A}^* + \mathbf{D}_v^*\right) + \mathbf{B}^* + \mathbf{D}_v^*\right] \tag{64}$$

where

$$\mathbf{A}^* = \mathbf{A}/V \tag{65}$$

$$\mathbf{B}^* = \mathbf{B}/V \tag{66}$$

$$\mathbf{D}_v^* = \mathbf{D}_v/V \tag{67}$$

Assigned pressure profiles.—For engine modeling it is often more useful to assign a flow pressure profile and compute the area profile that satisfies mass continuity after each numerical integration step. A new set of equations for the V, ρ, and T derivatives can be derived that use p and dp/dt instead of A and dA/dt. The momentum equation (eq. (53)) then becomes the velocity differential equation, and equation (51) is used to eliminate dA/dt and A. The resulting equations are

$$\frac{dV}{dt} = -\frac{1}{\rho V}\frac{dp}{dt} \tag{68}$$

$$\frac{d\rho}{dt} = \rho\left(\frac{1}{\gamma p}\frac{dp}{dt} - \mathbf{A} + \mathbf{D}_v\right) \tag{69}$$

$$\frac{dT}{dt} = T\left[\left(\frac{\gamma-1}{\gamma}\right)\frac{1}{p}\frac{dp}{dt} - \mathbf{B} - \mathbf{D}_v\right] \tag{70}$$

The last two equations are the same as equations (44) and (43) for a batch reaction, except for the definition of the enthalpy loss function. If distance is the integration variable, the assigned pressure equations become

$$\frac{dV}{dx} = -\frac{1}{\rho V}\frac{dp}{dx} \tag{71}$$

$$\frac{d\rho}{dx} = \rho\left(\frac{1}{\gamma p}\frac{dp}{dx} - \mathbf{A}^* + \mathbf{D}_v^*\right) \tag{72}$$

$$\frac{dT}{dx} = T\left[\left(\frac{\gamma-1}{\gamma}\right)\frac{1}{p}\frac{dp}{dx} - \mathbf{B}^* - \mathbf{D}_v^*\right] \tag{73}$$

Equations for Well-Stirred Reactor

We now consider the problem of highly backmixed reacting flow. The limiting case of zero-dimensional flow or instantaneous backmixing of the reacted gases with the cold unreacted mixture is assumed. This is the "well-stirred reactor," for which the theoretical equations are given in references 4 and 5. Although this model is a great simplification of highly turbulent reacting flow, it is a very useful first-order approximation to some practical reacting-flow systems.

A gas mixture with constant mass flow rate $\dot{m}$ enters a reactor of volume v and instantaneously mixes with the reacted mixture in a constant-pressure process. The resulting mixture reacts during an average residence time

$$\tau = \frac{\rho v}{\dot{m}} \tag{74}$$

where ρ is the reacting gas density, and then exits at flow rate $\dot{m}$. Because no mass accumulates in the reactor, we can write the following species continuity equation for each reacting species:

[Flow rate of species i into reactor per unit volume] − [Flow rate of species i out of reactor per unit volume] = [Net rate of destruction of species i per unit reactor volume]

The right side of this equation is just the negative of the species formation rate $\dot{W}_i$ in equation (8). Therefore we can write the set of conservation equations for each reacting species

$$\frac{\dot{m}}{v}(\sigma_i^* - \sigma_i) = -\rho^2 \sum_{j=1}^{J} (\upsilon_{ij}' - \upsilon_{ij}'')X_j$$

or

$$\rho^2 \sum_{j=1}^{J} (\upsilon_{ij}' - \upsilon_{ij}'')X_j + \frac{\dot{m}}{v}(\sigma_i^* - \sigma_i) = 0 \qquad i = 1,2,3,\ldots,N \tag{75}$$

where σ_i is the i^{th} species concentration within and leaving the reactor. Here the asterisk indicates the unreacted gas mixture and v is the reactor volume. The reactor temperature T is also unknown, so we need the energy conservation equation

$$\sum_{i=1}^{NS} (\sigma_i H_i - \sigma_i^* H_i^*) + \frac{\dot{Q}}{\dot{m}} = 0 \tag{76}$$

where $\dot{Q}$ is the (positive) heat loss rate from the reactor and the summation is over the total number of species NS including inerts. Equations (75) and (76) constitute a system of $N+1$ nonlinear algebraic equations in the variables σ_1, σ_2, ..., σ_N and T. They are solved by a Newton-Raphson iterative procedure using logarithmic increments in the variables to avoid numerical problems. Details of the derivation of the system of linear equations for the logarithmic variables and computation of the Jacobian for this system are given in appendix B.

Numerical Integration Procedure

GCKP84 uses a new implicit numerical integration procedure for sets of "stiff" differential equations developed by Zeleznik (ref. 2). This property of stiffness often arises in the differential equations of chemical kinetics because of widely varying rates of relaxation of the fluid dynamic and chemical processes toward the equilibrium conditions. This can cause an integration algorithm to take excessively small steps, out of proportion to the rate of change of the dependent variables. Reference 2 develops a generalized theory of implicit numerical integration that includes the methods of Gear and Nordsieck (refs. 6 and 7) as special cases. It also describes a practical computer code applying the theory to the solution of equations very similar to those presented in this report. This variable-order, predictor-corrector method selects the largest step size consistent with the gradients of the unknowns and with the accuracy requirements. See Appendix C for derivation of the partial derivatives needed in using this method.

Comparison tests have shown the new integration method to be anywhere from 10 to 20 times faster than the method in the original GCKP while maintaining the same accuracy. The coding for the control and use of the integration routine uses the method of Hindmarsh as described in reference 7.

General Description of Program Use

The GCKP84 code can compute the progress of many different types of batch and flow reactions, as already described. Computations can be performed for any homogeneous gas mixture containing up to 50 species that participate in a maximum of 150 chemical reactions. Of these reactions, no more than 35 may be of the catalytic third-body recombination-dissociation type. Any species may be used for which thermodynamic data are available in the form described below. This includes ionic and excited-state species. A maximum of 20 different species may be specified as third-body species. For these species, collisional efficiency ratios different from 1 may be specified for any third-body reaction.

For all problems the user must provide chemical reaction and rate-constant data and also initial values of the mixture composition and fluid variables. Nonzero initial time and position values may be given, if desired. Otherwise, these variables are initialized to zero. Heat transfer data for any problem may be given if the logical variable HTRAN is set equal to TRUE. If coefficients for $\dot{Q}$ in equation (25) are not given, the variable QMREAD must be set to FALSE and a separate dataset containing viscosity and thermal conductivity data must be provided. This dataset, which will be provided with the GCKP84 code, contains coefficients for curve-fitted equations giving viscosity (in $g/(cm\text{-}sec) \times 10^6$) and thermal conductivity (in $cal/(cm\text{-}sec\text{-}K) \times 10^6$) as a function of temperature for 20 species. The code reads in these coefficients and uses them with the mixture rules of reference 2 to compute the heat transfer coefficient $\mathfrak{IC}$ in either equation (27) or (30). If equation (27) is being used for a flow reaction, a value of the wall temperature T_w must also be given. If equation (30) for a batch reaction Otto-cycle model is used, the variable OTTO must be set to TRUE and values of T_w, engine speed (in revolutions per minute), and cylinder bore and stroke (in centimeters) must also be given. Note that the total mass must be given for a batch reaction if $\dot{Q}$ is read in by equation (25). However, the mass does not have to be given if the Otto-cycle option (eq. (30)) is used to compute the enthalpy loss.

Figure 1 gives a flow diagram of the necessary input and all of the options available. The input data preparation for all types of problem is described in detail in appendix D. Appendix E gives a discussion of some computational problems. In appendix F we list the complete input data for several test cases and also give selected results for these cases.

Problem Types

Batch reaction.—Batch reaction can be carried out either for constant volume or with an assigned pressure-versus-time profile. The method of specifying the profile is given in the next section. For a constant-volume case the variable RHOCON is set equal to TRUE. Initial values of T, ρ, and the σ_i's must be given. When an assigned pressure profile is given, only initial temperature and composition must be given. Either of these problems can be computed with temperature held constant by setting the logical variable TCON equal to TRUE. However, for an *assigned pressure case only*, the additional variable PCON must also be set equal to TRUE. This is to make the code skip the computation of $d\rho/dt$. If T and p are assigned, ρ is determined by the ideal-gas law, and the only variables in the differential equation system are the σ_i's.

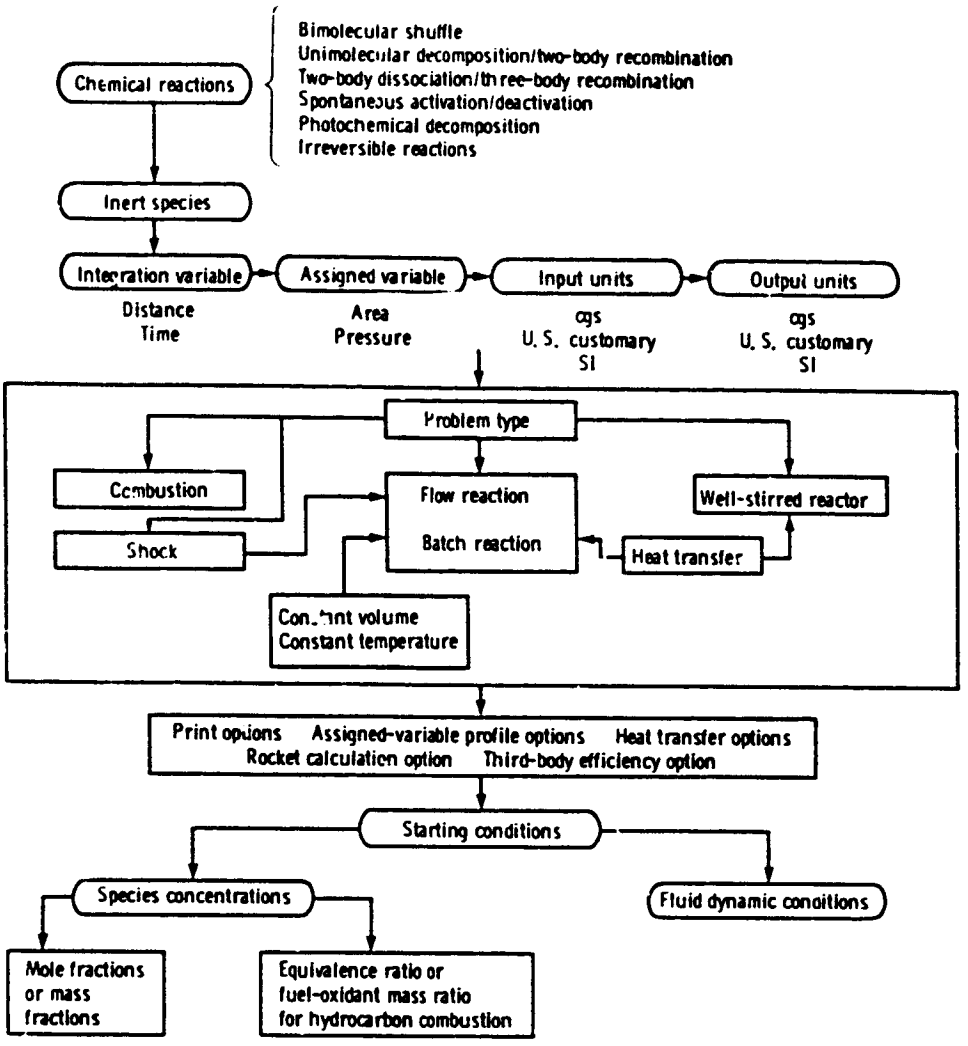

Figure 1.—Flow chart for inputs and options.

One-dimensional flow reaction.—As previously described, one-dimensional flow reaction can be done with either an assigned area or an assigned pressure profile. The user has a choice of either time or distance as the integration variable. The choice is made by using the word TIME or DISTANCE in the appropriate line of the input dataset. The assigned variable profile can be given as a function of time or distance independently of the choice of integration variable. The profile is given in either of the following ways:

(1) A table of the assigned variable as a function of time or distance

(2) Polynomial coefficients for the equation

$$V_{ass} = C_0 + C_1 q + C_2 q^2 + C_3 q^3 \qquad (77)$$

where V_{ass} is either pressure or area and q represents either t or x. A constant area or pressure is easily specified by setting C_1, C_2, and $C_3 = 0$ and C_0 equal to the desired constant value. *Note that these two methods also apply to specifying the pressure profile for an assigned-pressure batch reaction.* A flow reaction may also be run at constant temperature by setting TCON equal to TRUE.

The GCKP84 code permits the computation of several rocket performance parameters during a nozzle expansion process. For these computations the rocket combustion chamber pressure P_c and nozzle throat area A_t are specified as input.

The following variables are then computed:

(1) Specific impulse: $I_{sp} = \dfrac{V}{g}$

(2) Vacuum specific impulse: $I_{vac} = I_{sp} + \dfrac{pA}{\dot{m}}$

(3) Area ratio: $A_r = \frac{A}{A_t}$

(4) Characteristic velocity: $c^* = \frac{P_c A_t g}{\dot{m}}$

(5) Thrust coefficient: $c_f = \frac{V}{c^*}$

In these equations g is a units conversion factor. The computation of the rocket performance parameters is triggered by setting the logical variable ROCKET equal to TRUE. Starting conditions must be obtained by performing equilibrium combustion and nozzle flow computations with a code such as the one described in reference 8. The assumption can be made that the equilibrium nozzle pressure profile is the same as the kinetically limited pressure profile. This assumption is needed to a point just downstream of the throat where the flow just becomes supersonic and the Mach number exceeds 1.05. The validity of this approximation is quite good, except for very low chamber pressure (e.g., below 414 kPa (60 psia)). The rate-limited computation is done in two steps. The first part is started with all equilibrium conditions at a convenient point in the subsonic flow upstream of the nozzle throat. The equilibrium pressure profile is assigned and the computation carried through the throat until the Mach number just exceeds 1.05. The conditions at the end of this computation are then used to start the second part of the computation, which assigns the desired area profile of the expanding nozzle. For higher chamber pressures one can speed up this procedure by doing only the supersonic flow computation. The starting conditions are all the equilibrium data at a Mach number just larger than 1.05. The nozzle position where the kinetically limited fluid dynamic and composition data begin to differ significantly from the equilibrium results has to be determined for each particular situation.

Well-stirred reactor.—To solve the well-stirred-reactor (WSR) problem, the logical variable WELSTR must be set equal to TRUE. The code then solves the previously derived nonlinear algebraic equations by the method described in appendix B. The dependent variables are the N concentration values and either temperature or mass flow rate. The standard option is computing T as the $(N+1)^{th}$ variable and assigning increments in $\dot{m}$. The initial value of $\dot{m}$ is then given along with the desired $\dot{m}$ increment. If a temperature increment is to be assigned and $\dot{m}$ computed, the logical variable TASS is set equal to TRUE and the initial $\dot{m}$ and the temperature increment are given as input. For all WSR problems the unreacted-gas temperature and composition and the constant pressure for the reactions also must be specified. The code uses these data to compute the assigned-enthalpy and -pressure equilibrium reaction in order to obtain the initial estimates of the Newton-Raphson iterative solution for the first increment of $\dot{m}$ or T.

Shock-tube reaction.—The shock tube is one of the most frequently used instruments for generating a high-temperature environment for the study of rapid chemical reactions. The assumption is made that the shock wave instantaneously creates a high-temperature and high-pressure flowing system without changing the gas composition. Then the increased temperature and pressure behind the shock start a chemical reaction that can continue toward some new equilibrium conditions of temperature, pressure, and composition. The conservation equations for the change in conditions across the shock are

$$\rho_1^2 V_s^2 = \rho^2 V^2 \tag{78}$$

$$p_1 + \rho_1 V_s^2 = p + \rho V^2 \tag{79}$$

$$h_1 + \frac{V_s^2}{2} = h + \frac{V^2}{2} \tag{80}$$

In these equations the coordinate system is attached to the shock, which is considered to be stationary. The unshocked gas at conditions p_1, ρ_1, and T_1 flows past the shock with the experimental shock velocity V_s. Gas properties immediately after the shock passes are p, V, ρ, and T. The static enthalpy per gram of gas mixture is changed from h_1 to h by the shock. Since gas composition is unchanged, h is calculated for the initial composition at the new temperature T. These conditions are called the no-reaction or frozen shock conditions.

It is also possible to solve equations (78) to (80) for the equilibrium postshock conditions of particle velocity, temperature, pressure, and composition.

The preceding shock equations are solved by an iterative method for both frozen and equilibrium conditions. Estimates are made of the final temperature and pressure p_f and T_f. Then a Newton-Raphson method is used to calculate corrections to these estimates and converge on the correct values. The shock equations are transformed and combined for this solution. First, equation (78) gives

$$V^2 = \left(\frac{\rho_1}{\rho}\right)^2 V_s^2 \tag{81}$$

This equation is used in equations (79) and (80) to eliminate V and gives, after some rearrangement,

$$\left[1-\left(\frac{\rho_1 V_s^2}{p_1}\right)\left(\frac{\rho_1}{\rho}-1\right)\right]-\frac{F}{F_1}=0 \tag{82}$$

$$\left[h_1+\frac{V_s^2}{2}-\frac{V_s^2}{2}\left(\frac{\rho_1}{\rho}\right)^2\right]-h=0 \tag{83}$$

Using the equation of state (eq. (42)) for no change in gas composition gives

$$\frac{\rho_1}{\rho}=\left(\frac{p_1}{p}\right)\left(\frac{T}{T_1}\right)=\frac{\mathfrak{I}}{P} \tag{84}$$

where we have defined the new variables $\mathfrak{I}=T/T_1$ and $P=p/p_1$.

Equations (82) and (83) can now be written as functions of the pressure and temperature ratios across the shock:

$$\left[1-\left(\frac{\rho_1 V_s^2}{p_1}\right)\left(\frac{\mathfrak{I}}{P}-1\right)\right]-P=0 \tag{85}$$

$$\left[h_1+\frac{V_s^2}{2}-\frac{V_s^2}{2}\left(\frac{\mathfrak{I}}{P}\right)^2\right]-h=0 \tag{86}$$

These equations are solved iteratively for the final ratios $\mathfrak{I}_f$ and P_f across the shock. First estimates of $\mathfrak{I}$ and P are obtained from the following equations:

$$P_0=\frac{2\gamma\mathfrak{M}_s^2-\gamma+1}{\gamma+1} \tag{87}$$

$$\mathfrak{I}_0=\frac{P_0\left(\frac{2}{\mathfrak{M}_s^2}+\gamma-1\right)}{\gamma+1} \tag{88}$$

These are the exact solutions of equations (78) to (80) when heat capacity is assumed to be independent of temperature. Then the Newton-Raphson procedure is used to calculate corrections to ln P and ln $\mathfrak{I}$, where it is assumed that

$$\ln P_{n+1}=\ln P_n+\Delta\ln P \tag{89}$$

$$\ln \mathfrak{I}_{n+1}=\ln \mathfrak{I}_n+\Delta\ln \mathfrak{I} \tag{90}$$

where n indicates the n^{th} iteration step. Logarithmic differentiation is used to obtain rapid convergence of the procedure. We define the quantities

$$p^*=1-\left(\frac{\rho_1 V_s^2}{p_1}\right)\left(\frac{\mathfrak{I}}{P}-1\right) \tag{91}$$

$$h^*=h_1+\frac{V_s^2}{2}-\frac{V_s^2}{2}\left(\frac{\mathfrak{I}}{P}\right)^2 \tag{92}$$

Then equations (85) and (86) can be written as

$$F(\mathfrak{I},P)=P^*-P=0 \tag{93}$$

$$G(\mathfrak{I},P)=h^*-h=0 \tag{94}$$

Substituting equations (89) and (90) and using logarithmic differentiation give the following pair of linear equations for the corrections $\Delta\ln P$ and $\Delta\ln \mathfrak{I}$ in the Newton-Raphson method:

$$\left(\frac{\partial F}{\partial\ln \mathfrak{I}}\right)_n\Delta\ln \mathfrak{I}+\left(\frac{\partial F}{\partial\ln P}\right)_n\Delta\ln P=-F_n \tag{95}$$

$$\left(\frac{\partial G}{\partial\ln \mathfrak{I}}\right)_n\Delta\ln \mathfrak{I}+\left(\frac{\partial G}{\partial\ln P}\right)_n\Delta\ln P=-G_n \tag{96}$$

In these equations the subscript n indicates evaluation of either the function or its derivative for the estimated values P_n and $\mathfrak{I}_n$. This method of solution is the one used by Gordon and McBride (ref. 8). This procedure is used for both the equilibrium and frozen-shock conditions. The only difference in method for the two situations is the way the enthalpy is computed for the shocked gas. For the frozen-shock conditions, h is calculated at the estimated temperature T for the original gas composition. For equilibrium conditions the shocked-gas enthalpy depends on T and also on the changing gas composition due to reaction. Therefore the estimated T and p are first used to perform an equilibrium chemical reaction computation. This gives the estimated final composition of the shocked gas. This composition and the estimated T are then used to calculate the enthalpy h used in equation (94) to compute the function $G(\mathfrak{I},P)$ in the Newton-Raphson method.

The GCKP84 code contains an option for easily computing the progress of chemical reactions behind a shock wave. When the logical variable SHOCK is made TRUE, the input conditions are recognized as unshocked gas conditions. The velocity V is then the shock velocity V_s. The conservation equations are first solved to give the frozen flow conditions behind the shock wave. These new conditions and the initial composition are used to compute the progress of the one-dimensional flow reaction occurring in the high-temperature region behind the shock. The final equilibrium reaction conditions are also computed. In these shock-tube reactions a special area profile function is used to take account of laminar and

turbulent boundary layer losses according to the theory of Mirels (refs. 9 to 11). The special area function is

$$A = \frac{1}{1 - \left(\frac{x}{L_m}\right)^{\eta}} \tag{97}$$

The exponent η is given as input and is either 0.5 for laminar or 0.8 for a turbulent boundary layer. The characteristic length L_m may either be given as input or computed by the code. In the latter case three other quantities are given instead of L_m. These are the shock-tube hydraulic diameter D_h, the unshocked gas viscosity μ, and a boundary layer thickness parameter β, which can be computed from equations given in references 10 and 11. The code computes L_m by using equation (3) of reference 11 for a laminar boundary layer or equation (4) of reference 10 for a turbulent boundary layer. Note that the area profile is always given as a function of x for flow reaction behind a shock wave. However, either time or distance may still be selected as the integration variable. Also, equation (97) is used only for flow reactions behind a shock.

Combustion equilibrium computations.—An option is provided for computing final equilibrium conditions for batch or flow reaction constant-pressure combustion. Enthalpy is also assumed to be constant for these computations, which are triggered by setting the logical variable COMBUS equal to TRUE. The method of Gordon and McBride (ref. 8) is used for these computations.

Combined WSR plus plug flow problem.—The user may perform a combined well-stirred-reactor plus plug flow computation in a single computer run. The required input for the WSR reaction, including initial composition, pressure, and temperature is given. In addition, an assigned pressure or area profile for a normal flow reaction is given, and the logical variable WSFLOW is set equal to TRUE. The code then performs the WSR computation and uses the final values of composition, temperature, pressure, and mass flow rate as input to a subsequent normal flow reaction with the given area or pressure profile. When area is assigned, initial velocity for the flow reaction is computed from the known mass flow rate and density. When pressure is assigned, the initial velocity or Mach number for the flow reaction must be specified at input time. The code then computes an initial area consistent with the known mass flow rate. This combined process is sometimes used as a simplified model of part of a gas turbine combustion process.

Additional Options

Unit options.—A choice of three systems of units for input and output is provided. These are the cgs, U.S. customary, and SI systems. The choices for input and output are completely independent of each other. The exact units used for each system are given later in the Input and Output sections.

Third-body efficiencies.—The code allows the rate constant for any third-body recombination-dissociation reaction to be adjusted for the efficiencies of different collision catalysts. The user may read in values of the weighting factor m_{ij} described in equation (A14) of appendix A for any third-body reaction if the logical variable ALLM1 is set equal to FALSE. If no weighting factors are changed at input time, they are all set equal to 1.0 by the code.

Multiple cases.—Several different cases may be executed in one computer run without reading in a complete new dataset each time. This is accomplished by using an ACTION line in the data for each case after the first. The four options that may be used on the ACTION line are described in appendix D.

Standard options.—The code has a built-in standard choice for each of the options discussed. None of the given logical variables or code words (to be described later) need be given in the data unless a nonstandard option is desired. The standard values of all input codes are listed in appendix D.

Thermodynamic Data and Species Names

All species names and the thermodynamic data format for GCKP84 are identical to those used in the chemical equilibrium composition code of Gordon and McBride (ref. 8). Thermodynamic functions are computed by using polynomial equations for $(C_p)_i$, H_i, S_i, and G_i as a function of temperature. The polynomial coefficients are computed by using the thermodynamic properties code of McBride and Gordon (ref. 12). The data calculated from these equations agree with those tabulated in the JANAF thermochemical tables (refs. 13 to 17). Seven coefficients are used for each species in the following equations, where T is the Kelvin temperature.

$$\frac{(C_p)_i}{R} = A_1 + A_2T + A_3T^2 + A_4T^3 + A_5T^4 \tag{98}$$

$$\frac{H_i}{RT} = A_1 + \frac{A_2}{2}T + \frac{A_3}{3}T^2 + \frac{A_4}{4}T^3 + \frac{A_5}{5}T^4 + \frac{A_6}{T} \tag{99}$$

$$\frac{S_i}{R} = A_1 \ln T + A_2T + \frac{A_3}{2}T^2 + \frac{A_4}{3}T^3 + \frac{A_5}{4}T^4 + A_7 \tag{100}$$

$$\frac{G_i}{RT} = A_1(1 - \ln T) - \frac{A_2}{2}T - \frac{A_3}{6}T^2 - \frac{A_4}{12}T^3 - \frac{A_5}{20}T^4 + \frac{A_6}{T} - A_7 \tag{101}$$

The form in which these data are read by GCKP84 is discussed in appendix D.

To use any species, the user must permanently compile its name and molecular weight into the code. This is accomplished by placing them in a BLOCK DATA dataset that also contains other necessary alphanumeric data and logical tape assignment numbers. All names are listed in the array ALSP exactly as they are written on the first record of the thermodynamic data grouping for each species. Corresponding molecular weights are listed in the array ALMW in exactly the same order as the names. The name array has room now for 100 eight-character names, and this dimension can easily be increased. However, a new name may be substituted for one that is not being used if computer core storage is a critical factor.

A name for each species must also be listed in subroutine INIT, which reads in the starting composition and fluid dynamic data. In this subroutine the names are actually Fortran variables that represent the initial concentration of the given species, to simplify preparation of input data. The names, in the same order as in BLOCK DATA, are placed in a COMMON block called FAKE and in NAMELIST START. Usually the species name in INIT may be the same as it is in BLOCK DATA. However, for excited-state and ionic species the variable name cannot contain special characters such as +, −, or *. Thus letters must be used in place of these symbols. For example, *P* may be used for +, *A* for *, etc. Any desired name actually may be used for any species in INIT. The order of the variables identifies the initial concentration of any species. For example, suppose that the Σ^3 excited oxygen molecule, O_2^*, were listed as the twelfth species in BLOCK DATA under the name O2*. Then the twelfth species name in COMMON block FAKE and NAMELIST START could be O2A, and an initial concentration of O_2^* would be listed in the data as O2A = *n* in NAMELIST START. Here *n* is either the mass or mole fraction of the species. Table II gives examples of the names that may be used for different types of species. In listing the species variable names in subroutine INIT, any name beginning with I, J, K, L, M, or N must be declared a REAL variable. This applies to the name NOP in table II. Note that the BLOCK DATA name given to any species must be identical to the name given the species in the dataset for the thermodynamic data described in appendix D.

TABLE II. - SPECIES NAMES

Species	BLOCK DATA name	Name in COMMON block FAKE and NAMELIST START
H_2O	H2O	H2O
B_2O_3	B2O3	B2O3
NO^+	NO+	NOP
O^+	O+	OP
O^-	O-	OM
O_2	O2	O2
O_2^-	O2-	O2M
O_2^*	O2*	O2A

Accuracy Control

The accuracy of any computation is controlled primarily by the relative error parameter EMAX and, to a much smaller extent, by the initial step size HINT. The integration procedure is designed to increase the step size at any time to the highest value consistent with EMAX, the main accuracy control. The recommended values of this parameter range from 1×10^{-3} for a slow reaction to 1×10^{-6} for a very rapid process such as a combustion ignition. For any problem the user may choose the EMAX that gives the best compromise between speed of computation and the accuracy desired. If no values of the two error parameters are given, the code sets EMAX to 1×10^{-6} and HINT to 1×10^{-6} cm or 5×10^{-8} sec. The sensitivity of computed results to variation in EMAX for a relatively rapid hydrogen-air ignition is shown in table III. These results show that the species concentrations are, in general, more sensitive to the EMAX value than are the fluid dynamic variables. As might be expected, the trace concentrations, such as that for NO, are most sensitive to accuracy changes. The user can adjust EMAX over a wide range to give the desired combination of accuracy and computation speed. The data in table III show that, for this case, computing speed can be increased dramatically while keeping good accuracy by raising EMAX from 1×10^{-7} to 1×10^{-5}. No general quantitative correlation between accuracy and running time can be given. For any particular problem, test computations will have to be run to obtain the best EMAX value for the accuracy desired.

Input

In this section we give a general description of the data required to compute the progress of a general flow, batch, or well-stirred reaction. The exact format of each line (or card) in the dataset is given in appendix D.

Chemical reactions and species.—Each chemical reaction is listed on a separate line that has fields for two reactant names, two products, and the three rate-constant parameters A_j, n_j, and either E_j or c_j (eqs. (3) and (4)). The line also has fields for indicating a reversible or irreversible reaction and for indicating the special rate-constant equation (eq. (4)). The reactions may be put in any order, regardless of type. A maximum of 150 reactions is now permitted, of which no more than 35 may be third-body collision reactions. The code checks

TABLE III. - EFFECT OF RELATIVE ERROR PARAMETER EMAX
ON HYDROGEN-AIR IGNITION COMPUTATION

[Assigned distance, 6.096 cm; initial step size, $1x10^{-6}$ cm; distance integration.]

Parameter	EMAX value				
	$1.0x10^{-3}$	$1.0x10^{-4}$	$1.0x10^{-5}$	$1.0x10^{-6}$	$1.0x10^{-7}$
Computation time, sec	2.71	3.19	3.51	5.45	11.8
Reaction time, μsec	13.475	13.540	13.491	13.537	13.563
Pressure, p, atm	1.3642	1.3554	1.3418	1.3273	1.3215
Linear flow velocity, V, cm/sec	445120	445235	445428	445636	445719
Gas mixture density, ρ, g/cm^3	$1.59042x10^{-4}$	$1.59000x10^{-4}$	$1.58931x10^{-4}$	$1.58857x10^{-4}$	$1.58827x10^{-4}$
Absolute temperature, T, K	2285.8	2269.0	2243.6	2216.5	2205.6
Molecular weight	21.8669	21.8417	21.8054	21.7672	21.7518
Mole fractions:					
H	$7.6534x10^{-2}$	$7.7961x10^{-2}$	$7.9906x10^{-2}$	$8.1992x10^{-2}$	$8.2840x10^{-2}$
O_2	$3.0705x10^{-2}$	$3.0946x10^{-2}$	$3.1325x10^{-2}$	$3.1727x10^{-2}$	$3.1890x10^{-2}$
OH	$3.4395x10^{-2}$	$3.4005x10^{-2}$	$3.3463x10^{-2}$	$3.2857x10^{-2}$	$3.2609x10^{-2}$
O	$2.6547x10^{-2}$	$2.6812x10^{-2}$	$2.7209x10^{-2}$	$2.7616x10^{-2}$	$2.7778x10^{-2}$
H_2	$6.6925x10^{-2}$	$6.6762x10^{-2}$	$6.6673x10^{-2}$	$6.6536x10^{-2}$	$6.6476x10^{-2}$
H_2O	0.18497	0.18426	0.18314	0.18200	0.18154
HO_2	$1.7560x10^{-5}$	$1.7731x10^{-5}$	$1.7862x10^{-5}$	$1.8182x10^{-5}$	$1.8315x10^{-5}$
H_2O_2	$4.5578x10^{-6}$	$5.5466x10^{-6}$	$4.4177x10^{-6}$	$4.6040x10^{-6}$	$4.6776x10^{-6}$
NO	$5.2200x10^{-6}$	$3.4656x10^{-6}$	$2.7564x10^{-6}$	$2.1004x10^{-6}$	$1.8834x10^{-6}$

all species names against the master list in the BLOCK DATA array ALSP and automatically builds up the list of species being used in any problem. The code permits a maximum of 50 species for any problem.

Inert species.—The names of any species present, but not reacting, are listed, four per line, after the reactions.

Integration variable and units.—The next line lists the integration variable (TIME or DISTANCE) and the assigned variable (AREA or PRESSURE) for an integration problem. In addition, the code words for input and output units (cgs, U.S. customary, or SI) are listed for all problems. Table IV gives the input units required for each of the three systems.

Problem data.—Most of the data for any problem are listed next in a NAMELIST called PROB. It contains the logical variables that designate the options desired, such as a well-stirred-reactor problem (WSR), a shock kinetics problem, constant temperature or volume reaction, and the equilibrium combustion computation. PROB also contains all of the necessary data for either an integration problem or a WSR problem, except the initial composition and fluid dynamic variable values. Included are the assigned variable profile, printout information, and the assigned mass or temperature increments for a WSR problem. For an integration problem, printout may be obtained either at assigned t or x values or every n integration steps.

Efficiencies for third-body collisional reactions.—The third-body catalyst efficiencies are listed immediately after NAMELIST PROB. They are present only if the variable ALLM1 has been set equal to FALSE in NAMELIST PROB. Each line of these data contains a third-body reaction name (exactly as previously written) followed by one or two species names and their collisional efficiencies in the given reaction. No more than 20 of the species in any problem may be used as third-body species. The code automatically makes a separate list of all third-body species.

TABLE IV. - INPUT UNITS FOR THREE UNIT SYSTEMS[a]

Variable	Units		
	Internal (cgs)	U.S. customary	SI
Velocity	cm/sec	ft/sec	m/sec
Temperature	K	°R	K
Density	g/cm^3	lbm/ft^3	kg/m^3
Pressure[b]	atm	lbf/ft^2	N/m^2
Length	cm	ft	m
Area	cm^2	ft^2	m^2
Species concentration	Mole fraction or mass fraction	Mole fraction or mass fraction	Mole fraction or mass fraction

[a]Activation energy is always input in calories per mole, and reaction rate-constant preexponential factors are always input in cgs units.

[b]Pressure may also be specified as millimeters of mercury (torr) in all systems.

Starting conditions.—The final data listed are the initial reacting gas composition and starting values of the fluid dynamic variables. They are listed in a NAMELIST called START. Before this NAMELIST is read, initial values of time and distance are set to zero by the code, but nonzero values may be listed here for restart problems. The fluid dynamic variable options are as follows: for a constant-volume batch or WSR problem temperature T and either pressure p or density ρ must be given. For an assigned-pressure batch problem only T has to be given. For a flow integration problem T and either velocity V or Mach number $\mathfrak{M}$ must always be given. One more fluid dynamic variable, either p, ρ, $\dot{m}$, or A, must be specified. The choice is determined by the assigned variable chosen previously. If area has been assigned, only p, ρ, or $\dot{m}$ may be given here. If pressure has been assigned, only $\dot{m}$ or A may be specified in START. To conserve storage, the storage for A in a flow integration problem is used for reactor volume in a WSR problem. This volume and an initial $\dot{m}$ value must be given for a WSR problem.

As explained previously, initial mixture composition is specified by using the species variable name to list its mole or mass fraction. The names are interpreted as mole fractions unless the logical variable MOLEF is set equal to FALSE. For a combustion problem composition may alternatively be specified by giving either the equivalence ratio φ or the fuel-oxidant mass ratio f/o. Equations (17) and (19) to (24) are used to convert either of these ratios to the molar mixture composition. Complete details of the input for this method are given in appendix D.

Output

Numerical integration problem.—For a batch or one-dimensional flow problem the code provides both standard and optional output. The exact units used for each of the three systems, cgs, U.S. customary, and SI, are listed in table V. All computed results are completely independent of the print stations assigned. The code performs two-point linear interpolation by using results that bracket any assigned t or x value to obtain the results at the desired point. The following standard data will be listed if no special codes are used in the input:

(1) Reaction time (gas particle time for a shock reaction)

(2) Axial position and flow cross-sectional area

(3) Pressure, velocity, density, and temperature of the gas mixture

(4) Entropy and enthalpy per unit mass and frozen heat capacity ratio for the gas mixture, where entropy s is computed from

$$s = R \sum_{i=1}^{NS} \sigma_i \left(\frac{S_i}{R} - \ln \sigma_i - \ln(pM_w) \right) \tag{102}$$

(5) Local Mach number

(6) Mole fraction of each species in the gas mixture

(7) Molar concentration of each mixture species

(8) Net species production rate W_i, defined by equation (1). This is the net formation rate of the species due to all chemical reactions and, of course, is negative if the species is actually being destroyed.

(9) Net reaction conversion rate X_j for each reaction, defined by equations (A4), (A12), or (A24) in appendix A

(10) Rate-constant value for each reaction. The reference rate-constant formula is used for collisional-catalyst reactions.

(11) The equilibration factor defined by equation (3)

(12) Mixture molecular weight

(13) Mass fraction sum

(14) Total energy exchange rate given by

TABLE V. - OUTPUT UNITS FOR THREE UNITS SYSTEMS

Variable	Units		
	Internal (cgs)	U.S. customary	SI
Velocity	cm/sec	ft/sec	m/sec
Temperature	K	°R	K
Density	g/cm^3	lbm/ft^3	kg/m^3
Pressure	atm	lbf/ft^2	N/m^2
Time	sec	sec	sec
Length	cm	ft	m
Area	cm^2	ft^2	m^2
Species concentration	Mole fraction, mass fraction, (g/mole)/cm^3	Mole fraction, mass fraction, (lb mole)/ft^3	Mole fraction, mass fraction, (kg mole)/m^3
Species production rate	(g mole)/cm^3 sec	(lb mole)/ft^3 sec	kg mole)/m^3 sec
Net reaction conversion rate	$\frac{\text{g mole}}{\text{cm}^3\ \text{sec}} \Big/ \rho^2$	$\frac{\text{lb mole}}{\text{ft}^3\ \text{sec}} \Big/ \rho^2$	$\frac{\text{kg mole}}{\text{m}^3\ \text{sec}} \Big/ \rho^2$
Net energy exchange rate	$\frac{\text{cal}}{\text{cm}^3\ \text{sec}} \Big/ \rho^2$	$\frac{\text{Btu}}{\text{ft}^3\ \text{sec}} \Big/ \rho^2$	$\frac{\text{J}}{\text{m}^3\ \text{sec}} \Big/ \rho^2$
Reaction rate constant	cgs units[a]	cgs units[a]	cgs units[a]
dV/dq	(cm/sec)/unit q	(cm/sec)/unit q	(cm/sec)/unit q
dρ/dq	(g/cm^3)/unit q	(g/cm^3)/unit q	(g/cm^3)/unit q
dT/dq	K/unit q	K/unit q	K/unit q
$d\sigma_i/dq$	(g mole/g)/unit q	(g mole/g)/unit q	(g mole/g)/unit q
Mass flow rate	g/sec	lbm/sec	kg/sec
Entropy	cal/(g K)	Btu/(lb °R)	J/(kg K)
Enthalpy	cal/g	Btu/lb	J/kg

[a]Units for first-order reaction are sec^{-1}.
Units for bimolecular reaction are cm^3 mole^{-1} sec^{-1}.
Units for termolecular reaction are cm^6 mole^{-2} sec^{-1}.

$$X_H = \sum_{j=1}^{I} X_j\left(\Delta H^{\circ}_{298}\right)_j \tag{103}$$

This quantity is proportional to the net heat release rate for the entire complex reaction and may be useful in ignition processes.

(15) Heat loss rate if different from zero

(16) Integration indicators

(a) Steps from last print

(b) Average step size since last print

(c) Total number of derivative function evaluations during the integration

(d) Total number of Jacobian evaluations during the integration

The following optional output may be obtained by simple changes in the input data:

(1) Species mass fractions may be listed in place of molar concentrations by setting the logical variable CONC equal to FALSE in NAMELIST PROB.

(2) The net energy exchange rate for each reaction $X_{H,j}$, defined by equation (9), may be listed instead of the net conversion rate by setting the logical variable EXCHR equal to TRUE in NAMELIST PROB.

(3) Additional data or intermediate output may be listed if desired. These data are useful for studying the effect of individual reactions on gas composition or for diagnosing problems by using the code. This option is chosen by setting the variable DBUGO equal to TRUE in NAMELIST PROB. The following quantities are then listed:

(a) Derivatives of all dependent integration variables, V, ρ, T, and the σ_i's, with respect to the integration variable

(b) The mass and energy production functions **A** and **B** or **A*** and **B***

(c) For assigned area the quantities dA/dq, d^2A/dq^2, and either

$$\frac{1}{A}\frac{dA}{dq} - \mathbf{A}$$

or

$$\frac{1}{A}\frac{dA}{dq} - \mathbf{A}^{\bullet}$$

For assigned pressure the quantities dp/dq, d^2p/dq^2, and $(1/p)\,dp/dq$ are printed out. Here q is either t or x.

(d) The matrix Ω in which each element ω_{ij} is the rate of production of species i due to reaction j as defined by equation (6)

Well-stirred-reactor problem.—For each assigned mass flow or temperature increment the following data are automatically printed out after successful convergence:

(1) Initial and present values of pressure, temperature, entropy, density, enthalpy, molecular weight, and heat capacity ratio of the gas. Ratios of present to initial values are also given.

(2) Initial and present values of both the mole fraction and the mass fraction of each species

(3) The assigned reactor flow rate $\dot{m}$ and volume v as well as $\dot{m}/v$

(4) The average gas residence time given by equation (74)

(5) The number of iterations needed for convergence

(6) The heat loss term $\dot{Q}/\dot{m}$, when used

If the integer variable MPR in NAMELIST PROB is set to a value n greater than 1, this printout will occur only every n^{th} convergence. If the numerical solution encounters trouble, the DBUGO = TRUE switch is automatically turned on. This causes the printing out of the current values of all variables and their logarithmic increments as well as other useful data before the computation is terminated. The same DBUGO switch may be purposely turned on, as with an integration problem, to obtain useful intermediate output for following the details of the computation.

Program Organization

The GCKP84 code is organized into five major sections, consisting of the main program and 30 subroutines. These are (1) control, (2) input/output, (3) chemical kinetics, (4) numerical integration, (5) well-stirred reactor/shock combustion. We have tried to make these sections independent of each other, as much as possible, except for the reading and processing of input data. The well-stirred-reactor/shock-combustion section uses subroutine THRM from the chemical kinetics section as well as parts of DIFFUN and PEDERV but is otherwise self-contained. The numerical integration and chemical kinetics sections are completely self-contained. The following sections describe the function of each section of the code and of each subroutine in the section. The names of nonstandard entry points into a subroutine are given in parentheses after the subroutine name. Flow charts are given for important subroutines.

Control Section

The control section contains just the main program, GCKP84. It provides for problem setup via a series of subroutine calls. It selects the type of solution, either well-stirred-reactor or numerical integration problem. It monitors the latter type and provides an output call whenever a print station is reached (fig. 2).

Input/Output Section

This input/output section is called for all problems. It reads, converts, and writes out all input data and numerical integration results. It also performs the necessary bookkeeping functions such as building tables, setting option switches, and storing data for later use.

KINP (RINP).—Subroutine KINP processes all input data. It initializes, sets all standard options, reads all input data, and converts them to internal (cgs) units. This routine also calculates heats of reaction at a reference condition, builds tables, and provides calls for shock and equilibrium combustion computations (fig. 3).

CIMAGE.—Subroutine CIMAGE prints an image of the input dataset.

BLOCK DATA.—Subroutine BLOCK DATA contains, in block data format, the master species list and the molecular weight of each species in the list, as well as alphanumeric data for testing and input and logical tape unit numbers.

INIT.—Subroutine INIT reads in initial conditions via NAMELIST START and stores initial species compositions in a table provided by KINP.

OUT1.—Subroutine OUT1 prints out chemical reactions, reaction rate-constant parameters, third-body efficiencies, and information about the type of problem being done, including the assigned area or pressure profile, if used.

OUT2 (OUTSTR, OUT3).—Subroutine OUT2 prints out the initial thermophysical and chemical gas properties for all problems and the equilibrium combustion conditions that are used as starting estimates for a well-stirred reactor problem. Its main function is to provide general output for numerical integration problems at each assigned print station. For these problems it provides all output except shock and constant-pressure equilibrium combustion results. Output data are converted from internal units to the user's desired output units, and certain parameters are computed that are required only as output. These are total entropy and net energy exchange rates for the reactions.

RKTOUT.—Subroutine RKTOUT computes and prints out the rocket performance parameters listed previously

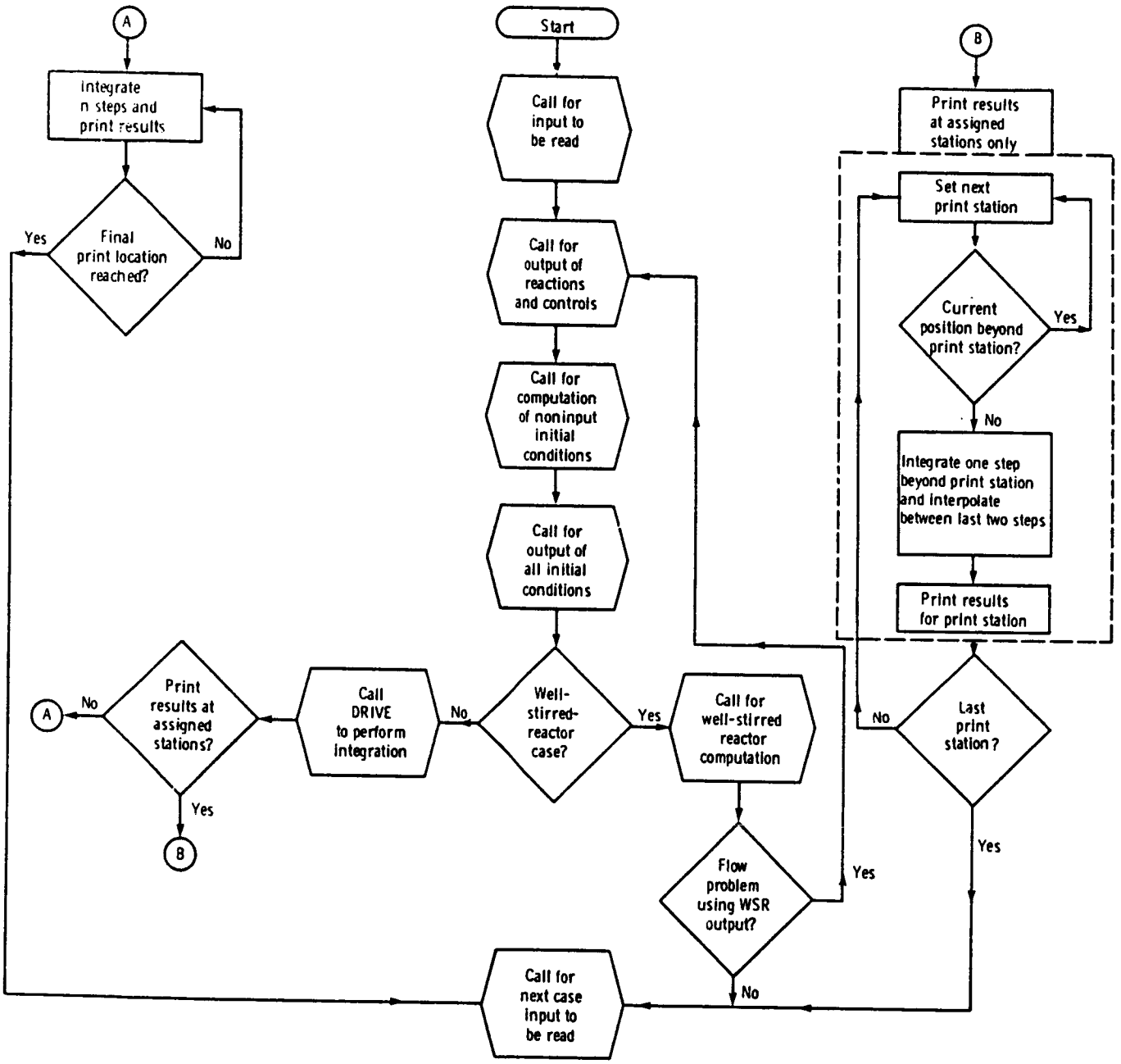

Figure 2.—GCKP84, main control program.

for rocket performance computation, when called from OUT2.

Chemical Kinetics Section

In the chemical kinetics section, called for all problems, all chemical and flow parameters are computed. In particular, thermodynamic functions are evaluated and net reaction and species production rates are computed as are enthalpy loss terms. All required total and partial derivatives are also evaluated.

DIFFUN (DIFFW, DIFFI).—Subroutine DIFFUN computes directly or calls for the computation of thermodynamic properties, net reaction rates, pressure, specific heat ratio, and Mach number. It uses these results to compute all total derivatives with respect to the independent variable for an integration problem (fig. 4).

PEDERV.—Subroutine PEDERV computes all partial derivatives for both integration and well-stirred-reactor problems and computes the Jacobian for each step of a numerical integration (fig. 5).

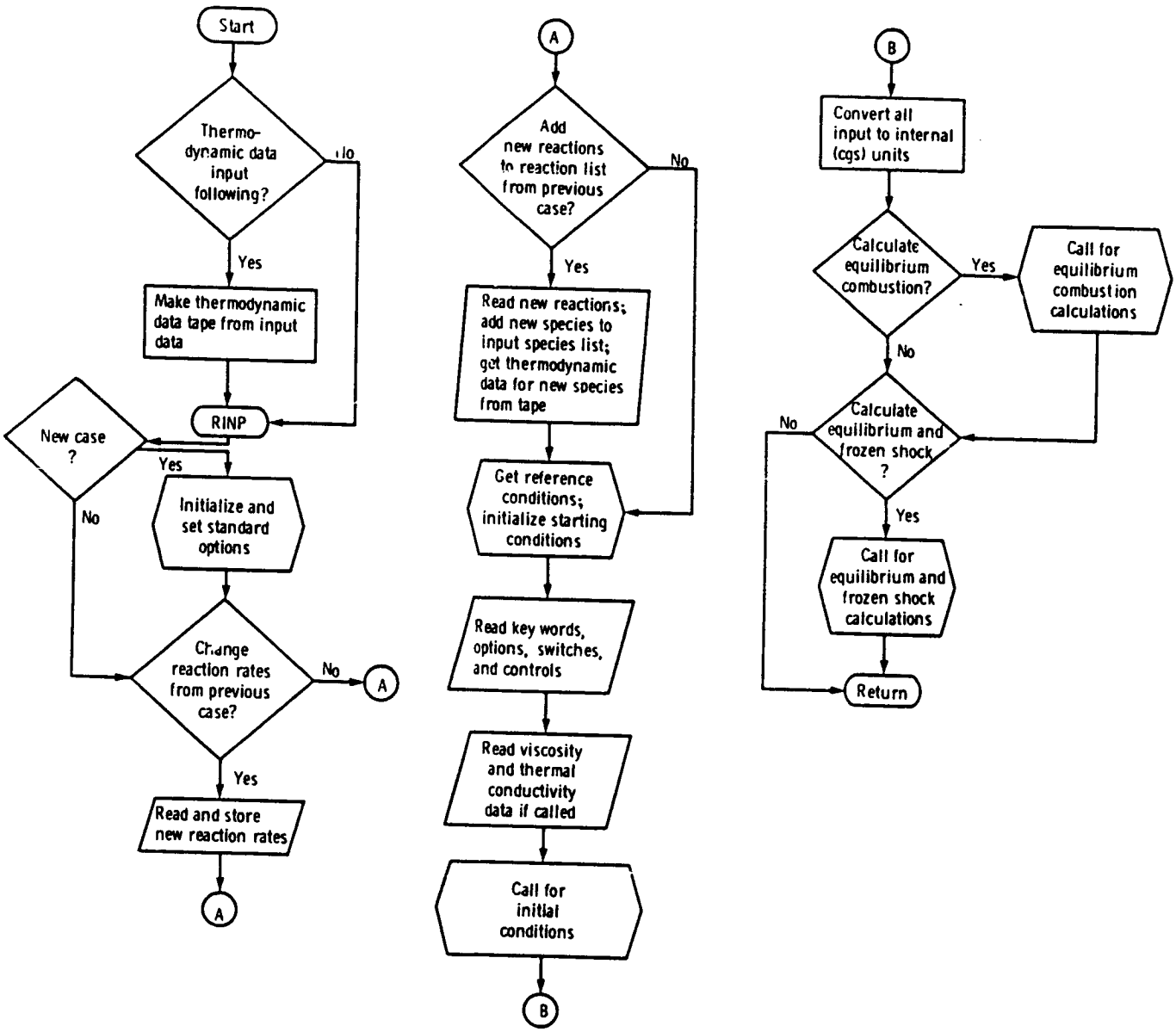

Figure 3.—Subroutine KINP, routine for reading in all data, initialization, and problem setup.

HETRAN (VISCON).—Subroutine HETRAN computes the heat transfer terms $\dot{Q}/\dot{m}$ (or Q/m) and **D** for all problems. It also reads in thermal conductivity and viscosity data, if they are used for the computation of $\dot{Q}/\dot{m}$.

THRM.—Subroutine THRM computes the dimensionless thermodynamic properties H_i/RT, G_i/RT, S_i/R, $(C_p)_i/R$, and $(dC_p/dT)_i/R$ from polynomial curvefit equations.

CUBS (CINP).—Subroutine CUBS computes assigned variable values and derivatives either by evaluating a polynomial or special function or by calling a cubic spline-fit routine when a table of values is given.

SPLINE.—Subroutine SPLINE performs a cubic spline fit by using the first-derivative method. The end conditions give parabolic runout.

Numerical Integration Section

The numerical integration section is called for batch and one-dimensional flow reaction problems.

DRIVE.—Subroutine DRIVE controls the numerical integration routine. It makes repeated calls to the core integrator subroutine and calls for interpolation when an assigned print station is reached. It also sets error flags and gives appropriate messages when the integration runs into difficulties (fig. 6).

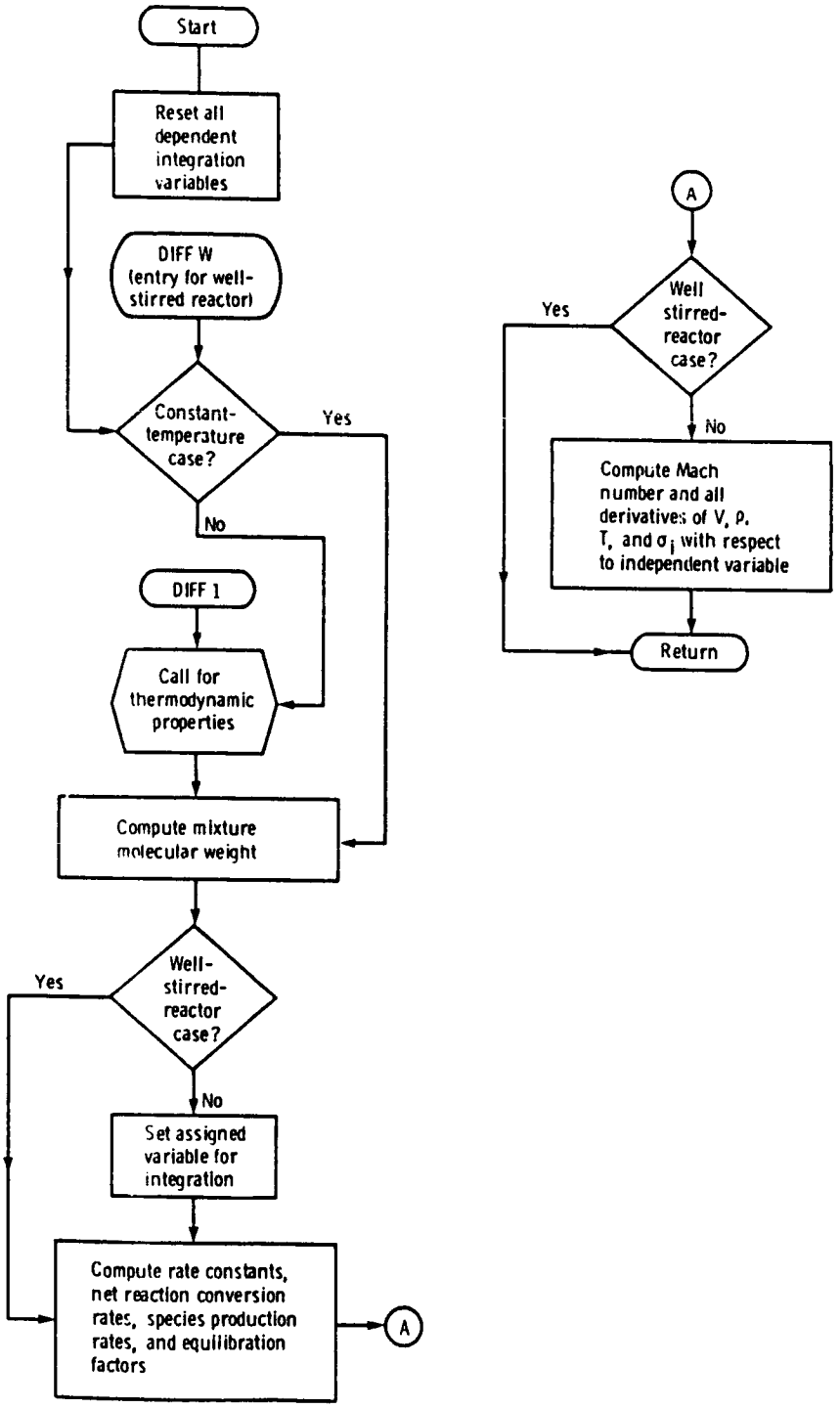

Figure 4.—Subroutine DIFFUN, routine for computing reaction rate data and all derivatives of integration variables.

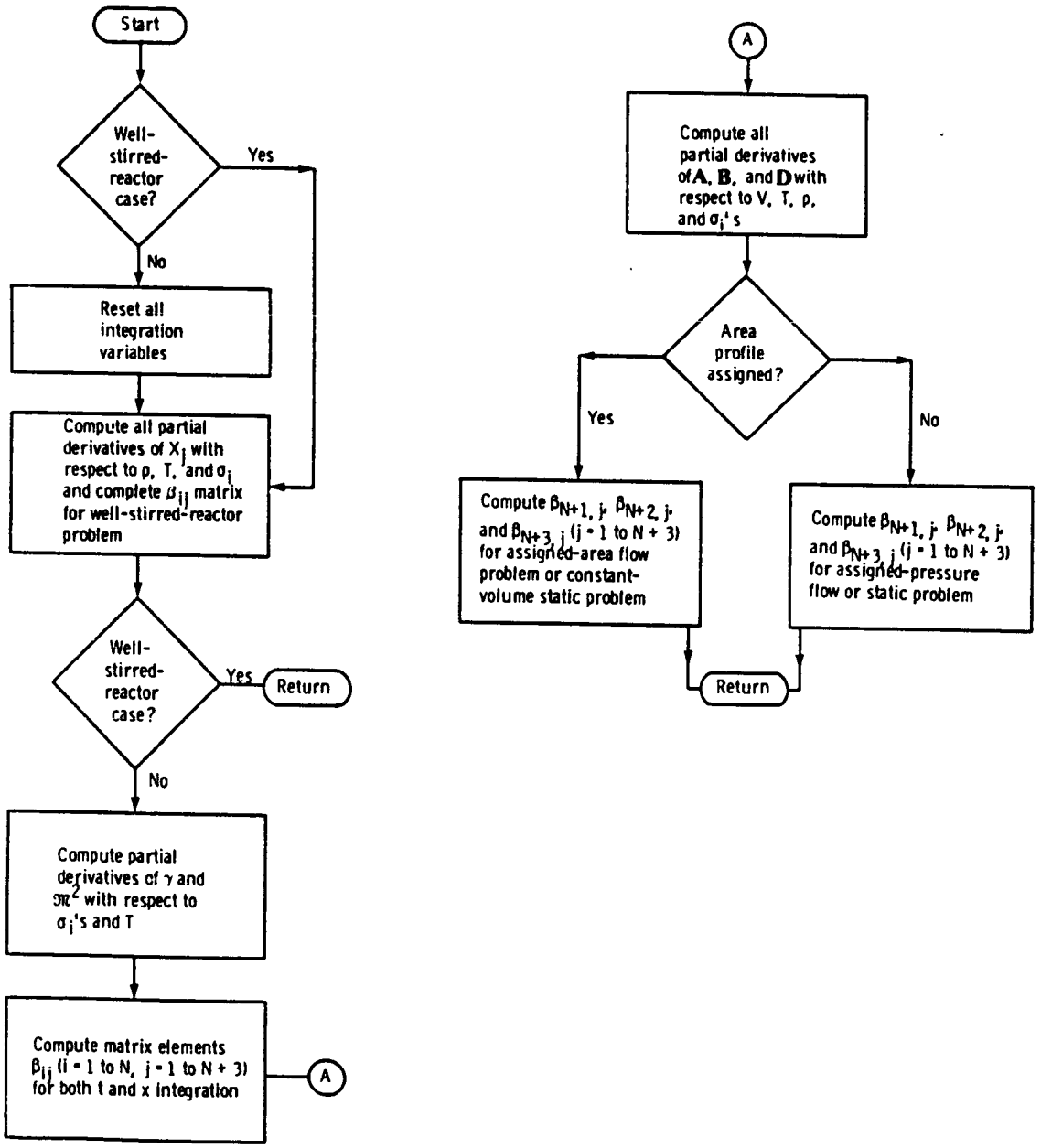

Figure 5.—Subroutine PEDERV, routine for computing all partial derivatives and Jacobian setup.

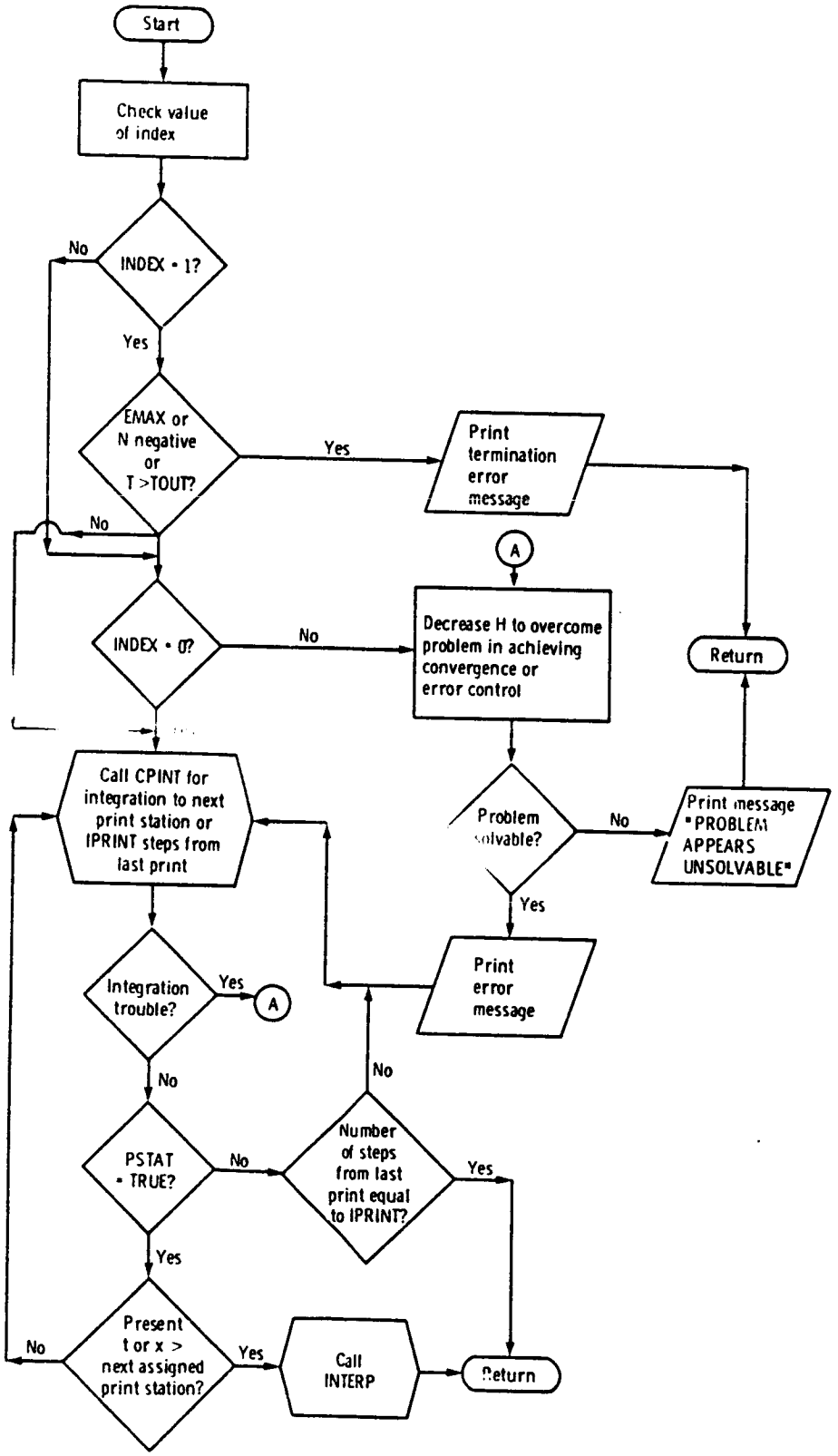

Figure 6.—Subroutine DRIVE, control routine for controlling integration problem.

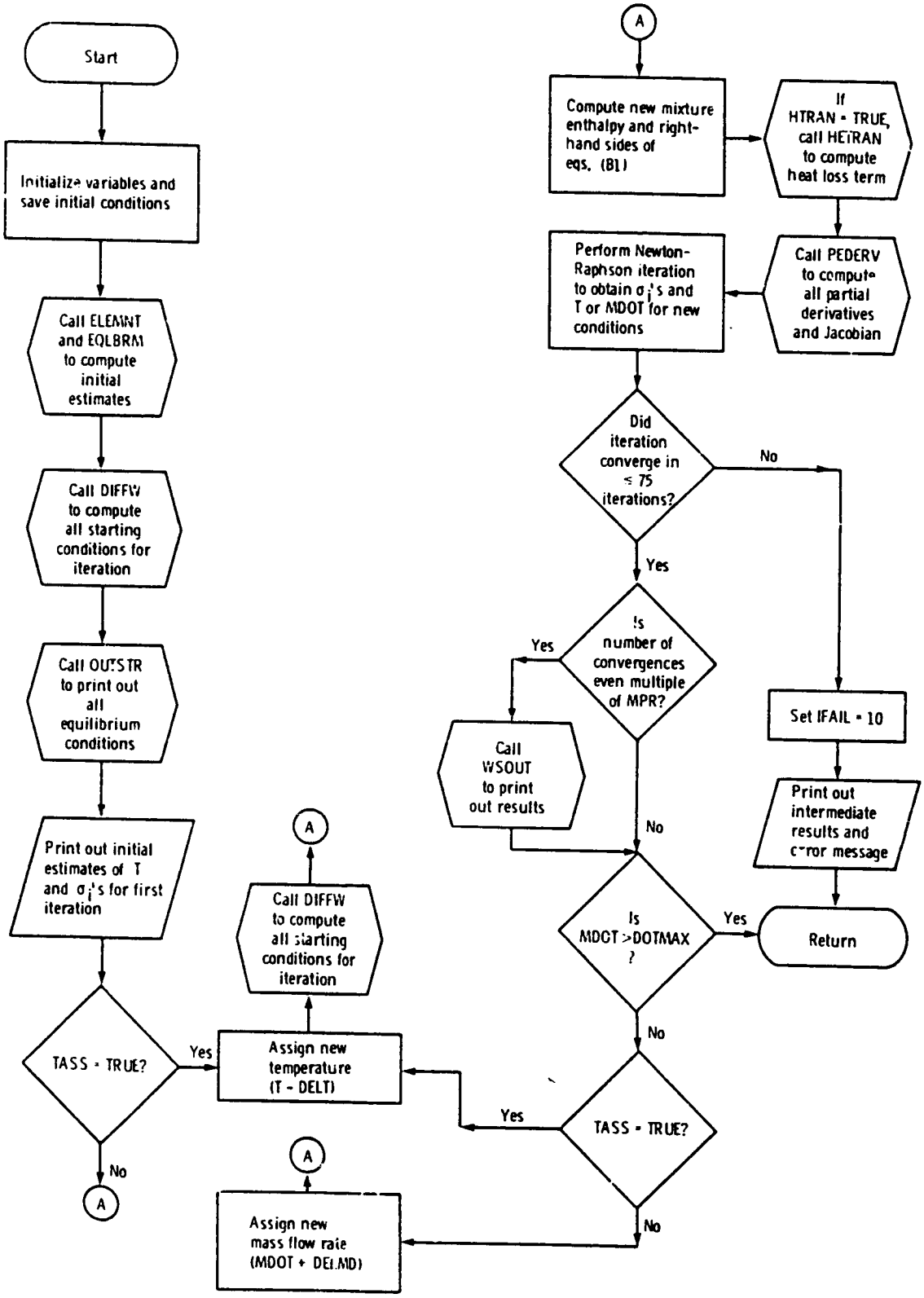

Figure 7.—Subroutine WSR, routine for computing well-stirred-reactor problem.

CPINT.—Subroutine CPINT is the core integrator subroutine. It uses an implicit predictor-corrector method for stiff differential equation systems to perform one step of the numerical integration and checks that the error is within required limits.

INTERP.—Subroutine INTERP interpolates between two integration steps to obtain values of the dependent variables at an assigned print station.

COSET.—Subroutine COSET is called by subroutine CPINT and sets coefficients used there.

PSET.—Subroutine PSET is called by subroutine CPINT to obtain the Jacobian (by calling PEDERV). Using the Jacobian it computes a related matrix **P**, which is used later by CPINT for solving linear systems.

DEC.—Subroutine DEC is called by PSET to triangularize the matrix **P** by Gaussian elimination.

SOL.—Subroutine SOL is called by CPINT to solve a linear system whose coefficient matrix was obtained by DEC.

Well-Stirred-Reactor/Shock-Combustion Section

In the well-stirred-reactor/shock-combustion section well-stirred-reactor computations as well as frozen and equilibrium combustion and shock computations are performed. Output is converted and written within the section. Provision is also made here for the transfer of frozen shock results to the input/output section to be used as initial conditions for the kinetic computations.

WSR.—Subroutine WSR sets up the Jacobian for each step of a well-stirred-reactor computation and performs the complete iterative solution. It calls subroutines DIFFUN and PEDERV to obtain starting conditions and Jacobian elements for each iteration at a given mass flow rate. It also calls subroutine EQLBRM to compute initial estimates ($\dot{m} = 0$) of density, temperature, and gas composition and subroutine MATRIX for solving the set of linear equations for the logarithmic corrections (fig. 7).

WSOUT.—Subroutine WSOUT converts and prints out final results of a well-stirred-reactor solution for a given $\dot{m}$ value. It is called by WSR.

COMB.—Subroutine COMB provides the setup and necessary subroutine calls to perform a constant-pressure equilibrium combustion computation and print out the results. It is used when a constant-pressure ignition problem is being integrated if the user wants to know how far from completion the reaction is at any reaction time.

SHOK.—Subroutine SHOK provides the setup and subroutine calls for computing both frozen and equilibrium shock processes.

SHOCKS.—Subroutine SHOCKS solves the shock-wave continuity equations for both equilibrium and frozen cases.

ELEMENT.—Subroutine ELEMENT sets up a table of all elements present and their concentrations in atoms per gram of mixture. These data are used for equilibrium shock and combustion computations.

EQLBRM.—Subroutine EQLBRM performs the equilibrium shock and combustion computations using subroutines GAUSS and MATRIX. These three subroutines are modifications of those used in the Gordon-McBride chemical equilibrium code (ref. 8).

MATRIX.—Subroutine MATRIX sets up the matrices required for the iterative numerical solution of equilibrium reaction problems by using subroutine EQLBRM.

GAUSS.—Subroutine GAUSS solves the linear equations set up by subroutine MATRIX.

SPOUT (ECOUT, ESOUT, FSOUT).—Subroutine SPOUT provides for the printout of all results of shock and equilibrium combustion computations. It converts output data to the user's requested units, transfers frozen shock results to the input/output section, and computes the characteristic shock-tube reaction length L_m in centimeters if this computation is required.

Concluding Remarks

A general chemical kinetics computer code, GCKP84, has been described that computes the progress of many types of complex gas-phase reaction. This new code replaces the original GCKP code and offers greatly improved efficiency as well as several new capabilities and convenience features. The code now permits solving the general differential equations for flow, batch, and shock-tube reactions and the nonlinear algebraic equations for the highly backmixed well-stirred reactor. In addition, heat loss or addition to any reaction may be simulated. The flexibility and efficiency of the code have been improved, especially by the use of a significantly faster numerical integration method. Comparisons have shown the new code to be 10 to 20 times faster than the original one while maintaining the same accuracy. A set of 12 typical test problems (appendix F) gives individual case running times ranging from 0.74 to 25.9 sec on the IBM 370/3033 computer. Reactions and species considered are specified by the user. In its present form the code permits a maximum of 50 species and 150 reactions to be considered for any problem. The new code allows the use of additional types of chemical reaction, including photochemical reactions and those involving excited-state species. The new code is written in Fortran V and was developed on the IBM 370/3033 computer. It may be available through the COSMIC organization at the University of Georgia in Athens; additional information about it can be obtained from the authors.

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Appendix A

General Net Reaction Rate Expressions and Partial Derivatives

Non-Third-Body Catalyst Reaction

Because the GCKP84 code allows at most two reactant and two product species, equation (2) will be written in the more specific form

$$\nu_{1j}S_1 + \nu_{2j}S_2 \underset{k_{-j}}{\overset{k_j}{\rightleftharpoons}} \nu_{3j}S_3 + \nu_{4j}S_4 \tag{A1}$$

Here subscripts 1 and 2 represent the specific reactant species and subscripts 3 and 4 represent the particular product species for reaction j. We define n_i to be the concentration of S_i in moles per unit volume and note that

$$n_i = \rho\sigma_i \tag{A2}$$

The net molar reaction rate is

$$R_j - R_{-j} = k_j n_1^{\nu_{1j}} n_2^{\nu_{2j}} - \frac{k_j}{K_j} n_3^{\nu_{3j}} n_4^{\nu_{4j}} \tag{A3}$$

Using the definition of X_j (eq. (7)) and equations (5) and (A2) we get for X_j the expression

$$X_j = k_j \left\{ \rho^{\nu_{1j}+\nu_{2j}-2} \sigma_1^{\nu_{1j}} \sigma_2^{\nu_{2j}} - \frac{\rho^{\nu_{3j}+\nu_{4j}-2} \sigma_3^{\nu_{3j}} \sigma_4^{\nu_{4j}}}{K_j} \right\} \tag{A4}$$

We need the derivatives of X_j with respect to ρ, T, and the σ_i's.

$$\frac{\partial X_j}{\partial \rho} = k_j \left\{ (\nu_{1j}+\nu_{2j}-2)\rho^{\nu_{1j}+\nu_{2j}-3} \sigma_1^{\nu_{1j}} \sigma_2^{\nu_{2j}} - \frac{(\nu_{3j}+\nu_{4j}-2)\rho^{\nu_{3j}+\nu_{4j}-3} \sigma_3^{\nu_{3j}} \sigma_4^{\nu_{4j}}}{K_j} \right\} \tag{A5}$$

$$\frac{\partial X_j}{\partial T} = \frac{k_j \rho^{\nu_{1j}+\nu_{4j}-2} \sigma_3^{\nu_{3j}} \sigma_4^{\nu_{4j}}}{K_j} \frac{d\ln K_j}{dT} + X_j \frac{d\ln k_j}{dT} \tag{A6}$$

$$\frac{\partial X_j}{\partial \sigma_1} = k_j \nu_{1j} \rho^{\nu_{1j}+\nu_{2j}-2} \sigma_1^{\nu_{1j}-1} \sigma_2^{\nu_{2j}} \tag{A7}$$

$$\frac{\partial X_j}{\partial \sigma_2} = k_j \nu_{2j} \rho^{\nu_{1j}+\nu_{2j}-2} \sigma_1^{\nu_{1j}} \sigma_2^{\nu_{2j}-1} \tag{A8}$$

$$\frac{\partial X_j}{\partial \sigma_3} = \frac{-k_j \nu_{3j} \rho^{\nu_{3j}+\nu_{4j}-2} \sigma_3^{\nu_{3j}-1} \sigma_4^{\nu_{4j}}}{K_j} \tag{A9}$$

$$\frac{\partial X_j}{\partial \sigma_4} = \frac{-k_j \nu_{4j} \rho^{\nu_{3j}+\nu_{4j}-2} \sigma_3^{\nu_{3j}} \sigma_4^{\nu_{4j}-1}}{K_j} \tag{A10}$$

If either species S_1 or S_4 or both are absent, the corresponding ν_{ij} factor is set to 0 and the σ_i factor to 1.

Third-Body Dissociation Reaction

We shall write the general reaction as

$$M + \nu_{2j}S_2 \underset{k_{-j}}{\overset{k_j}{\rightleftharpoons}} \nu_{3j}S_3 + \nu_{4j}S_4 + M \tag{A11}$$

where M, the catalyst collision partner, may be any species present. The X_j for this reaction is

$$X_j = \frac{k_j}{\rho^2} \left(n_M n_{S_2}^{\nu_{2j}} - \frac{n_M n_{S_3}^{\nu_{3j}} n_{S_4}^{\nu_{4j}}}{K_j} \right) \tag{A12}$$

The total concentration of catalyst molecules n_M is given by

$$n_M = \rho M_j \tag{A13}$$

where

$$M_j = \sum_{i=1}^{NS} m_{ij}\sigma_i \tag{A14}$$

Here M_j is the third-body efficiency factor for reaction j, and m_{ij} is the third-body efficiency factor for species i in reaction j. This is a correction only on the preexponential factor A_j of the rate-constant expression (eq. (3) or (4)) and is defined as

$$m_{ij} = \frac{(A_j)_i}{(A_j)_0} \tag{A15}$$

where $(A_j)_0$ is the A_j value for a reference species as collision partner and is the value used in the rate-constant data for a computation. Using equations (A2) and (A13) in (A12) gives

$$X_j = k_j M_j \left(\rho^{\nu_{2j}-1} \sigma_2^{\nu_{2j}} - \frac{\rho^{\nu_{3j}+\nu_{4j}-1} \sigma_3^{\nu_{3j}} \sigma_4^{\nu_{4j}}}{K_j} \right) \quad \text{(A16)}$$

The partial derivatives of X_j are

$$\frac{\partial X_j}{\partial \rho} = k_j M_j \left[(\nu_{2j}-1)\rho^{\nu_{2j}-2} \sigma_2^{\nu_{2j}} - \frac{(\nu_{3j}+\nu_{4j}-1)\rho^{\nu_{3j}+\nu_{4j}-2} \sigma_3^{\nu_{3j}} \sigma_4^{\nu_{4j}}}{K_j} \right] \quad \text{(A17)}$$

$$\frac{\partial X_j}{\partial T} = \frac{k_j M_j \rho^{\nu_{3j}+\nu_{4j}-1} \sigma_3^{\nu_{3j}} \sigma_4^{\nu_{4j}}}{K_j} \frac{d \ln K_j}{dT} + X_j \frac{d \ln k_j}{dT} \quad \text{(A18)}$$

$$\frac{\partial X_j}{\partial \sigma_2} = k_j M_j \nu_{2j} \rho^{\nu_{2j}-1} \sigma_2^{\nu_{2j}-1} + \frac{X_j}{M_j} m_{2j} \quad \text{(A19)}$$

$$\frac{\partial X_j}{\partial \sigma_3} = \frac{-k_j M_j \nu_{3j} \rho^{\nu_{3j}+\nu_{4j}-1} \sigma_3^{\nu_{3j}-1} \sigma_4^{\nu_{4j}}}{K_j} + \frac{X_j}{M_j} m_{3j} \quad \text{(A20)}$$

$$\frac{\partial X_j}{\partial \sigma_4} = \frac{-k_j M_j \nu_{4j} \rho^{\nu_{3j}+\nu_{4j}-1} \sigma_3^{\nu_{3j}} \sigma_4^{\nu_{4j}-1}}{K_j} + \frac{X_j}{M_j} m_{4j} \quad \text{(A21)}$$

Since M_j is an explicit function of all σ_k's, whether or not the species concentration is changed by reaction j, we also have the nonzero derivatives

$$\frac{\partial X_j}{\partial \sigma_k} = \frac{X_j}{M_j} m_{kj} \quad \text{(A22)}$$

where species k is only a third-body catalyst for the reaction.

Third-Body Recombination Reaction

We write the general reaction as follows:

$$M + \nu_{1j} S_1 + \nu_{2j} S_2 \underset{k_{-j}}{\overset{k_j}{\rightleftharpoons}} \nu_{3j} S_3 + M \quad \text{(A23)}$$

The X_j for this reaction becomes

$$X_j = k_j M_j \left(\rho^{\nu_{1j}+\nu_{2j}-1} \sigma_1^{\nu_{1j}} \sigma_2^{\nu_{2j}} - \frac{\rho^{\nu_{3j}-1} \sigma_3^{\nu_{3j}}}{K_j} \right) \quad \text{(A24)}$$

The partial derivatives are

$$\frac{\partial X_j}{\partial \rho} = k_j M_j \left[(\nu_{1j}+\nu_{2j}-1)\rho^{\nu_{1j}+\nu_{2j}-2} \sigma_1^{\nu_{1j}} \sigma_2^{\nu_{2j}} - \frac{(\nu_{3j}-1)\rho^{\nu_{3j}-2} \sigma_3^{\nu_{3j}}}{K_j} \right] \quad \text{(A25)}$$

$$\frac{\partial X_j}{\partial T} = \frac{k_j M_j \rho^{\nu_{3j}-1} \sigma_3^{\nu_{3j}}}{K_j} \frac{d \ln K_j}{dT} + X_j \frac{d \ln k_j}{dT} \quad \text{(A26)}$$

$$\frac{\partial X_j}{\partial \sigma_1} = k_j M_j \nu_{1j} \rho^{\nu_{1j}+\nu_{2j}-1} \sigma_1^{\nu_{1j}-1} \sigma_2^{\nu_{2j}} + \frac{X_j}{M_j} m_{1j} \quad \text{(A27)}$$

$$\frac{\partial X_j}{\partial \sigma_2} = k_j M_j \nu_{2j} \rho^{\nu_{1j}+\nu_{2j}-1} \sigma_1^{\nu_{1j}} \sigma_2^{\nu_{2j}-1} + \frac{X_j}{M_j} m_{2j} \quad \text{(A28)}$$

$$\frac{\partial X_j}{\partial \sigma_3} = \frac{-k_j M_j \nu_{3j} \rho^{\nu_{3j}-1} \sigma_3^{\nu_{3j}-1}}{K_j} + \frac{X_j}{M_j} m_{3j} \quad \text{(A29)}$$

$$\frac{\partial X_j}{\partial \sigma_k} = \frac{X_j}{M_j} m_{kj} \quad \text{(A30)}$$

where species k is only a catalyst molecule for the reaction.

Appendix B

Numerical Solution for Well-Stirred Reactor

The set of algebraic equations (75) and (76) is solved by a Newton-Raphson numerical technique. First, they are rewritten in the form

$$\left.\begin{aligned} f_i(\vec{\sigma}, T) &= \rho^2 \sum_{j=1}^{I} (\nu'_{ij} - \nu_{ij}) X_j + \frac{\dot{m}}{v}(\sigma_i^* - \sigma_i) = 0 \\ & \qquad i = 1,2,\ldots,N \\ f_{N+1}(\vec{\sigma}, T) &= \sum_{i=1}^{NS} (\sigma_i H_i - \sigma_i^* H_i^*) + \frac{\dot{Q}}{\dot{m}} = 0 \end{aligned}\right\} \quad \text{(B1)}$$

where the vector $\vec{\sigma}$ is a shorthand representation of the concentration variables.

$$\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3, \ldots, \sigma_N) \quad \text{(B2)}$$

In these equations N is the number of reacting species, NS is the total number of species present, including inerts, and I is the total number of reactions.

The f_i's of equation (B1) are expanded in a Taylor series about the values at the next point $(\vec{\sigma}_{n+1}, T_{n+1})$:

$$f_i\left(\vec{\sigma}_{n+1}, T_{n+1}\right) = f_i(\vec{\sigma}_n, T_n) + \sum_{k=1}^{N} \left(\frac{\partial f_i}{\partial \sigma_k}\right)_n \delta\sigma_{k,n} + \left(\frac{\partial f_i}{\partial T}\right)_n \delta T_n \qquad i = 1,2,3,\ldots,N+1 \quad \text{(B3)}$$

In this linearized expansion $\delta\sigma_{k,n}$ and δT_n are the corrections to the unknowns in going from the n^{th} to the $(n+1)^{\text{th}}$ iteration. If proper initial estimates are chosen, the new corrections will ultimately make all of the f_i's approach zero, which they must do at convergence, according to equations (B1). Thus setting the left sides of equation (B3) equal to zero gives a set of $N+1$ linear equations in the $N+1$ correction variables:

$$\sum_{k=1}^{N} \left(\frac{\partial f_i}{\partial \sigma_k}\right)_n \delta\sigma_{k,n} + \left(\frac{\partial f_i}{\partial T}\right)_n \delta T_n = -f_i(\vec{\sigma}_n, T_n) \qquad i = 1,2,3,\ldots,N+1 \quad \text{(B4)}$$

To avoid negative concentrations in the iteration procedure, it is necessary to convert to logarithmic correction variables. If q is any variable, we have

$$\frac{\partial f_i}{\partial q} = \frac{\partial f_i}{\partial \ln q} \frac{d \ln q}{dq} = \frac{1}{q} \frac{\partial f_i}{\partial \ln q}$$

and also $\delta q/q = \delta(\ln q)$.

Therefore we get immediately

$$\frac{\partial f_i}{\partial q} \delta q = \frac{\partial f_i}{\partial \ln q} \delta(\ln q)$$

and the system of equations (B4) can be rewritten as

$$\sum_{k=1}^{N} \left(\frac{\partial f_i}{\partial \ln \sigma_k}\right)_n \delta \ln \sigma_{k,n} + \left(\frac{\partial f_i}{\partial \ln T_n}\right)_n \delta \ln T_n = -f_i(\vec{\sigma}_n, T_n) \qquad i = 1,2,3,\ldots,N+1 \quad \text{(B5)}$$

This set of linear equations in the logarithmic correction variables is solved in an iterative procedure until the corrections approach zero within a specified accuracy. The Jacobian elements $(\partial f_i/\partial \ln \sigma_k)_n$ and $(\partial f_i/\partial \ln T)_n$ can be computed from equation (B1). In differentiating, the density ρ is treated as a function of the σ_i's and T obtained by combining equations (41) and (42)

$$\rho = \frac{p}{RT\sigma_M} \quad \text{(B6)}$$

where $\sigma_M = \sum_{i=1}^{NS} \sigma_i$. The resulting formulas, after some simplification, can be written

$$\frac{\partial f_i}{\partial \ln \sigma_k} = \rho^2 \sigma_k \sum_{j=1}^{I} (\nu'_{ij} - \nu_{ij}) \frac{DX_j}{D\sigma_k} - \frac{2\sigma_k W_i}{\sigma_M} - \frac{\dot{m}\sigma_k}{v} \delta_{ik}$$

$$k = 1,2,\ldots,N;\ i = 1,2,\ldots,N \quad \text{(B7)}$$

where δ_{ik} is the Kronecker delta

$$\frac{\partial f_i}{\partial \ln T} = \rho^2 T \sum_{j=1}^{I} (\nu'_{ij} - \nu_{ij}) \frac{DX_j}{DT} - 2W_i$$

$$i = 1,2,\ldots,N \quad \text{(B8)}$$

$$\frac{\partial f_{N+1}}{\partial \ln \sigma_k} = \sigma_k H_k \qquad k = 1,2,\ldots,N \tag{B9}$$

$$\frac{\partial f_{N+1}}{\partial \ln T} = T \sum_{k=1}^{NS} \sigma_k (C_p)_k + \frac{T}{\dot{m}} \frac{\partial \dot{Q}}{\partial T} \tag{B10}$$

The derivatives $DX_j/D\sigma_k$ and DX_j/DT are related to the partial derivatives of X_j obtained in appendix A in the following way: for the well-stirred reactor we have

$$X_j = X_j(\rho, T, \vec{\sigma_k}) \tag{B11}$$

where

$$\rho = g(T, \vec{\sigma_k}) = \frac{p}{RT\sigma_M} \tag{B6}$$

The chain rule gives

$$\frac{DX_j}{D\sigma_k} = \frac{\partial X_j}{\partial \sigma_k} + \frac{\partial X_j}{\partial \rho} \frac{\partial \rho}{\partial \sigma_k} \tag{B12}$$

and

$$\frac{DX_j}{DT} = \frac{\partial X_j}{\partial T} + \frac{\partial X_j}{\partial \rho} \frac{\partial \rho}{\partial T} \tag{B13}$$

By using the results $\partial\rho/\partial\sigma_k = -\rho/\sigma_M$ and $\partial\rho/\partial T = -\rho/T$, we get for equations (B12) and B(13)

$$\frac{DX_j}{D\sigma_k} = \frac{\partial X_j}{\partial \sigma_k} - \frac{\rho}{\sigma_M} \frac{\partial X_j}{\partial \rho} \tag{B14}$$

$$\frac{DX_j}{DT} = \frac{\partial X_j}{\partial T} - \frac{\rho}{T} \frac{\partial X_j}{\partial \rho} \tag{B15}$$

In applying this solution method, initial estimates are obtained by performing an equilibrium combustion computation for the assigned initial enthalpy and constant pressure and $\dot{m} = 0$. The equilibrium conditions along with a small assigned $\dot{m}$ of less than 100 g/sec are then used to obtain the first WSR solution for a near-equilibrium situation. The results of this solution are then used with another small $\dot{m}$ increment to obtain a second WSR solution. The process is continued with additional mass flow increments until the solution for the desired $\dot{m}$ is obtained. It was found necessary to set minimum values for all species concentrations at all times, including the initial equilibrium estimates. A minimum value of $\sigma_i = 1 \times 10^{-10}$ moles/g is used in the code at present.

It is sometimes convenient to interchange the roles of T and $\dot{m}$ in this computation. If desired, a temperature increment can be assigned and the $\dot{m}$ increment can be made the $(N+1)^{th}$ variable. This option is built into the code. The only changes needed are the replacement of derivatives of the f_i's with respect to T by derivatives with respect to $\dot{m}$. From equation (B1) we obtain

$$\frac{\partial f_i}{\partial(\ln \dot{m})} = \frac{\dot{m}}{v}(\sigma_i^* - \sigma_i) \qquad i = 1,2,\ldots,N \tag{B16}$$

$$\frac{\partial f_{N+1}}{\partial(\ln \dot{m})} = \dot{m} \frac{\partial}{\partial \dot{m}} \left(\frac{\dot{Q}}{\dot{m}} \right)$$

Usually $\dot{Q}$ will be specified as a quadratic function of temperature (eq. (25)) so that we may write the last equation as

$$\frac{\partial f_{N+1}}{\partial(\ln \dot{m})} = -\frac{\dot{Q}}{\dot{m}} \tag{B17}$$

Equations (B16) and (B17) replace equations (B8) and (B10).

Appendix C
Partial Derivatives for Numerical Integration

A number of partial derivatives must be computed in implementing the multistep numerical integration procedure for solving the general system

$$\frac{dY_i}{dq} = f_i(q, Y_1, Y_2, \ldots, Y_m) \tag{C1}$$

where

$q = t$ or x

$i = 1,2,\ldots,m$

At each step a Jacobian is set up that consists of the elements

$$\beta_{ij} = \frac{\partial f_i}{\partial Y_j} \qquad i,j = 1,2,\ldots,m \tag{C2}$$

For the GCKP84 code the following variables are identified:

$Y_i = \sigma_i \qquad i = 1,2,\ldots,N$

$Y_{N+1} = V$

$Y_{N+2} = \rho$

$Y_{N+3} = T$

Here N is the number of reacting species in the gas mixture. The following simplified notation will be used for the derivatives of the Y_i's:

$$f_i = \frac{d\sigma_i}{dq} \qquad i = 1,2,\ldots,N$$

$$f_{N+1} = \frac{dV}{dq}$$

$$f_{N+2} = \frac{d\rho}{dq}$$

$$f_{N+3} = \frac{dT}{dq}$$

In the following equations the symbols $\mathbf{A}^*$, $\mathbf{B}^*$, and $\mathbf{D}_v^*$ will not be used. The symbols $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{D}_v$ will be assumed to have definitions consistent with the particular f_i definitions being used.

Assigned Area Flow Equations

The following equations obtained from equations (34), (56) to (58), and (8) are used for the f_i's:

$$f_i = \frac{\rho^2}{Z} \sum_{s=1}^{I} (\nu'_{is} - \nu_{is}) \qquad i = 1,2,3,\ldots,N \tag{C3}$$

where $Z = \rho$ for $q = t$ and $Z = \rho V$ for $q = x$.

$$f_{N+1} = \frac{V}{\mathfrak{M}^2 - 1}\left(\frac{1}{A}\frac{dA}{dq} - \mathbf{A} + \mathbf{D}_v\right) \tag{C4}$$

$$f_{N+2} = -\rho\left[\frac{\mathfrak{M}^2}{\mathfrak{M}^2 - 1}\left(\frac{1}{A}\frac{dA}{dq} - \mathbf{A} + \mathbf{D}_v\right) + \mathbf{A} - \mathbf{D}_v\right] \tag{C5}$$

$$f_{N+3} = -T\left[\frac{(\gamma - 1)\mathfrak{M}^2}{\mathfrak{M}^2 - 1}\left(\frac{1}{A}\frac{dA}{dq} - \mathbf{A} + \mathbf{D}_v\right) + \mathbf{B} - \mathbf{D}_v\right] \tag{C6}$$

First, the derivatives for β_{ij} for $i,j = 1,2,\ldots,N$ are

$$\beta_{ij} = \frac{\partial f_i}{\partial \sigma_j} = \frac{\rho^2}{Z} \sum_{s=1}^{I} (\nu'_{is} - \nu_{is}) \frac{\partial X_s}{\partial \sigma_j} \tag{C7}$$

Next for $i = 1,2,\ldots,N$ we have

$$\beta_{i,N+1} = \frac{\partial f_i}{\partial V} = \begin{cases} 0 & \text{if } q = t \\ -\dfrac{f_i}{V} & \text{if } q = x \end{cases} \tag{C8}$$

$$\beta_{i,N+2} = \frac{\partial f_i}{\partial \rho} = \frac{f_i}{\rho} + \frac{\rho^2}{Z} \sum_{s=1}^{I} (\nu'_{is} - \nu_{is}) \frac{\partial X_s}{\partial \rho} \tag{C9}$$

$$\beta_{i,N+3} = \frac{\partial f_i}{\partial T} = \frac{\rho^2}{Z} \sum_{s=1}^{I} (\nu'_{is} - \nu_{is}) \frac{\partial X_s}{\partial T} \tag{C10}$$

Next we write the derivatives of f_{N+1}. For $i=1,2,\ldots,N$ we have

$$\beta_{N+1,i}=\frac{\partial f_{N+1}}{\partial \sigma_i}=\frac{1}{\mathfrak{M}^2-1}\left(-V\frac{\partial \mathbf{A}}{\partial \sigma_i}+V\frac{\partial \mathbf{D}_v}{\partial \sigma_i}-f_{N+1}\frac{\partial \mathfrak{M}^2}{\partial \sigma_i}\right) \tag{C11}$$

Then

$$\beta_{N+1,N+1}=\frac{\partial f_{N+1}}{\partial V}=\frac{1}{\mathfrak{M}^2-1}\left(-V\frac{\partial A}{\partial V}+V\frac{\partial \mathbf{D}_v}{\partial V}+\frac{1}{A}\frac{dA}{dq}-\mathbf{A}+\mathbf{D}_v-f_{N+1}\frac{\partial \mathfrak{M}^2}{\partial V}\right) \tag{C12}$$

$$\beta_{N+1,N+2}=\frac{\partial f_{N+1}}{\partial \rho}=\frac{V}{\mathfrak{M}^2-1}\left(-\frac{\partial \mathbf{A}}{\partial \rho}+\frac{\partial \mathbf{D}_v}{\partial \rho}\right) \tag{C13}$$

$$\beta_{N+1,N+3}=\frac{\partial f_{N+1}}{\partial T}=\frac{V}{\mathfrak{M}^2-1}\left(-\frac{\partial \mathbf{A}}{\partial T}+\frac{\partial \mathbf{D}_v}{\partial T}\right)-\frac{f_{N+1}}{\mathfrak{M}^2-1}\frac{\partial \mathfrak{M}^2}{\partial T} \tag{C14}$$

Next we write the derivatives of f_{N+2}. For $i=1,2,\ldots,N$ we have

$$\beta_{N+2,i}=\frac{\partial f_{N+2}}{\partial \sigma_i}=\frac{\rho}{\mathfrak{M}^2-1}\left(\frac{\partial \mathbf{A}}{\partial \sigma_i}-\frac{\partial \mathbf{D}_v}{\partial \sigma_i}\right)+\frac{\rho}{(\mathfrak{M}^2-1)^2}\times\left(\frac{1}{A}\frac{dA}{dq}-\mathbf{A}+\mathbf{D}_v\right)\frac{\partial \mathfrak{M}^2}{\partial \sigma_i} \tag{C15}$$

Then

$$\beta_{N+2,N+1}=\frac{\partial f_{N+2}}{\partial V}=\frac{\rho}{(\mathfrak{M}^2-1)^2}\left(\frac{1}{A}\frac{dA}{dq}-\mathbf{A}+\mathbf{D}_v\right)\times\frac{\partial \mathfrak{M}^2}{\partial V}+\frac{\rho}{\mathfrak{M}^2-1}\left(\frac{\partial \mathbf{A}}{\partial V}-\frac{\partial \mathbf{D}_v}{\partial V}\right) \tag{C16}$$

$$\beta_{N+2,N+2}=\frac{\partial f_{N+2}}{\partial \rho}=\frac{\rho}{\mathfrak{M}^2-1}\left(\frac{\partial \mathbf{A}}{\partial \rho}-\frac{\partial \mathbf{D}_v}{\partial \rho}\right)+\frac{f_{N+2}}{\rho} \tag{C17}$$

$$\beta_{N+2,N+3}=\frac{\partial f_{N+2}}{\partial T}=\frac{\rho}{\mathfrak{M}^2-1}\left(\frac{\partial \mathbf{A}}{\partial T}-\frac{\partial \mathbf{D}_v}{\partial T}\right)+\frac{\rho}{(\mathfrak{M}^2-1)^2}\left(\frac{1}{A}\frac{dA}{dq}-\mathbf{A}+\mathbf{D}_v\right)\frac{\partial \mathfrak{M}^2}{\partial T} \tag{C18}$$

Finally we write the derivatives of f_{N+3}. For $i=1,2,\ldots,N$ we get

$$\beta_{N+3,i}=\frac{\partial f_{N+3}}{\partial \sigma_i}=\frac{T(\gamma-1)\mathfrak{M}^2}{\mathfrak{M}^2-1}\frac{\partial \mathbf{A}}{\partial \sigma_i}-\frac{T(\gamma\mathfrak{M}^2-1)}{\mathfrak{M}^2-1}\frac{\partial \mathbf{D}_v}{\partial \sigma_i}+\frac{(\gamma-1)T}{(\mathfrak{M}^2-1)^2}\left(\frac{1}{A}\frac{dA}{dq}-\mathbf{A}+\mathbf{D}_v\right)\frac{\partial \mathfrak{M}^2}{\partial \sigma_i}-\frac{T\mathfrak{M}^2}{\mathfrak{M}^2-1}\times\left(\frac{1}{A}\frac{dA}{dq}-\mathbf{A}+\mathbf{D}_v\right)\frac{\partial \gamma}{\partial \sigma_i}-T\frac{\partial \mathbf{B}}{\partial \sigma_i} \tag{C19}$$

Then

$$\beta_{N+3,N+1}=\frac{\partial f_{N+3}}{\partial V}=\frac{(\gamma-1)T\mathfrak{M}^2}{\mathfrak{M}^2-1}\frac{\partial \mathbf{A}}{\partial V}+\frac{(\gamma-1)T}{(\mathfrak{M}^2-1)^2}\times\left(\frac{1}{A}\frac{dA}{dq}-\mathbf{A}+\mathbf{D}_v\right)\frac{\partial \mathfrak{M}^2}{\partial V}-\frac{T(\gamma\mathfrak{M}^2-1)}{\mathfrak{M}^2-1}\frac{\partial \mathbf{D}_v}{\partial V}-T\frac{\partial \mathbf{B}}{\partial V} \tag{C20}$$

$$\beta_{N+3,N+2}=\frac{\partial f_{N+3}}{\partial \rho}=\frac{(\gamma-1)T\mathfrak{M}^2}{\mathfrak{M}^2-1}\frac{\partial \mathbf{A}}{\partial \rho}-\frac{T(\gamma\mathfrak{M}^2-1)}{\mathfrak{M}^2-1}\frac{\partial \mathbf{D}_v}{\partial \rho}-T\frac{\partial \mathbf{B}}{\partial \rho} \tag{C21}$$

$$\beta_{N+3,N+3}=\frac{\partial f_{N+3}}{\partial T}=\frac{f_3}{T}+\frac{(\gamma-1)T\mathfrak{M}^2}{\mathfrak{M}^2-1}\frac{\partial \mathbf{A}}{\partial T}-\frac{T(\gamma\mathfrak{M}^2-1)}{\mathfrak{M}^2-1}\frac{\partial \mathbf{D}_v}{\partial T}+\frac{(\gamma-1)T}{(\mathfrak{M}^2-1)^2}\times\left(\frac{1}{A}\frac{dA}{dq}-\mathbf{A}+\mathbf{D}_v\right)\frac{\partial \mathfrak{M}^2}{\partial T}-\frac{T\mathfrak{M}^2}{\mathfrak{M}^2-1}\times\left(\frac{1}{A}\frac{dA}{dq}-\mathbf{A}+\mathbf{D}_v\right)\frac{\partial \gamma}{\partial T}-T\frac{\partial \mathbf{B}}{\partial T} \tag{C22}$$

Assigned-Pressure Flow Equations

For this system the equations for f_i, $i=1,2,\ldots,N$, are unchanged and given by equation (C3). The remaining f_i's are defined from equations (68) to (70) as

$$f_{N+1}=-\frac{1}{\rho V}\frac{dp}{dq} \tag{C23}$$

$$f_{N+2}=\rho\left(\frac{1}{\gamma p}\frac{dp}{dq}-\mathbf{A}+\mathbf{D}_v\right) \tag{C24}$$

$$f_{N+3} = T\left[\left(\frac{\gamma-1}{\gamma}\right)\frac{1}{p}\frac{dp}{dq} - \mathbf{B} - \mathbf{D}_v\right] \tag{C25}$$

The required new matrix elements are given by

$$\beta_{N+1,i} = \frac{\partial f_{N+1}}{\partial \sigma_i} = 0 \qquad i = 1,2,\ldots,N \tag{C26}$$

$$\beta_{N+1,N+1} = \frac{\partial f_{N+1}}{\partial V} = \frac{-f_{N+1}}{V} \tag{C27}$$

$$\beta_{N+1,N+2} = \frac{\partial f_{N+1}}{\partial \rho} = \frac{-f_{N+1}}{\rho} \tag{C28}$$

$$\beta_{N+1,N+3} = \frac{\partial f_{N+1}}{\partial T} = 0 \tag{C29}$$

$$\beta_{N+2,i} = \frac{\partial f_{N+2}}{\partial \sigma_i} = \frac{-\rho}{\gamma^2 p}\frac{dp}{dq}\frac{\partial \gamma}{\partial \sigma_i} - \rho\frac{\partial \mathbf{A}}{\partial \sigma_i} + \rho\frac{\partial \mathbf{D}_v}{\partial \sigma_i} \qquad i = 1,2,\ldots,N \tag{C30}$$

$$\beta_{N+2,N+1} = \frac{\partial f_{N+2}}{\partial V} = -\rho\left(\frac{\partial \mathbf{A}}{\partial V} - \frac{\partial \mathbf{D}_v}{\partial V}\right) \tag{C31}$$

$$\beta_{N+2,N+2} = \frac{\partial f_{N+2}}{\partial \rho} = \frac{f_{N+2}}{\rho} - \rho\left(\frac{\partial \mathbf{A}}{\partial \rho} - \frac{\partial \mathbf{D}_v}{\partial \rho}\right) \tag{C32}$$

$$\beta_{N+2,N+3} = \frac{\partial f_{N+2}}{\partial T} = -\rho\left\{\frac{1}{\gamma^2 p}\frac{dp}{dq}\frac{\partial \gamma}{\partial T} + \frac{\partial \mathbf{A}}{\partial T} - \frac{\partial \mathbf{D}_v}{\partial T}\right\} \tag{C33}$$

$$\beta_{N+3,i} = \frac{\partial f_{N+3}}{\partial \sigma_i} = T\left\{\frac{1}{\gamma^2 p}\frac{dp}{dq}\frac{\partial \gamma}{\partial \sigma_i} - \frac{\partial \mathbf{B}}{\partial \sigma_i} - \frac{\partial \mathbf{D}_v}{\partial \sigma_i}\right\} \qquad i = 1,2,\ldots,N \tag{C34}$$

$$\beta_{N+3,N+1} = \frac{\partial f_{N+3}}{\partial V} = -T\left(\frac{\partial \mathbf{B}}{\partial V} + \frac{\partial \mathbf{D}_v}{\partial V}\right) \tag{C35}$$

$$\beta_{N+3,N+2} = \frac{\partial f_{N+3}}{\partial \rho} = -T\left(\frac{\partial \mathbf{B}}{\partial \rho} + \frac{\partial \mathbf{D}_v}{\partial \rho}\right) \tag{C36}$$

$$\beta_{N+3,N+3} = \frac{\partial f_{N+3}}{\partial T} = \frac{f_{N+3}}{T} + \frac{T}{\gamma^2 p}\frac{dp}{dq}\frac{\partial \gamma}{\partial T} - T\left(\frac{\partial \mathbf{B}}{\partial T} + \frac{\partial \mathbf{D}_v}{\partial T}\right) \tag{C37}$$

Batch Reaction Equations

The equations for species concentration change with time (eqs. (34)) are the same as for flow reactions. We only need new formulas for β_{ij}, where $i = N+1$, $N+2$, and $N+3$.

Constant-volume reaction.—Since density is an assigned constant and velocity is zero, the only variables to be solved for are the σ_i's and T. The only changed Jacobian elements are obtained from the temperature equation (eq. (50)). We define

$$f_{N+3} = -T[\mathbf{B} - (\gamma-1)\mathbf{A} + \gamma\mathbf{D}] \tag{C38}$$

and obtain the following new formulas:

$$\beta_{N+3,i} = \frac{\partial f_{N+3}}{\partial \sigma_i} = -T\left[\frac{\partial \mathbf{B}}{\partial \sigma_i} - (\gamma-1)\frac{\partial \mathbf{A}}{\partial \sigma_i} + (\mathbf{D}-\mathbf{A})\frac{\partial \gamma}{\partial \sigma_i} + \gamma\frac{\partial \mathbf{D}}{\partial \sigma_i}\right] \qquad i = 1,2,\ldots,N \tag{C39}$$

$$\beta_{N+3,N+3} = \frac{\partial f_{N+3}}{\partial T} = -T\left[\frac{\partial \mathbf{B}}{\partial T} - (\gamma-1)\frac{\partial \mathbf{A}}{\partial T} + (\mathbf{D}-\mathbf{A})\frac{\partial \gamma}{\partial T} + \gamma\frac{\partial \mathbf{D}}{\partial T}\right] + \frac{f_{N+3}}{T} \tag{C40}$$

The values of $\beta_{N+3,N+1}$ and $\beta_{N+3,N+2}$ are zero when this type of problem is solved, as are all the $\beta_{N+1,i}$ and $\beta_{N+2,i}$ elements.

Variable-volume-assigned-pressure problem.—For this situation the variables to be solved for are ρ, T, and the σ_i's. The temperature and density derivative equations are given by equations (43) and (44) and we make the definitions

$$f_{N+2} = \rho\left(\frac{1}{\gamma p}\frac{dp}{dt} - \mathbf{A} + \mathbf{D}\right) \tag{C41}$$

$$f_{N+3} = T\left[\left(\frac{\gamma-1}{\gamma}\right)\frac{1}{p}\frac{dp}{dt} - \mathbf{B} - \mathbf{D}\right] \tag{C42}$$

The new formulas for the Jacobian elements are then

$$\beta_{N+2,i} = \frac{\partial f_{N+2}}{\partial \sigma_i} = \frac{-\rho}{\gamma^2 p}\frac{dp}{dt}\frac{\partial \gamma}{\partial \sigma_i} - \rho\frac{\partial \mathbf{A}}{\partial \sigma_i} + \rho\frac{\partial \mathbf{D}}{\partial \sigma_i}$$

$$i = 1,2,\ldots,N \qquad \text{(C43)}$$

$$\beta_{N+2,N+2} = \frac{\partial f_{N+2}}{\partial \rho} = \frac{f_{N+2}}{\rho} - \rho\left(\frac{\partial \mathbf{A}}{\partial \rho} - \frac{\partial \mathbf{D}}{\partial \rho}\right) \qquad \text{(C44)}$$

$$\beta_{N+2,N+3} = \frac{\partial f_{N+2}}{\partial T} = -\rho\left(\frac{1}{\gamma^2 p}\frac{dp}{dt}\frac{\partial \gamma}{\partial T} + \frac{\partial \mathbf{A}}{\partial T} - \frac{\partial \mathbf{D}}{\partial T}\right) \qquad \text{(C45)}$$

$$\beta_{N+3,i} = \frac{\partial f_{N+3}}{\partial \sigma_i} = T\left(\frac{1}{\gamma^2 p}\frac{dp}{dt}\frac{\partial \gamma}{\partial \sigma_i} - \frac{\partial \mathbf{B}}{\partial \sigma_i} - \frac{\partial \mathbf{D}}{\partial \sigma_i}\right)$$

$$i = 1,2,\ldots,N \qquad \text{(C46)}$$

$$\beta_{N+3,N+2} = \frac{\partial f_{N+3}}{\partial \rho} = -T\left(\frac{\partial \mathbf{B}}{\partial \rho} + \frac{\partial \mathbf{D}}{\partial \rho}\right) \qquad \text{(C47)}$$

$$\beta_{N+3,N+3} = \frac{\partial f_{N+3}}{\partial T} = \frac{f_{N+3}}{T} - T\left(\frac{\partial \mathbf{B}}{\partial T} + \frac{\partial \mathbf{D}}{\partial T}\right) + \frac{T}{\gamma^2 p}\frac{dp}{dt}\frac{\partial \gamma}{\partial T} \qquad \text{(C48)}$$

Additional Partial Derivatives

In using the differentiation formulas just given, several additional formulas for the derivatives of X_j, $\mathbf{A}$, $\mathbf{B}$, $\mathbf{D}$, $\mathbf{D}_v$, $\mathfrak{M}^2$, and γ are needed. The derivatives of the X_j factors were computed in appendix A. Formulas for the derivatives of $\mathbf{A}$, $\mathbf{B}$, $\mathfrak{M}^2$, and γ were derived in appendix C of reference 1 and will not be repeated here. The necessary derivatives of $\mathbf{D}$ and $\mathbf{D}_v$ are obtained from equations (49) and (59).

$$\frac{\partial \mathbf{D}}{\partial \sigma_i} = \mathbf{D}\left[\frac{1}{\gamma(\gamma-1)}\frac{\partial \gamma}{\partial \sigma_i} - M_w\right] \qquad i = 1,2,\ldots,N \qquad \text{(C49)}$$

$$\frac{\partial \mathbf{D}}{\partial \rho} = \mathbf{D}\frac{\partial}{\partial \rho}\ln\left(\frac{\dot{Q}}{\dot{m}}\right) \qquad \text{(C50)}$$

$$\frac{\partial \mathbf{D}}{\partial T} = \mathbf{D}\frac{\partial}{\partial T}\ln\left(\frac{\dot{Q}}{\dot{m}}\right) - \frac{\mathbf{D}}{T} + \frac{\mathbf{D}}{\gamma(\gamma-1)}\frac{\partial \gamma}{\partial T} \qquad \text{(C51)}$$

The derivatives of $\mathbf{D}_v$ for a flow reaction are the same as for $\mathbf{D}$, except that $\dot{m}$ is replaced by $\dot{m}$, the mass flow rate, and we also compute $\partial \mathbf{D}_v/\partial V$

$$\frac{\partial \mathbf{D}_v}{\partial \sigma_i} = \mathbf{D}_v\left(\frac{1}{\gamma(\gamma-1)}\frac{\partial \gamma}{\partial \sigma_i} - M_w\right) \qquad \text{(C52)}$$

$$\frac{\partial \mathbf{D}_v}{\partial V} = \frac{\mathbf{D}_v}{V} + \mathbf{D}_v\frac{\partial}{\partial V}\left(\ln\frac{\dot{Q}}{\dot{m}}\right) \qquad \text{(C53)}$$

$$\frac{\partial \mathbf{D}_v}{\partial \rho} = \mathbf{D}_v\frac{\partial}{\partial \rho}\ln\left(\frac{\dot{Q}}{\dot{m}}\right) \qquad \text{(C54)}$$

$$\frac{\partial \mathbf{D}_v}{\partial T} = \mathbf{D}_v\frac{\partial}{\partial T}\ln\left(\frac{\dot{Q}}{\dot{m}}\right) - \frac{\mathbf{D}_v}{T} + \frac{\mathbf{D}_v}{\gamma(\gamma-1)}\frac{\partial \gamma}{\partial T} \qquad \text{(C55)}$$

The derivatives of the heat transfer terms are computed by using either equation (25) or equations (28) to (34).

Appendix D
Input Data Preparation and Error Messages

We have divided the description of the input data into two parts. First, we describe the dataset for a single case in detail. We then describe the additional data needed for any subsequent problems. This will show the user how to run several cases at one time without making a complete new dataset for each case. Finally we list some of the code error messages and briefly explain them.

Input Preparation

Thermodynamic data.—The necessary thermodynamic data for all cases in a single computer run are entered first, before any of the individual problem data. The first line of a dataset tells the code where to find the thermodynamic data. Columns 1 to 4 of this line must contain either the word CARD or TAPE. If the word CARD appears, the code reads the thermodynamic data from the lines that immediately follow this line. If the word TAPE is used, the code reads the thermodynamic data from a separate dataset that must be referenced to logical tape unit 4. A copy of the NASA Lewis master thermodynamic dataset is provided with the GCKP84 code. Note that, when CARD is used, the data are written out on logical unit 4 after being read. The user should be careful not to accidentally overwrite a master dataset when using the "CARD" option. The format of this dataset is identical to that of the Gordon-McBride equilibrium chemistry code and is described in their report (ref. 8) as well as in appendix D of reference 1. We only mention here that the data for the last species must be followed by a line with END written in columns 1 to 3.

First-case data.—The data lines for a single (or first) case are now described in the order of their listing in the dataset. *All names must be left adjusted in their fields.*

(1) Title—The first line of the data after the thermodynamic data information is a title, which is read with format (20A4) and printed out at the top of the first page of output.

(2) Chemical reactions—chemical reactions are listed, one per line, in any order. The line contains participating species names and stoichiometric coefficients (if different from 1) and the rate-constant parameters A_j, n_j, and either E_j or c_j (eqs. (3) and (4)). The exact format of each line, which is different from the format used in the original GCKP code, is as follows:

Columns	Format	Content and explanation
1–3	F3.1	Stoichiometric coefficient of first reactant; if left blank, 1 is used
4–11	2A4	(a) Name of first reactant, if two reactants are present (b) Letter M in column 4 if a collisional decomposition (c) HNU in columns 4 to 6 if a photochemical decomposition
12		Not read
13–15	F3.1	Stoichiometric coefficient of second reactant (only reactant if a decomposition reaction)
16–23	2A4	Name of second (or only) reactant
24		Not read
25	A1	Equal sign if reaction is reversible; any other symbol if it is irreversible
26–28	F3.1	Stoichiometric coefficient of first product
29–36	2A4	Name of first product
37		Not read
38–40	F3.1	Stoichiometric coefficient of second product
41–48	2A4	Name of second product, if present
49		Not read
50	A1	Leave blank for equation (3); write "S" if equation (4) is used for k_j
51–60	E10.4	A_j for equation (3) or (4)
61–62		Not read
63–70	F8.4	n_j for equation (3) or (4)
71–72		Not read
73–80	F8.4	E_j for equation (3) or c_j for equation (4)

In the current version of GCKP84 the total number of reactions may not exceed 150. Of these no more than 35 may be collisional recombination or dissociation reactions requiring third-body efficiencies m_{ij} (eq. (A14)). *The end of the reaction list is signaled by a blank line after the last reaction has been written.* Note that the code makes up its own list of reacting species from the names of the species in the reaction list. No separate reacting species list is needed in the data.

(3) Inert species—The names of any nonreacting species are listed, four per card, starting in columns 1, 17, 33, and 49. The format is (4(2A4,8X)). *The end of the inert species list is signaled by a blank field after the last species name.* If there are no inert species, a blank line must be placed here. If there is an exact multiple of four inert species, a blank line must follow the last species line. The total number of reacting plus inert species must not exceed 50 in the present code.

(4) Version and units—A single line specifies the variable of integration, the assigned variable (area or pressure), and the desired input and output units. Its exact format is as follows:

Columns	Content	Explanation
1-8	TIME	Time is the integration variable
	DISTANCE	Distance is the integration variable
11-18	PRESSURE	Pressure profile is assigned
	AREA	Area profile is assigned
	Blank	Velocity is zero; no assigned pressure. Volume must be constant
21-23	CGS or blank	Input in internal (cgs) units
	FPS	Input in U.S. customary units
	SI	Input in SI units
31-33	CGS or blank	Output in internal (cgs) units
	FPS	Output in U.S. customary units
	SI	Output in SI units

(5) Problem selection and controls—Problem selection and all logical control variables are set in the NAMELIST called PROB. The names of all variables in PROB are given below. If no value is given for a variable, the code sets a default value or zero. The standard options are shown by an underscore.

Name	Value	Explanation
ALLM1	TRUE	All collisional efficiencies for third-body reactions are equal to 1; none are listed in data
	FALSE	Some collisional third-body efficiencies are to be read in
COMBUS	TRUE	Perform equilibrium combustion calculations
	FALSE	Do not perform equilibrium combustion calculations
CONC	TRUE	Composition to be output as moles per unit volume
	FALSE	Composition to be output as mass fractions
DBUGO	TRUE	Print intermediate output
	FALSE	Do not print intermediate output
EMAX		Relative error control parameter per integration step; set equal to 1×10^{-6} if defaulted
EXCHR	TRUE	Net energy exchange rate to be output for each reaction
	FALSE	Net conversion rate to be output for each reaction
HINT		Initial step size for integration in centimeters or seconds; default values are 5×10^{-8} sec or 1×10^{-6} cm
ITPSZ	1	An area or pressure table of values will be input
	2	Area or pressure will be specified by a polynomial equation (eq. (77))
	3	LSUBM and ETA will be input for special area equation (eq. (97))
	4	D, VISC, BETA, and ETA will be input for special area equation (eq. (97))
	5	Zero-velocity case—no assigned pressure
IPRCOD	1	Distance versus area profile is given
	2	Distance versus pressure profile is given
	3	Time versus area profile is given
	4	Time versus pressure profile is given

PCON	TRUE	Pressure is assigned and temperature is held constant for a batch reaction
	FALSE	Temperature is changing in an assigned-pressure batch reaction
RHOCON	TRUE	Hold volume (density) constant
	FALSE	Do not hold volume (density) constant
SHOCK	TRUE	Perform frozen and equilibrium shock calculations
	FALSE	Do not perform shock calculations
TCON	TRUE	Hold temperature constant
	FALSE	Do not hold temperature constant
ATB	------	Array for area or pressure half of assigned-variable table; must be in user's chosen input units
NTB	------	Total number of stations in input area or pressure table; must be less than or equal to 40
XTB	------	Array for time or distance half of assigned-variable table; must be in user's chosen input units
CX3	------	Coefficient of q^3 in pressure/area equation (eq. (77))
CX2	------	Coefficient of q^2 in equation (77)
CX1	------	Coefficient of q in equation (77)
CX0	------	Constant term in equation (77)
LSUBM	------	Characteristic shock-tube reaction length for special area equation (eq. (97))—must be given in centimeters
ETA	------	Dimensionless exponent in special area equation (eq. (97)) for boundary layer correction
D	------	Hydraulic diameter of shock tube, cm
VISC	------	Viscosity coefficient, g/(cm-sec)
BETA	------	Dimensionless boundary layer parameter; last three variables used to have code compute LSUBM, if desired. Set ITPSZ = 4
PSTAT	FALSE	Printout requested every n integration steps
	TRUE	A list of print stations is given
END	------	Final print station in user's chosen input units; must be a time if time is the integration variable and conversely for distance; only used if output is made every n steps
IPRINT	------	Number of steps, n, between printouts if PSTAT = FALSE. Default value is 5
PRINT	------	Array of values of the variable of integration at which output is desired; must be in user's chosen input units. Number of values equals NPRNTS
APRINT	------	Array of areas or pressures at which output is desired; may only be used if table of assigned pressures or areas is given and must be in user's chosen input units. Number of values equals NPRNTS
NPRNTS	------	Total number of input print stations; must be less than or equal to 50
HTRAN	TRUE	Heat transfer between reacting system and environment will be considered
	FALSE	Reaction is adiabatic.
QMREAD	TRUE	Heat transfer rate Q will be specified by the quadratic expression (eq. (25))
	FALSE	Code will use viscosity and thermal conductivity data and appropriate engineering correlation equations to compute Q. The viscosity and thermal conductivity data must be available in a separate dataset
HT2	------	Coefficient of T^2 in equation (25)
HT1	------	Coefficient of T in equation (25)
HT0	------	Constant term in equation (25)
TWALL	------	Wall temperature for heat transfer computation. See equations (26) to (32). Used only when QMREAD = FALSE

TOTMAS	------	Total mass of reacting gas for a batch reaction. Used only when both HTRAN and QMREAD are TRUE
OTTO	TRUE	Correlations of reference 2 for the internal combustion engine are used to compute heat transfer coefficient and Q for batch reaction with cylindrical geometry. QMREAD must be set equal to FALSE
	FALSE	Correlations of reference 2 not used for heat transfer computation
STROKE	------	Length of piston stroke, cm. Used for heat transfer coefficient computation when OTTO = TRUE
BORE	------	Diameter of piston, cm. Used for heat transfer coefficient computation when OTTO = TRUE
FREQ	------	Engine speed, rpm. Used for heat transfer coefficient computation when OTTO = TRUE
ROCKET	TRUE	Rocket performance will be computed and results printed for each print station
	FALSE	Rocket performance will not be computed
PC	------	Chamber pressure, psia, for rocket performance computation. Used only when ROCKET = TRUE
ATHROT	------	Rocket nozzle throat area, in^2. Used only when ROCKET = TRUE
WELSTR	TRUE	A well-stirred-reactor problem is to be done
	FALSE	A numerical integration problem is to be done
WSFLOW	TRUE	A numerical integration reacting flow problem will be done after a well-stirred-reactor problem, using the final WSR results for ρ, T, and the σ_i's as input
	FALSE	No integration problem will be done after a WSR problem
DELMD	------	Desired mass flow rate increment for WSR problem using assigned mass flow rate. Used only if TASS = FALSE
DELT	------	Desired temperature decrement (absolute value) for WSR problem using assigned temperature. Used only if TASS = TRUE
TASS	TRUE	Temperature assigned for a WSR problem
	FALSE	Mass flow rate assigned for a WSR problem
DOTMAX	------	Maximum mass flow rate desired for a WSR problem. Computation ends when this value is exceeded.
MPR	------	Control variable for WSR problem printout. Default value is 1 for printout after every convergence. If set equal to integer n, printout occurs only every n^{th} convergence (value of assigned $\dot{m}$ or T)
RICH	TRUE	Special control of iteration in a WSR problem will be used for rich hydrocarbon combustion mixtures to improve convergence
	FALSE	Standard iteration control will be used in a WSR problem
RITE	TRUE	Extra debug output will be printed out for a well-stirred-reactor problem
	FALSE	No extra debug output will be printed

(6) Optional viscosity and thermal conductivity data—If HTRAN is TRUE and QMREAD is FALSE in NAMELIST PROB, a special dataset containing viscosity and thermal conductivity coefficients for 20 species must be available for reading in just after PROB. This dataset is provided with the GCKP84 code. The data are read in by subroutine HETRAN and used later to compute the mixture heat transfer coefficient.

(7) Third-body efficiencies—To read in collisional efficiencies m_{ij} different from 1 for third-body reactions, the variable ALLM1 is set equal to FALSE. Otherwise no data of this type will be present. Only efficiencies different from 1 must be read in. The efficiencies are listed, up to two per line, in the following format, which is different from that in the original GCKP.

Columns	Content	Explanation
1-48	Third-body reaction	These columns must be identical to columns 1 to 48 of the reaction line for the particular reaction

49–56	Species name; format 2A4	Third-body species name; must be left adjusted
57		Not read
58–63	Efficiency; format F6.3	Efficiency value for species in columns 49 to 56
64–65		Not read
66–73	Species name; format 2A4	Third-body species name
74		Not read
75–80	Efficiency; format F6.3	Efficiency value for species in columns 66 to 73

The efficiency data lines may be in any order and the third-body species may be listed in any order, one or two per line. *The end of the third-body list is indicated by a blank line following the last set of efficiencies.*

(8) Initial conditions—The initial conditions are input through a NAMELIST called START. This NAMELIST contains the names of all the species in the master species list as variable names. Therefore initial concentrations are input by "species name = initial concentration." For example, one of the NAMELIST lines could look like

COL 2

|

& START H2 = 0.5, O2 = 0.375, H = 0.015, OH = 0.015, H20 = 0.095,

All species concentrations are initialized to zero so only those concentrations that are initially nonzero actually need to be read in. The names of the other variables in START along with standard options are given next. All parameters except pressure must be in the user's chosen input units. Note that only one of the names P, RHO, MDOT, and AREA is used for any case. For the possible choices see the section Starting conditions under Input in the section General Description of Program Use.

Name	Value	Explanation
AIRMW	------	Molecular weight of oxidant. Needed only if FLAIR is specified. Default value is 28.9644 for "standard air" (table I)
AREA	------	Initial area for flow reaction or initial volume for a well-stirred-reactor problem
ARAT	------	Ar/O_2 mole ratio in oxidant for special combustion input. Default value is 0.044487 for "standard air" (table I)
CRAT	------	CO_2/O_2 ratio in oxidant for special combustion input. Default value is 0.001432 for "standard air" (table I)
ERATIO	------	Equivalence ratio of initial combustible mixture. Used when individual mole or mass fractions are not specified
FLAIR	------	Initial fuel-oxidant mass ratio of combustible mixture. May be specified *instead of* ERATIO when individual species concentrations are not given
FRO2	------	Mole (or volume) fraction of molecular oxygen in the oxidant. Needed only if FLAIR or ERATIO is specified. Default value is 0.2095 for "standard air" (table I)
FUEL	------	Name of fuel species when special combustion input is used. The name must be spelled exactly as in the master species list and is enclosed in single quotes: e.g., FUEL = 'CH3OH'
MACH	------	Mach number
MDOT	------	Mass flow rate
MFUEL	------	Molecular weight of fuel. Must be listed *only* when FLAIR is specified
MMHG	TRUE	Input pressure has units of millimeters of mercury
	FALSE	Input pressure is given in the user's chosen input units
MOLEF	TRUE	Species concentrations will be input as mole fractions
	FALSE	Species concentrations will be input as mass fractions

NOXRAT	------	N_2/O_2 mole ratio in oxidant for special combustion input. Default value is 3.72735 for "standard air" (table I)
P	------	Pressure
RHO	------	Density
SCC	------	Stoichiometric coefficient of carbon in fuel. Used only when equivalence ratio or mass fuel-air ratio is specified for a combustion
SCH	------	Stoichiometric coefficient of hydrogen in fuel
SCOX	------	Stoichiometric coefficient of oxygen in fuel
T	------	Temperature
TIME	------	Time, sec
V	------	Velocity
X	------	Axial position

(9) Final line—Each case must end with a line containing the word FINIS in columns 1 to 5.

Multiple cases.—At the end of each case the code tries to read data for another case. Hence several cases can be computed during one computer run. As mentioned earlier, the code was designed to eliminate the necessity of repeating data that do not change from case to case. This objective was accomplished by adding one switch, called the ACTION switch, to the input list for the second and all following cases of a computer run. By using the ACTION switch the user can tell the code to retain much of the data from the previous case for use by the present case. This means that only those data that change between the present case and the previous case must actually be input. The input lines for each case after the first must correspond to the following specifications. Notice particularly that each case after the first case of a computer run must contain an ACTION line. Each number corresponds to a line or group of lines.

(1) Title—The first line of each subsequent case must be the title line. The format is the same as before.

(2) ACTION switch—The value of the ACTION switch is put in columns 1 to 6. The possible values are any one of the words NEW, REPEAT, CHANGE, or ADD.

If the word NEW is input, the code will completely reinitialize. The remainder of the case data must be exactly like the case data for a first case. The user has told the program not to retain any of the data from the previous case.

The REPEAT option tells the code to use the reactions, rate constants, and inert species that are stored at the time the switch is read. The REPEAT option may either follow the title line or a CHANGE action. In the former case, all reaction and inert species data from the previous case are used, unchanged.

The CHANGE option allows the user to change rate-constant parameters for any of the reactions used in the previous case. A set of reaction lines, in any order, must follow the word CHANGE. Each reaction must be written the same as it was in the previous case. Only the rate-constant parameters are changed. The end of the change list is indicated by a blank line after the last changed reaction. If a REPEAT switch follows the CHANGE action, all unchanged rate constants and the newly changed ones are used in the new case.

The ADD switch tells the code to save the reaction and species data it has and to prepare to read in more reactions and, possibly, new reacting species as well. A set of new reaction lines follows the ADD switch. Again the end of the new list is signaled by a blank line. The word ADD may either directly follow the new title line or may be used after a CHANGE list. *Note that no other ACTION switch ever follows REPEAT or ADD, but either one of these last two switches must follow a CHANGE action.*

The use of the ACTION switch has two limitations. First, and most important, no new reacting species may be introduced by the ADD option if any inert species has been used in the previous case. Inert species must always be at the end of the species list for any case. Second, no new inert species may ever be introduced in a case after the first one.

(3) Version and units—The information on this line must be reset for every case. It is prepared just as for the first case.

(4) Controls—Only those data that are to be changed must be listed in NAMELIST PROB. If nothing is to be changed, a dummy line simply indicating the beginning and end of PROB must be inserted.

(5) Third-body efficiencies—If ALLM1 was FALSE in the previous case, any desired changes in third-body efficiencies may be made here by putting in the same type of line as for the first case, listing the new efficiencies. A blank line must be inserted either to end the list of new efficiencies *or to indicate that no changes are being made in the previous list.* If ALLM1 was TRUE in the previous case and is still kept TRUE for the present case, no additional data lines appear between NAMELIST PROB and START.

(6) All the data in NAMELIST START must be listed in the usual way since they are always initialized to zero or their default value before each case.

(7) Final line—The usual line with FINIS in columns 1 to 5 ends every case.

Error Messages

Most error messages contain two pieces of information: The first is the name of the subroutine that generated the message. The second is a statement of the error condition and, whenever possible, a list of the current value of pertinent parameters. Following is a list of several error messages that the program can generate and a brief explanation of each message.

Subroutine	Message	Explanation
(GCKP)	END OF THIS CASE—READ DATA FOR NEXT CASE	Normal end of case reached
(GCKP)	A FATAL ERROR HAS OCCURRED—CASE TERMINATED	Case ended due to unrecoverable error condition
(KINP)	THE INPUT REACTION LIST DOES NOT CONTAIN THE REACTION $S_1+S_2=S_3+S_4$	Error in entering third-body efficiencies or in changing a reaction rate by using the ACTION switch
(KINP)	THE MASTER SPECIES LIST DOES NOT CONTAIN THE SPECIES ____	The given species is not in the master species list ALSP in the BLOCK DATA
(KINP)	THE INPUT SPECIES LIST DOES NOT CONTAIN THE SPECIES ____.	Error in entering third-body species
(KINP)	INVALID INPUT COMPOSITION SUM = x.xxxx	Input mole or mass fractions do not sum to 1.0
(SHOCKS)	FROZEN SHOCK CALCULATION FAILED	Iteration of frozen shock equations failed to converge
(SHOCKS)	EQUILIBRIUM SHOCK CALCULATION FAILED	Failed convergence of equilibrium shock equations
(EQLBRM)	DERIVATIVE MATRIX SINGULAR	Singular derivative matrix encountered in equilibrium calculation
(EQLBRM)	SINGULAR MATRIX	Singular matrix encountered in equilibrium calculation
(EQLBRM)	RESTART	Equilibrium calculation restarted
(EQLBRM)	xx ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMENTS	Iteration of equilibrium equations failed to converge
(OUT2)	INVALID COMPOSITION	Mass fraction sum not equal to 1.0
(DIFFUN)	WARNING MACH NUMBER = x.xxxx IS APPROACHING 1.0	$0.94 < \mathfrak{M} < 1.05$; numerical problems occur if Mach number gets close to 1.0 for assigned-area computations
(THRM)	ERROR T = xxxx.xx IS OUT OF RANGE	Temperature (K) is above range of thermodynamic data
(THRM)	WARNING T = xxxx.xx IS OUT OF RANGE EXTRAPOLATED VALUES RETURNED	Temperature (K) is below range of the thermodynamic data

The numerical integration subroutines DRIVE and CPINT also contain several error messages pointing out both recoverable and fatal errors. Most are self-explanatory and some that are not are described in appendix E, where some causes of trouble are discussed along with possible ways of overcoming the problems.

Appendix E
Discussion of Computational Problems

In this appendix we attempt to give the user the benefit of our experience in overcoming certain problems that are often encountered in some integration and well-stirred-reactor cases. It is not meant to be a comprehensive discussion, but we hope it will aid the new user in using the code successfully.

Numerical Integration Computations

Quite often problems can occur at the very beginning of an integration during the period when there may be some very large concentration gradients. This is especially true during a combustion ignition. Only fuel and oxidant are present as various free radical species begin to be formed and subsequently destroyed rather rapidly. The integration routine will have difficulty in satisfying the error criteria and also in the convergence of its predictor-corrector technique. In addition, negative concentrations of some trace species may be encountered. Error messages are printed out for these situations that show how the step size is being reduced to cope with the problem. Often the problem will correct itself, but sometimes the computation will be aborted with the message "PROBLEM APPEARS UNSOLVABLE." We have found that one way to alleviate this situation is to put in very small (about 10^{-10} to 10^{-8} mole fraction) concentrations of one or two of the species that are showing negative concentrations (e.g., test case 10). The reader will notice that this has been done in several test cases to suppress many error messages and make the computation smoother.

A problem with small step size may also occur at the end of a combustion problem, when near equilibrium has been achieved. The integration method becomes very inefficient for these conditions and H is drastically reduced. If the computation is not terminated, the following message will be given for some value of the integration variable T: WARNING...T+H=T ON NEXT STEP. Computer time will be wasted if these computations are not terminated when near equilibrium is achieved.

Finally the integration control routine, DRIVE, prints out several messages starting with ILLEGAL INPUT... One of these continues (TO−TOUT)*H.GE.0. This means that the initial value of the integration variable is beyond the first print station value asked for in a print list in NAMELIST PROB. In our experience this usually means that the variable PSTAT was not set to TRUE to tell the code to expect a print list.

Well-Stirred-Reactor Computations

The well-stirred reactor subroutine, WSR, allows 75 iterations in an attempt to converge to a solution for any set of assigned conditions. Convergence is always hardest for the first assigned mass flow or temperature. If convergence is not achieved, a message to this effect is printed out, and then the current values of many variables are printed out before the computation is aborted. The greatest convergence success has been achieved for all problems by using an initial mass flow rate (MDOT in NAMELIST START) of 25 to 100 g/sec. Often this initial value will have to be varied to find the one that works properly. Too small values of MDOT as well as too large values will be unsuccessful.

The chemical system that we have found most difficult to compute with is a very rich propane-air mixture. We really do not have a completely accurate chemical mechanism for the oxidation process. Also, solid carbon is formed in the combustion of these mixtures. A typical characteristic of the iterations for such a problem is a positive temperature gradient at first instead of a negative one. The computation can converge at a temperature higher than the first estimate (the equilibrium combustion temperature). However, this is a false convergence and MDOT must be changed to obtain convergence to a temperature less than the first estimate. For very rich hydrocarbon mixtures a slightly modified iteration control sometimes improves convergence. This option may be used by setting the variable RICH equal to TRUE in NAMELIST PROB. In summary, it is clear that a certain amount of experimenting may be necessary to obtain good convergence for some chemical systems, especially rich hydrocarbon oxidations.

Appendix F
Test Case Data and Results

In this appendix we list data for 12 test cases that illustrate the variety of problems which GCKP84 handles and many of the code options previously described. The data are set up as a single computer run to illustrate the various uses of the ACTION switch options for multiple cases. The test cases are described first, and then the complete dataset for executing them is listed. Finally, selected output results of the execution of this dataset are given.

Description of Test Cases

Case 1.—Test case 1 is the dissociation of Br_2 in a shock tube. It shows the use of the shock kinetics option and the Mirels boundary layer equation (eq. (97)). Running time is 0.74 sec of CPU time.

Case 2.—Test case 2 is a hydrogen-air ignition in supersonic flow with heat transfer computed as a linear function of temperature. A constant-area profile is used. Only two reactions involving H_2O_2 are used in the abbreviated chemical mechanism. Starting composition is specified by giving the equivalence ratio. Running time will be given for cases 2 and 3, which must be run together.

Case 3.—Test case 3 is the same problem as case 2 and illustrates the use of the CHANGE and ADD options for the ACTION switch. The rate constant of the reaction $2HO_2 - H_2O_2 + O_2$ is changed, and reactions of O, OH, and H with H_2O_2 are added. In addition, input is given in U.S. customary units for temperature, pressure, area, and print stations. Note that Q is given in calories per second, no matter what other input units are specified. Initial composition is specified by giving the mass fuel-oxidant ratio. Running time for cases 2 and 3 together is 4.3 sec.

Case 4.—Test case 4 is a hydrogen-oxygen ignition in subsonic flow with cgs input and U.S. customary output. Pressure is held constant and initial Mach number, temperature, and area are given in START. This case illustrates composition input for combustion problems using a nonstandard air oxidant, namely pure oxygen. The fraction of O_2 in the oxidant is 1, and the oxidant molecular weight is that of O_2. Running time is 2.7 sec.

Case 5.—Test case 5 is a batch methane-air ignition in a rich mixture with an assigned-pressure profile. The mechanism contains several reactions of the CH radical that are only needed for a rich mixture. Heat transfer is computed by using the Otto-cycle option. Only temperature and composition have to be given in NAMELIST START. Running time is 16.8 sec.

Case 6.—Test case 6 is a lean methane-air ignition problem in supersonic flow at constant pressure. All CH reactions have been removed from the mechanism since this radical has a quite negligible concentration except in rich mixtures. Running time will be given for cases 6 and 7, which must be run together.

Case 7.—Test case 7 is the same as case 6 and shows the use of the REPEAT option. However, we now assign the point-by-point area profile generated by case 6 to see if we compute the constant pressure and other results of case 6. Results were quite sensitive to the choice of EMAX and somewhat less dependent on the selection of x values for the area profile. After several trials good agreement was obtained, as is shown by the results given in the next section. Running time is 12.6 sec for cases 6 and 7.

Case 8.—Test case 8 is a constant-volume batch ignition of a methanol-air mixture and illustrates the use of equivalence ratio input for a fuel containing oxygen. Running time is 16.5 sec.

Case 9.—Test case 9 is a well-stirred-reactor problem with assigned mass flow rate, followed by a supersonic flow reaction. The chemical reactions illustrate a fairly complete rich propane-air ignition and combustion mechanism. (See refs. 18 to 26 for sources of rate-constant data.) This case illustrates the use of the option to compute rocket performance parameters. Running time is 20.9 sec.

Case 10.—Test case 10 is a high-temperature air ionization reaction in constant-area flow. It illustrates the use of ionic species and also of the DEBUG output option. Notice that a small initial concentration of O2 – is listed in NAMELIST START by using its variable name from subroutine INIT, namely O2M. Running time is 2.1 sec.

Case 11.—Test case 11 is a batch, constant-volume, high-temperature reaction of 1 percent CO in gaseous hydrogen. It illustrates the ability of the numerical integration routine to compute the results for very long reaction times very efficiently when the reaction is very slow. Running time is 6.6 sec.

Case 12.—Test case 12 is a photolytic ignition of hydrogen and oxygen in a constant-volume batch system at low initial temperature. It illustrates the use of photochemical reactions. Running time is 4.1 sec.

Listing of Test Case Dataset

```
TAPE
GCKP84                    BROMINE DISSOCIATION IN A SHOCK TUBE                    CASE 1
   M        +   BR2       = 2 BR                                  6.99E+11  0.50      35500.

XE
DISTANCE  AREA
 &PROB    ITPSZ=3,LSUBM=32200.,ETA=0.50,    SHOCK=.TRUE.,
   PRINT= .05, .2, .5, 2., 4.,   NPRNTS = 5,
  ALLM1= F, PSTAT= T, MF=21,                          EMAX=1.E-5, HINT=1.E-6 &END
   M        +   BR2       = 2 BR                        BR2       3.80

 &START    P=0.1227,MACH=3.2646,T=299.9,    BR2=0.01,XE=0.99,    &END
FINIS
  GCKP84  HYD - AIR TEST WITH HEAT TRANSFER          STOICH  CASE 2
NEW
   H        +   O2        =   OH       +   O          2.2E+14   0.        16790.
   O        +   H2        =   OH       +   H          1.8E+10   1.        8900.
   H2       +   OH        =   H2O      +   H          5.2E+13   0.        6500.
   OH       +   OH        =   O        +   H2O        6.3E+12   0.        1093.
   H        +   O2        =   HO2      +   M          1.5E+15    0.       -1000.
   O        +   O         =   O2       +   M          5.7E+13   0.        -1788.
   H        +   H         =   H2       +   M          8.3E+17   -1.        0.
   H        +   OH        =   H2O      +   M          8.4E+21   -2.       0.
   H2       +   HO2       =   H2O      +   OH         7.2E+11   0.        18700.
   M        +   H2O2      = 2 OH                      1.3E+17   0.       45500.
   H2       +   O2        = 2 OH                     1.00E+13   0.       43000.
   H        +   HO2       =   OH       +   OH         2.5E+14   0.        1900.
   O        +   HO2       =   OH       +   O2         5.0E+13   0.        1000.
   OH       +   HO2       =   H2O      +   O2         5.0E+13   0.        1000.
              2 HO2       =   H2O2     +   O2        1.00E+12   0.       0.
   HO2      +   NO        =   NO2      +   OH         1.2E+13    0.       2380.
   O        +   NO2       =   NO       +   O2         1.0E+13     0.      596.
   NO       +   O         =   NO2      +   M         5.62E+15   0.        -1160.
   NO2      +   H         =   NO       +   OH         2.9E+14   0.        795.
   N        +   O2        =   NO       +   O          6.4E+9    1.        6250.
   O        +   N2        =   NO       +   N          1.8E+14   0.       76250.
   N        +   OH        =   NO       +   H          4.0E+13   0.        0.
   M        +   N2O       =   N2       +   O         1.42E+14   0.        51280.
   O        +   N2O       =   N2       +   O2        6.23E+13   0.       24520.
   O        +   N2O       = 2 NO                      3.1E+13   0.        21800.
              2 NO2       = 2 NO       +   O2         4.0E+12   0.        26900.
   N        +   NO2       = 2 NO                      3.6E+12   0.        0.
   OH       +   N2        =   N2O      +   H          3.2E+12   0.        80280.

CO2               AR
DISTANCE  AREA
 &PROB  HINT =1.E-6,  ITPSZ=2,  CX0 = 2000.,  ALLM1 = F,
   PRINT= 3.048, 4.572, 6.096, 7.620, 15.24,  NPRNTS = 5,
   EMAX=1.E-4,  MF= 21, PSTAT= T,
   HTRAN = T, QMREAD= T,  HT1= 5.863, HT0= -42.88   &END
   H        +   O2        =   HO2      +   M        H2        5.0     O2        2.0
   H        +   O2        =   HO2      +   M        H2O      32.5     N2        2.0
   H            H         =   H2       +   M        O2        2.0     H2        5.0
   H            H         =   H2       +   M        H2O      15.0     N2        2.0
   M        +   H2O2      = 2 OH                    O2        0.78     H2O       6.0
   M        +   H2O2      = 2 OH                    H2O2      6.6      H2        2.3
   H        +   OH        =   H2O      +   M        H2        4.0      N2        1.6
   H        +   OH        =   H2O      +   M        H2O      20.0      O2        1.6

 &START      P=0.9560,  T=1559., MACH=5.0,
  ERATIO =1, SCC= 0, SCH= 2, SCOX= 0, FUEL= 'H2'  &END
FINIS
  GCKP84  HYD - AIR TEST WITH HEAT TRANSFER        FULL MECH  CASE 3
CHANGE
              2 HO2       =   H2O2     +   O2          1.80E+12  0.        0.
```

```
ADD
   OH      +   H2O2     =   H2O     +   HO2          1.0E+13   0.        1800.
   O       +   H2O2     =   OH      +   HO2          8.0E+13   0.        1000.
   H       +   H2O2     =   H2O     +   OH           3.2E+14   0.        9000.

DISTANCE  AREA       FPS
 &PROB    EXCHR = T, CX0= 2.15278, PRINT = 0.1, 0.2, 0.25, 0.5, NPRNTS=4, &END

 &START          P=2023.09, T=2806.2, MACH=5.0,
  FLAIR = .029163, SCC= 0, SCH= 2, SCOX= 0, FUEL= 'H2',
   MFUEL = 2.0159                          &END
FINIS
  GCKP84  HYD - OXYGEN CASE WITH HEAT TRANSFER                    CASE 4
NEW
   H       +   O2       =   OH      +   O            2.2E+14   0.        16790.
   O       +   H2       =   OH      +   H            1.8E+10   1.        8900.
   H2      +   OH       =   H2O     +   H            5.2E+13   0.        6500.
   OH      +   OH       =   O       +   H2O          6.3E+12   0.        1093.
   H       +   O2       =   HO2     +   M            1.5E+15    0.       -1000.
   O       +   O        =   O2      +   M            5.7E+13   0.        -1788.
   H       +   H        =   H2      +   M            8.3E+17   -1.         0.
   H       +   OH       =   H2O     +   M            8.4E+21   -2.       0.
   H2      +   HO2      =   H2O     +   OH           7.2E+11   0.        18700.
   M       +   H2O2     = 2 OH                       1.3E+17   0.        45500.
   H2      +   O2       = 2 OH                      1.00E+13   0.        43000.
   H       +   HO2      =   OH      +   OH           2.5E+14   0.        1900.
   O       +   HO2      =   OH      +   O2           5.0E+13   0.        1000.
   OH      +   HO2      =   H2O     +   O2           5.0E+13   0.        1000.
             2 HO2      =   H2O2    +   O2          1.80E+12   0.        0.
   OH      +   H2O2     =   H2O     +   HO2          1.0E+13   0.        1800.
   O       +   H2O2     =   OH      +   HO2          8.0E+13   0.        1000.
   H       +   H2O2     =   H2O     +   OH           3.2E+14   0.        9000.


DISTANCE  PRESSURE              FPS
 &PROB  HINT =1.E-6,  ITPSZ=2,   CX0 = 5., CX1= .01,  ALLM1 = F,
  PRINT = 6, 20, 22.81, 22.83, 22.84, 22.845,  NPRNTS = 6,
   EMAX=1.E-6,  MF= 21, PSTAT= T,
    HTRAN = T, QMREAD = T,  HT1=5.863, HT0=-42.88     &END
   H       +   O2       =   HO2     +   M        H2        5.0     O2        2.0
   H       +   O2       =   HO2     +   M        H2O      32.5
   H           H        =   H2      +   M        O2        2.0     H2        5.0
   H           H        =   H2      +   M        H2O      15.0
   M       +   H2O2     = 2 OH                   O2        0.78    H2O       6.0
   M       +   H2O2     = 2 OH                   H2O2      6.6     H2        2.3
   H       +   OH       =   H2O     +   M        H2       4.0
   H       +   OH       =   H2O     +   M        H2O      20.0     O2        1.6

 &START     T=1075., MACH=0.5,  FUEL = 'H2',
   AIRMW = 31.994,  FRO2 = 1,  AREA = 2000,
  ERATIO =1, SCC= 0, SCH= 2, SCOX= 0, NOXRAT=0, ARAT= 0, CRAT=0  &END
FINIS
  GCKP84 CH4 - AIR RICH MECH. BATCH RXN WITH OTTO CYCLE HEAT LOSS -  CASE 5
NEW
               CH4      =   CH3     +   H            2.0E+15   0.        104000.
   H       +   CH4      =   CH3     +   H2          1.26E+14   0.        11900.
   O       +   CH4      =   CH3     +   OH           2.0E+13   0.        9200.
   OH      +   CH4      =   CH3     +   H2O          3.0E+13   0.        6000.
   CH      +   O2       =   HCO     +   O            1.0E+13   0.        0.
   CH2     +   O2       =   CH2O    +   O            1.0E+14   0.        3700.
   CH3     +   O2       =   CH2O    +   OH           1.7E+12   0.        14000.
   CH3     +   O        =   CH2O    +   H            6.8E+13   0.        0.
   CH2O    +   H        =   HCO     +   H2           2.E+13   0.        3300.
   CH2O    +   O        =   HCO     +   OH           5.E+13   0.        4570.
   CH2O    +   OH       =   HCO     +   H2O          5.E+15   0.        13000.
   M       +   CH2O     =   HCO     +   H            5.0E+16   0.        72000.
   O       +   HCO      =   H       +   CO2          5.3E+13   0.        0.
   HCO     +   O        =   CO      +   OH           3.E+13    0.        0.
   HCO     +   H        =   CO      +   H2           2.E+13    0.        0.
   HCO     +   OH       =   CO      +   H2O          3.E+13   0.        0.
   M       +   HCO      =   H       +   CO           3.E+14    0.        14700.
   CO      +   OH       =   CO2     +   H            4.0E+12   0.        8000.
   CO      +   O        =   CO2     +   M            2.8E+13   0.        -4540.
```

```
   CO      +   O2      =   CO2     +   O       1.2E+11    0.      35000.
   H       +   O2      =   OH      +   O       2.2E+14    0.      16790.
   O       +   H2      =   OH      +   H       1.8E+10    1.        890.
   H2      +   OH      =   H2O     +   H       5.2E+13    0.       6500.
   OH      +   OH      =   O       +   H2O     6.3E+12    0.       1093.
   H       +   O2      =   HO2     +   M       1.5E+15     0.      -1000.
   O       +   O       =   O2      +   M       5.7E+13    0.      -1788.
   H       +   H       =   H2      +   M       8.3E+17   -1.        0.
   H       +   OH      =   H2O     +   M       8.4E+21   -2.       0.
   O       +   H       =   OH      +   M       6.2E+16   -.6        0.
   H       +   CH3     =   H2      +   CH2     2.7E+11   .67     25700.
   O       +   CH3     =   OH      +   CH2     1.9E+11    .68    25700.
   OH      +   CH3     =   H2O     +   CH2     2.7E+11    .67    25700.
   HO2     +   NO      =   NO2     +   OH      1.2E+13     0.    2380.
   O       +   NO2     =   NO      +   O2      1.0E+13      0.     596.
   NO      +   O       =   NO2     +   M     5.62E+15     0.     -1160.
   NO2     +   H       =   NO      +   OH      2.9E+14    0.       795.
   N       +   O2      =   NO      +   O       6.4E+9     1.      6250.
   O       +   N2      =   NO      +   N       1.8E+14    0.     76250.
   N       +   OH      =   NO      +   H       4.0E+13    0.        0.
   CH      +   N2      =   HCN     +   N       1.5E+11    0.     19000.
   CN      +   H2      =   HCN     +   H       6.0E+13    0.      5300.
   O       +   HCN     =   H       +   NCO     5.2E+12   .68     8100.
   OH      +   HCN     =   HNCO    +   H       4.0E+11    0.      2800.
   CN      +   O       =   CO      +   N       1.2E+13    0.        0.
   CN      +   OH      =   NCO     +   H       2.5E+14    0.      6000.
   CN      +   O2      =   NCO     +   O       3.2E+13    0.      1000.
   CN      +   CO2     =   NCO     +   CO      3.7E+12    0.        0.
   O       +   NCO     =   NO      +   CO      2.0E+13     0.       0.
   N       +   NCO     =   N2      +   CO      1.0E+13     0.       0.
   H       +   NCO     =   NH      +   CO      2.0E+13    0.        0.
   H2      +   NCO     =   HNCO    +   H       1.0E+14    0.      9000.
   HNCO    +   H       =   NH2     +   CO      1.0E+14    0.      8500.
   NH      +   OH      =   N       +   H2O     5.0E+11    .5      1999.
   CH      +   CO2     =   HCO     +   CO      3.7E+12    0.        0.
   CH      +   NO      =   N       +   HCO     1.0E+14    0.       0.
   CH      +   NO      =   O       +   HCN     1.0E+13    0.       0.
   H       +   CH2     =   H2      +   CH      2.9E+11    .7     26000.
   O       +   CH2     =   OH      +   CH      3.2E+11    .5     26000.
   OH      +   CH2     =   H2O     +   CH      5.0E+11    .5      6000.
   H       +   HO2     =   OH      +   OH      1.4E+14    0.      1070.
   H       +   HO2     =   O       +   H2O     1.0E+13    0.      1000.
   O       +   HO2     =   OH      +   O2      1.6E+13    0.      1070.
   OH      +   HO2     =   H2O     +   O2      7.9E+12    0.        0.
   CH3     +   OH      =   CH2O    +   H2      7.4E+12    0.        0.
   H2      +   HO2     =   H2O     +   OH      7.2E+11    0.      18700.
   HCO     +   O2      =   CO      +   HO2     3.0E+13    0.        0.

TIME      PRESSURE
 &PROB  HINT=1.E-10, EMAX= 5.E-5, ITPSZ=2, MF =21,  CX0=2, CX1=700,
   PRINT =  5.E-5, 5.E-4,  5.5E-4, 5.85E-4,  NPRNTS=4, IPRCOD= 4,
  ALLM1= F, HTRAN= T, QMREAD= F, OTTO= T, BORE= 8.5, STROKE= 7, FREQ= 2500,
   TWALL = 1000,  PSTAT = T                          &END
   H       +   O2      =   HO2     +   M       O2        2.0    N2        2.0
   H       +   O2      =   HO2     +   M       H2O      32.5    CO2       7.5
   H       +   O2      =   HO2     +   M       CO        2.0    CH4       5.0
   H       +   O2      =   HO2     +   M       H2        5.0
   H       +   OH      =   H2O     +   M       O2        1.6    H2O      20.
   H       +   OH      =   H2O     +   M       N2        1.6    CO2       7.5
   H       +   OH      =   H2O     +   M       CO        1.6

 &START  CH4= .1725, O2= .1725,  N2= .65492,   T= 1510,
       N =1.E-5, CH= 3.E-5, CN=1.E-5, CH2=1.E-5  &END
FINIS
 GCKP84  METHANE - AIR LEAN MECH - NO CH REACTIONS     CASE 6
NEW
               CH4     =   CH3     +   H       2.0E+15    0.     104000.
   H       +   CH4     =   CH3     +   H2     1.26E+14    0.      11900.
   O       +   CH4     =   CH3     +   OH      2.0E+13    0.       9200.
   OH      +   CH4     =   CH3     +   H2O     3.0E+13    0.       6000.
   CH2     +   O2      =   CH2O    +   O       1.0E+14    0.       3700.
   CH3     +   O2      =   CH2O    +   OH      1.7E+12    0.      14000.
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CH3     +  O      =  CH2O   +  H        6.8E+13   0.      0.
CH2O    +  H      =  HCO    +  H2        2.E+13   0.   3300.
CH2O    +  O      =  HCO    +  OH        5.E+13   0.   4570.
CH2O    +  OH     =  HCO    +  H2O       5.E+15   0.  13000.
M       +  CH2O   =  HCO    +  H       5.0E+16   0.  72000.
O       +  HCO    =  H      +  CO2     5.3E+13   0.      0.
HCO     +  O      =  CO     +  OH        3.E+13    0.    0.
HCO     +  H      =  CO     +  H2        2.E+13    0.    0.
HCO     +  OH     =  CO     +  H2O       3.E+13   0.      0.
M       +  HCO    =  H      +  CO        3.E+14    0.  14700.
CO      +  OH     =  CO2    +  H       4.0E+12   0.   8000.
CO      +  O      =  CO2    +  M       2.8E+13   0.  -4540.
CO      +  O2     =  CO2    +  O       1.2E+11    0.  35000.
H       +  O2     =  OH     +  O       2.2E+14   0.  16790.
O       +  H2     =  OH     +  H       1.8E+10   1.   8900.
H2      +  OH     =  H2O    +  H       5.2E+13   0.   6500.
OH      +  OH     =  O      +  H2O     6.3E+12   0.   1093.
H       +  O2     =  HO2    +  M       1.5E+15    0.  -1000.
O       +  O      =  O2     +  M       5.7E+13   0.  -1788.
H       +  H      =  H2     +  M       8.3E+17   -1.     0.
H       +  OH     =  H2O    +  M       8.4E+21   -2.   0.
O       +  H      =  OH     +  M       6.2E+16   -.6     0.
O       +  CH3    =  H2     +  CH2     2.7E+11   .67  25700.
OH      +  CH3    =  OH     +  CH2     1.9E+11   .68  25700.
HO2     +  NO     =  H2O    +  CH2     2.7E+11   .67  25700.
O       +  NO2    =  NO     +  OH      1.2E+13    0.  2380.
NO      +  O      =  O2     +  NO      1.0E+13     0.   596.
NO2     +  H      =  NO     +  M     5.62E+15   0.   -1160.
N       +  O2     =  NO     +  OH      2.9E+14   0.    795.
O       +  N2     =  NO     +  O        6.4E+9   1.   6250.
N       +  OH     =  NO     +  N       1.8E+14   0.  76250.
CN      +  H2     =  HCN    +  H       4.0E+13   0.      0.
O       +  HCN    =  H      +  NCO     6.0E+13   0.   5300.
OH      +  HCN    =  HNCO   +  H       5.2E+12   .68  8100.
CN      +  O      =  CO     +  N       4.0E+11   0.   2800.
CN      +  OH     =  NCO    +  H       1.2E+13   0.      0.
CN      +  O2     =  NCO    +  O       2.5E+14   0.   6000.
CN      +  CO2    =  NCO    +  CO      3.2E+13   0.   1000.
O       +  NCO    =  NO     +  CO      3.7E+12   0.      0.
N       +  NCO    =  N2     +  CO      2.0E+13    0.    0.
H       +  NCO    =  NH     +  CO      1.0E+13    0.    0.
H2      +  NCO    =  HNCO   +  H       2.0E+13   0.      0.
HNCO    +  H      =  NH2    +  CO      1.0E+14   0.   9000.
NH      +  OH     =  N      +  H2O     1.0E+14   0.   8500.
H       +  HO2    =  OH     +  OH      5.0E+11   .5   1999.
H       +  HO2    =  O      +  H2O     1.4E+14   0.   1070.
O       +  HO2    =  OH     +  O2      1.0E+13   0.   1000.
OH      +  HO2    =  H2O    +  O2      1.6E+13   0.   1070.
CH3     +  OH     =  CH2O   +  H2      7.9E+12   0.      0.
H2      +  HO2    =  H2O    +  OH      7.4E+12   0.      0.
HCO     +  O2     =  CO     +  HO2     7.2E+11   0.  18700.
                                       3.0E+13   0.      0.

DISTANCE  PRESSURE
 &PROB  ITPSZ=2, CX0=1.730, HINT=  1.E-6, EMAX=1.E-6, PSTAT=T, MF =21,
   PRINT = 10, 25, 35, 40, 42,    NPRNTS = 5,
   COMBUS = T,  ALLM1 = F,   EXCHR =T, IPRCOD=2      &END
   H       +  O2     =  HO2    +  M       O2        2.0     N2        2.0
   H       +  O2     =  HO2    +  M       H2O      32.5     CO2       7.5
   H       +  O2     =  HO2    +  M       CO        2.0     CH4       5.0
   H       +  O2     =  HO2    +  M       H2        5.0
   H       +  OH     =  H2O    +  M       O2        1.6     H2O      20.
   H       +  OH     =  H2O    +  M       N2        1.6     CO2       7.5
                                          CO        1.6

 &START  AREA= 1000,  MACH =2,  T= 1645,  CH4 = .049768 ,
          CN=1.E-7, O2 = .199072 ,  N2= .75116       &END
FINIS
  GCKP84  CH4 - AIR WITH AREA PROFILE OF CASE 6          CASE 7
REPEAT
DISTANCE  AREA
 &PROB   ITPSZ=1,IPRCOD=1,   HINT= 5.E-5,    MF= 21,
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   COMBUS=.FALSE.,   ALLM1=.FALSE.,   PSTAT = T,
   XTB=0.,5.,10.,15.,20.,25.,30.,35.,37.,38.,38.5,39., 39.5, 40, 40.5, 41,
  41.5, 42, 42.5, 43,                          NTB = 20,
   ATB= 1000, 1000.36, 1002.12, 1005.61, 1011.43, 1021.36, 1038.85,
  1073.32,  1097.49, 1114.04,1124.04, 1135.66, 1149.48, 1166.51, 1188.72,1220.48,
  1273.43, 1361.17, 1401.17, 1411.70,
   PRINT= 10, 25, 35, 40, 42,   NPRNTS = 5,
    EMAX = 1.24E-6   &END

 &START T= 1645, MACH =2,  P= 1.730,  CN= 1.E-7,
       CH4=0.049768, O2=0.199072, N2=0.75116,   &END
FINIS
   GCKP84   METHANOL - AIR  COMBUSTION       CASE 8
NEW
   M       +   CH3OH     =   CH3     +   OH        3.2E+18   0.        80000.
   O2      +   CH3OH     =   CH2OH   +   HO2       4.0E+13   0.        50900.
   OH      +   CH3OH     =   CH2OH   +   H2O       4.0E+12   0.        2000.
   O       +   CH3OH     =   CH2OH   +   OH        1.6E+12   0.        2300.
   H       +   CH3OH     =   CH2OH   +   H2        3.2E+13   0.        7000.
   H       +   CH3OH     =   CH3     +   H2O       5.0E+12   0.        5300.
   CH3     +   CH3OH     =   CH2OH   +   CH4       2.0E+11   0.        9800.
   HO2     +   CH3OH     =   CH2OH   +   H2O2      6.3E+12   0.        19400.
   M       +   CH2OH     =   CH2O    +   H         2.5E+13   0.        29000.
   O2      +   CH2OH     =   CH2O    +   HO2       1.0E+12   0.        6000.
               CH4       =   CH3     +   H         2.0E+15   0.        104000.
   H       +   CH4       =   CH3     +   H2      1.26E+14   0.        11900.
   O       +   CH4       =   CH3     +   OH        2.0E+13   0.        9200.
   OH      +   CH4       =   CH3     +   H2O       3.0E+13   0.        6000.
   CH      +   O2        =   HCO     +   O         1.0E+13   0.        0.
   CH2     +   O2        =   CH2O    +   O         1.0E+14   0.        3700.
   CH3     +   O2        =   CH2O    +   OH        1.7E+12   0.        14000.
   CH3     +   O         =   CH2O    +   H         6.8E+13   0.        0.
   CH2O    +   H         =   HCO     +   H2        2.E+13    0.        3300.
   CH2O    +   O         =   HCO     +   OH        5.E+13    0.        4570.
   CH2O    +   OH        =   HCO     +   H2O       5.E+15    0.        13000.
   HCO     +   O         =   CO      +   OH        3.E+13     0.       0.
   HCO     +   H         =   CO      +   H2        2.E+13     0.       0.
   HCO     +   OH        =   CO      +   H2O       3.E+13    0.        0.
   M       +   HCO       =   H       +   CO        3.E+14     0.       14700.
   CO      +   OH        =   CO2     +   H         4.0E+12   0.        8000.
   CO      +   O         =   CO2     +   M         2.8E+13   0.        -4540.
   CO      +   O2        =   CO2     +   O         1.2E+11    0.       35000.
   H       +   O2        =   OH      +   O         2.2E+14   0.        16790.
   O       +   H2        =   OH      +   H         1.8E+10   1.        8900.
   H2      +   OH        =   H2O     +   H         5.2E+13   0.        6500.
   OH      +   OH        =   O       +   H2O       6.3E+12   0.        1093.
   H       +   O2        =   HO2     +   M         1.5E+15    0.       -1000.
   O       +   O         =   O2      +   M         5.7E+13   0.        -1788.
   H       +   H         =   H2      +   M         8.3E+17   -1.        0.
   H       +   OH        =   H2O     +   M         8.4E+21   -2.       0.
   H       +   CH3       =   H2      +   CH2       2.7E+11   .67       25700.
   O       +   CH3       =   OH      +   CH2       1.9E+11   .68       25700.
   OH      +   CH3       =   H2O     +   CH2       2.7E+11   .67       25700.
   H       +   CH2       =   H2      +   CH        2.9E+11   .7        26000.
   O       +   CH2       =   OH      +   CH        3.2E+11   .5        26000.
   OH      +   CH2       =   H2O     +   CH        5.0E+11   .5        6000.
   HO2     +   NO        =   NO2     +   OH        1.2E+13    0.      2380.
   O       +   NO2       =   NO      +   O2        1.0E+13     0.      596.
   NO      +   O         =   NO2     +   M       5.62E+15    0.       -1160.
   NO2     +   H         =   NO      +   OH        2.9E+14   0.        795.
   N       +   O2        =   NO      +   O          6.4E+9   1.        6250.
   O       +   N2        =   NO      +   N         1.8E+14   0.        76250.
   N       +   OH        =   NO      +   H         4.0E+13   0.        0.
   CN      +   H2        =   HCN     +   H         6.0E+13   0.        5300.
   O       +   HCN       =   H       +   NCO       5.2E+12   .68       8100.
   OH      +   HCN       =   HNCO    +   H         4.0E+11   0.        2800.
   CN      +   O         =   CO      +   N         1.2E+13   0.        0.
   CN      +   OH        =   NCO     +   H         2.5E+14   0.        6000.
   CN      +   O2        =   NCO     +   O         3.2E+13   0.        1000.
   CN      +   CO2       =   NCO     +   CO        3.7E+12   0.        0.
   O       +   NCO       =   NO      +   CO        2.0E+13    0.       0.
   N       +   NCO       =   N2      +   CO        1.0E+13    0.       0.
   H       +   NCO       =   NH      +   CO        2.0E+13   0.        0.
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   H2      +   NCO     =   HNCO    +   H       1.0E+14   0.      9000.
   HNCO    +   H       =   NH2     +   CO      1.0E+14   0.      8500.
   NH      +   OH      =   N       +   H2O     5.0E+11   .5      1999.
   H       +   HO2     =   OH      +   OH      1.4E+14   0.      1070.
   H       +   HO2     =   O       +   H2O     1.0E+13   0.      1000.
   O       +   HO2     =   OH      +   O2      1.6E+13   0.      1070.
   OH      +   HO2     =   H2O     +   O2      7.9E+12   0.         0.
   CH3     +   OH      =   CH2O    +   H2      7.4E+12   0.         0.
   H2      +   HO2     =   H2O     +   OH      7.2E+11   0.     18700.
   HCO     +   O2      =   CO      +   HO2     3.0E+13   0.         0.
   OH      +   H2O2    =   H2O     +   HO2     1.0E+13   0.      1800.
   O2      +   H2O2    = 2 HO2                 4.0E+13   0.     42600.
   H       +   H2O2    =   HO2     +   H2      1.6E+12   0.      3800.
   M       +   H2O2    = 2 OH                  1.3E+17   0.     45500.

AR
TIME
 &PROB  MF=21, PSTAT= T,  ALLM1 =F,  RHOCON =T, EMAX=5.E-6,
   PRINT= 3.E-4,  5.6E-4,   6.E-4,  6.2E-4,
        NPRNTS = 4, HINT= 1.E-10  &END
   H       +   O2      =   HO2     +   M       O2        2.0    N2        2.0
   H       +   O2      =   HO2     +   M       H2O      32.5    CO2       7.5
   H       +   O2      =   HO2     +   M       CO        2.0
   H       +   OH      =   H2O     +   M       O2        1.6    H2O      20.
   H       +   OH      =   H2O     +   M       N2        1.6    CO2       7.5
   H       +   OH      =   H2O     +   M       CO        1.6

 &START   T= 1300, MMHG=T, P= 760,  ERATIO= 2.0,  SCC=1,  SCH= 4, SCOX= 1,
  CN = 1.E-6, CH=1.E-5, N= 1.E-6, FUEL ='CH3OH'              &END
FINIS
 C3H8 - AIR WELL-STIRRED REACTOR +  ROCKET EXPANSION PROB.   GCKP84 CASE 9
NEW
               C3H8    =   C2H5    +   CH3      4.5E+16   0.      84900.
               C2H5    =   C2H4    +   H       3.16E+13   0.      40700.
   O       +   C2H4    =   CH2O    +   CH2      2.5E+13   0.      5000.
   O       +   C2H4    =   CH3     +   HCO     2.26E+13   0.      2700.
   CH3     +   C3H8    =   CH4     +   C3H7     2.0E+13   0.     10300.
               C3H7    =   C2H4    +   CH3      4.0E+13   0.     33100.
   H       +   CH4     =   CH3     +   H2      1.26E+14   0.     11900.
   O       +   CH4     =   CH3     +   OH       2.0E+13   0.      9200.
   OH      +   CH4     =   CH3     +   H2O      3.0E+13   0.      6000.
   CH      +   O2      =   HCO     +   O        1.0E+13   0.         0.
   CH2     +   O2      =   CH2O    +   O        1.0E+14   0.      3700.
   CH3     +   O2      =   CH2O    +   OH       1.7E+12   0.     14000.
   CH3     +   O       =   CH2O    +   H        6.8E+13   0.         0.
   CH2O    +   H       =   HCO     +   H2        2.E+13   0.      3300.
   CH2O    +   O       =   HCO     +   OH        5.E+13   0.      4570.
   CH2O    +   OH      =   HCO     +   H2O       5.E+15   0.     13000.
   HCO     +   O       =   CO      +   OH        3.E+13   0.         0.
   HCO     +   H       =   CO      +   H2        2.E+13   0.         0.
   HCO     +   OH      =   CO      +   H2O       3.E+13   0.         0.
   M       +   HCO     =   H       +   CO        3.E+14   0.     14700.
   CO      +   OH      =   CO2     +   H       4.0E+12   0.      8000.
   CO      +   O       =   CO2     +   M       2.8E+13   0.     -4540.
   CO      +   O2      =   CO2     +   O       1.2E+11   0.     35000.
   H       +   O2      =   OH      +   O       2.2E+14   0.     16790.
   O       +   H2      =   OH      +   H       1.8E+10   1.      8900.
   H2      +   OH      =   H2O     +   H       5.2E+13   0.      6500.
   OH      +   OH      =   O       +   H2O     6.3E+12   0.      1093.
   H       +   O2      =   HO2     +   M       1.5E+15   0.     -1000.
   O       +   C       =   O2      +   M       5.7E+13   0.     -1788.
   H       +   H       =   H2      +   M       8.3E+17  -1.         0.
   H       +   OH      =   H2O     +   M       8.4E+21  -2.         0.
   H       +   CH3     =   H2      +   CH2      2.7E+11   .67    25700.
   O       +   CH3     =   OH      +   CH2      1.9E+11   .68    25700.
   OH      +   CH3     =   H2O     +   CH2      2.7E+11   .67    25700.
   HO2     +   NO      =   NO2     +   OH       1.2E+13   0.      2380.
   O       +   NO2     =   NO      +   O2       1.0E+13   0.       596.
   NO      +   O       =   NO2     +   M       5.62E+15   0.     -1160.
   NO2     +   H       =   NO      +   OH       2.9E+14   0.       795.
   N       +   O2      =   NO      +   O        6.4E+9    1.      6250.
   O       +   N2      =   NO      +   N       1.8E+14   0.     76250.
   N       +   OH      =   NO      +   H       4.0E+13   0.         0.
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   CH      +   N2      =   HCN     +   N          1.5E+11   0.        19000.
   CN      +   H2      =   HCN     +   H          6.0E+13   0.        5300.
   O       +   HCN     =   OH      +   CN         1.4E+11   .68       16900.
   OH      +   HCN     =   HNCO    +   H          4.0E+11   0.        2800.
   CN      +   O       =   CO      +   N          1.2E+13   0.        0.
   CN      +   OH      =   NCO     +   H          2.5E+14   0.        6000.
   H2      +   NCO     =   HNCO    +   H          1.0E+14   0.        9000.
   HNCO    +   H       =   NH2     +   CO         1.0E+14   0.        8500.
   CN      +   O2      =   NCO     +   O          3.2E+13   0.        1000.
   CN      +   CO2     =   NCO     +   CO         3.7E+12   0.        0.
   O       +   NCO     =   NO      +   CO         2.0E+13   0.        0.
   N       +   NCO     =   N2      +   CO         1.0E+13   0.        0.
   H       +   NCO     =   NH      +   CO         2.0E+13   0.        0.
   NH      +   OH      =   N       +   H2O        5.0E+11   0.5       2000.
   CH      +   CO2     =   HCO     +   CO         3.7E+12   0.        0.
   H       +   C2H4    =   H2      +   C2H3       1.1E+14   0.        8500.
   OH      +   C2H4    =   H2O     +   C2H3       1.0E+14   0.        3500.
   M       +   C2H3    =   C2H2    +   H          3.0E+16   0.        40500.
   O       +   C2H2    =   CH2     +   CO         5.2E+13   0.        3700.
   H       +   CH2     =   H2      +   CH         2.9E+11   .7        26000.
   O       +   CH2     =   OH      +   CH         3.2E+11   .5        26000.
   OH      +   CH2     =   H2O     +   CH         5.0E+11   .5        6000.
   CH      +   NO      =   N       +   HCO        1.0E+14   0.        0.
   CH      +   NO      =   O       +   HCN        1.0E+13   0.        0.
   CH3     +   OH      =   CH2O    +   H2         7.4E+12   0.        0.
   H2      +   HO2     =   H2O     +   OH         7.2E+11   0.        18700.
   HCO     +   O2      =   CO      +   HO2        3.0E+13   0.        0.
   C2H5    +   O2      =   C2H4    +   HO2        1.5E+12   0.        4860.
   H       +   C2H5    =   C2H4    +   H2         4.8E+13   0.        0.
   CH3     +   CH2     =   C2H4    +   H          2.0E+13   0.        0.
   OH      +   C2H2    =   C2H     +   H2O        6.0E+12   0.        7000.
   C2H     +   O       =   CO      +   CH         1.4E+13   0.        3150.
   C2H     +   O2      =   HCO     +   CO         1.0E+13   0.        7000.
   C2H2    +   O2      = 2 HCO                    4.0E+12   0.        28000.
   M       +   C2H2    =   C2H     +   H          1.0E+14   0.        114000.
   O       +   C2H2    =   C2H     +   OH         3.2E+15   -.6       17000.
   M       +   C2H5    =   C2H4    +   H          6.8E+17   0.        31800.

AR
DISTANCE  AREA
 &PROB WELSTR=T, TASS= F,DOTMAX= 1600,DELMD= 800, CONC=F,MPR=1, ALLM1=F,
  ITPSZ=2, IPRCOD=1,  CX0= 15, CX1= 20, PRINT = .4, .7, 2, 3, 4, NPRNTS=5,
    ROCKET=T,  WSFLOW=T, PSTAT=T, EMAX=1.E-4, HINT=1.E-5,
  HTRAN =T, QMREAD=T,  HT1= .05, HT0= -42.88 ,
  PC = 300, ATHROT = 2.2          &END
   H       +   O2      =   HO2     +   M      O2       2.0    N2        2.0
   H       +   O2      =   HO2     +   M      H2O      32.5   CO2       7.5
   H       +   O2      =   HO2     +   M      CO       2.0
   H       +   OH      =   H2O     +   M      O2       1.6    H2O       20.
   H       +   OH      =   H2O     +   M      N2       1.6    CO2       7.5
   H       +   OH      =   H2O     +   M      CO       1.6

 &START T= 614, P = 5, AREA= 6026,  MDOT= 85,  MOLEF= F, C3H8=.0873262,
   N2= .6892887, O2= .211232, AR= .0117370, CO2= 4.162E-4, X=.2 &END
FINIS
GCKP84          HIGH TEMPERATURE AIR IONIZATION      CASE 10
NEW
   N       +   O2      =   NO      +   O          6.4E+09   1.        6250.
   O       +   N2      =   NO      +   N          1.8E+14   0.        76250.
   N       +   O       =   NO      +   M         6.40E+16   -0.5      0.
   O       +   O       =   O2      +   M          5.7E+13   0.        -1788.
             2 N       =   N2      +   M         2.80E+17   -0.75     0.
   NO      +   O       =   NO2     +   M         5.62E+15   0.        -1160.
   M       +   N2O     =   N2      +   O          1.42E+14   0.        51280.
   O       +   N2O     =   N2      +   O2         6.23E+13   0.        24520.
   NO+     +   E       =   N       +   O          1.45E+21   -1.5      0.
   O+      +   E       =   O       +   M          2.00E+26   -2.5      0.
   O2      +   E       =   O2-     +   M          1.52E+21   -1.       1190.
   O2      +   O-      =   O2-     +   O          6.00E+12   0.        0.
```

```
DISTANCE  AREA
 &PROB  HINT= 3.E-9, MF= 21, ITPSZ= 2, CX0= 1000.,  ALLM1 = F,
   PSTAT= T,  DBUGO= T, EMAX= 1.E-5,
  PRINT = .02, .06, .10, .50, .70,  NPRNTS = 5   &END
   N      +  O      =  NO     +  M      N2O     2.25
   NO     +  O      =  NO2    +  M      N2      1.55
   O+     +  E      =  O      +  M      N       0.03    O2      4.5
   O+     +  E      =  O      +  M      NO      50.     O       0.03
   O2     +  E      =  O2-    +  M      N2      .00002

 &START  P=1.6803, V=47002, T=4820., N2=0.7905, O2=0.2095, O2M=1.E-9 &END
FINIS
 GCKP84    HIGH PRESSURE H2  -  CO REACTION       CASE 11
NEW
   CH3    +  OH     =  CH2O   +  H2        7.4E+12   0.        0.
             CH4    =  CH3    +  H         2.0E+15   0.      104000.
   H      +  CH4    =  CH3    +  H2       1.26E+14   0.      11900.
   O      +  CH4    =  CH3    +  OH        2.0E+13    0.0     9200.
   OH     +  CH4    =  CH3    +  H2O       3.0E+13   0.      6000.
   CH2O   +  H      =  HCO    +  H2         2.E+13   0.      3300.
   CH2O   +  O      =  HCO    +  OH        2.0E+13   0.        0.
   CH2O   +  OH     =  HCO    +  H2O       2.3E+13   0.        0.
   M      +  CH2O   =  H      +  HCO       5.0E+16   0.      72000.
   O      +  HCO    =  H      +  CO2       5.3E+13   0.        0.
   HCO    +  O      =  CO     +  OH       1.26E+14    0.        0.
   HCO    +  H      =  CO     +  H2        1.0E+14    0.        0.
   HCO    +  OH     =  CO     +  H2O       1.0E+14   0.        0.
   M      +  HCO    =  H      +  CO        5.0E+14   0.      19000.
   CO     +  OH     =  CO2    +  H         4.0E+12   0.0     8000
   CO     +  O      =  CO2    +  M         2.8E+13   0.      -4540.
   O      +  H2     =  OH     +  H         1.8E+10   1.      8900.
   H2     +  OH     =  H2O    +  H         5.2E+13   0.      6500.
   OH     +  OH     =  O      +  H2O       6.3E+12   0.      1093.
   H      +  H      =  H2     +  M         8.3E+17   -1.       0.
   H      +  OH     =  H2O    +  M         8.4E+21   -2.     0.

TIME
 &PROB     ITPSZ = 5, EMAX = 5.E-6,  PRINT =  1, 100, 1.E+4,
        1.E+6,  1.E+8, 1.E+9,    NPRNTS =  6,
   ALLM1 =F, PSTAT = T, RHOCON = T, MF= 21,  HINT= 1.E-15,TCON= T  &END
   H      +  OH     =  H2O    +  M       H2        4.0
   H      +  H      =  H2     +  M       H2        1.7     CO      2.0
   H      +  H      =  H2     +  M       H2O       9.6     CO2     3.5
   M      +  HCO    =  H      +  CO      H2        5.0     CO      2.0

 &START T= 1000, P= 100,  H2= .99, CO = .01, O=1.E-7, OH=1.E-9,
   CH2O = 1.E-8          &END
FINIS
   GCKP84    HYDROGEN - OXYGEN LOW TEMP PHOTOLYTIC IGNITION       CASE 12
NEW
   H      +  O2     =  OH     +  O         2.2E+14   0.      16790.
   O      +  H2     =  OH     +  H         1.8E+10   1.      8900.
   H2     +  OH     =  H2O    +  H         5.2E+13   0.      6500.
   OH     +  OH     =  O      +  H2O       6.3E+12   0.      1093.
   H      +  O2     =  HO2    +  M         1.5E+15    0.     -1000.
   O      +  O      =  O2     +  M         5.7E+13   0.      -1788.
   H      +  H      =  H2     +  M         8.3E+17   -1.       0.
   H      +  OH     =  H2O    +  M         8.4E+21   -2.     0.
   H2     +  HO2    =  H2O    +  OH        7.2E+11   0.      18700.
   M      +  H2O2   =  2 OH               1.3E+17   0.      45500.
   H2     +  O2     =  2 OH              1.00E+13   0.      43000.
   H      +  HO2    =  OH     +  OH        2.5E+14   0.      1900.
   O      +  HO2    =  OH     +  O2        5.0E+13   0.      1000.
   OH     +  HO2    =  H2O    +  O2        5.0E+13   0.      1000.
          2 HO2    =  H2O2   +  O2       1.80E+12   0.      0.
   OH     +  H2O2   =  H2O    +  HO2       1.0E+13   0.      1800.
   O      +  H2O2   =  OH     +  HO2       8.0E+13   0.      1000.
   H      +  H2O2   =  H2O    +  OH        3.2E+14   0.      9000.
   HNU    +  H2     > 2 H                    .003    0.        0.
   HNU    +  O2     > 2 O                    .005     0.       0.
```

```
TIME
 &PROB  HINT =5.E-7,  ITPSZ=5,    ALLM1 = F,  RHOCON =T, IPRINT=90,
   EMAX=5.E-7,  MF= 21, END = 1.147479          &END
   H       +   O2      =   HO2     +   M       H2       5.0     O2       2.0
   H       +   O2      =   HO2     +   M       H2O     32.5
   H           H       =   H2      +   M       O2       2.0     H2       5.0
   H           H       =   H2      +   M       H2O     15.0
   M       +   H2O2    = 2 OH                  O2       0.78    H2O      6.0
   M       +   H2O2    = 2 OH                  H2O2     6.6     H2       2.3
   H       +   OH      =   H2O     +   M       H2       4.0
   H       +   OH      =   H2O     +   M       H2O     20.0     O2       1.6

 &START T= 700, P = 2,  H2=  .667, O2= .333  &END
FINIS
```

Selected Test Case Results

```
                                        ** DATA CARDS **
                1         2         3         4         5         6         7         8
CC 12345678901234567890123456789012345678901234567890123456789012345678901234567890

    GCKP84
      M       +   BR2       = 2 BR                                          CASE 1
                                BROMINE DISSOCIATION IN A SHOCK TUBE
                                                    6.99E+11  0.50          35500.
    XE
                                    - BLANK CARD -
    DISTANCE  AREA
     &PROB   ITPSZ=3,LSUBM=32200.,ETA=0.50,   SHOCK=.TRUE.,
       PRINT= .05, .2, .5, 2., 4.,  NPRNTS = 5,
      ALLM1= F, PSTAT= T, MF=21,
       M       +   BR2       = 2 BR                  EMAX=1.E-5, HINT=1.E-6 &END
                                                       BR2       3.80
                                    - BLANK CARD -
     &START   P=0.1227,MACH=3.2646,T=299.9,   BR2=0.01,XE=0.99,   &END
    FINIS

      BR2             BR2
 0.44479494E 01  0.10051207E-03 -0.16393813E-07  0.22685621E-11 -0.10236773E-15  0.23659939E 04  0.40888424E 01
 0.38469572E 01  0.26111840E-02 -0.40034147E-05  0.28120688E-08 -0.7325620_E-12  0.24846982E 04  0.69696980E 01

      BR              BR
 0.20843281E 01  0.71949465E-03 -0.27419924E-06  0.42422649E-10 -0.23791569E-14  0.12858836E 05  0.90837994E 01
 0.24611549E 01  0.33319253E-03 -0.10080648E-05  0.12262125E-08 -0.44283506E-12  0.12711918E 05  0.69496724E 01

      XE              XE
 0.25000000E 01  0.00000000  0.00000000  0.00000000  0.00000000 -0.74537500E 03  0.61512737E 01
 0.25000000E 01  0.00000000  0.00000000  0.00000000  0.00000000 -0.74537476E 03  0.61512737E 01

                        ** EQUILIBRIUM SHOCK CALCULATION **

                                INITIAL STATE          FINAL STATE          FINAL/INITIAL RATIO

    PRESSURE
     (ATM)                          0.1227                1.6130                13.1462
    VELOCITY
     (CM/SEC)                   57875.77              18107.37                   0.3129
    DENSITY
     (GM/CM**3)                 6.56092E-04           2.09704E-03                3.1963
    TEMPERATURE
     (DEG K)                      299.90                1231.19                  4.1053
    ENTROPY
     (CAL/GM/DEG K)                 0.3421                0.3576                1.0451
    MACH NUMBER                     3.2646                0.5171                0.1584

    GAMMA                           1.6586                1.5730                0.9484

    *ONIC VELOCITY
     (CM/SEC)                   17728.29              35014.29                   1.9751

                                                  SPECIES     MOLE FRACTION
                                                   BR2         8.11959E-03
                                                   BR          3.72400E-03
                                                   XE          9.88161E-01

    MIXTURE MOLECULAR WEIGHT                        131.34019

    D(LOG VOLUME)/D(LOG T)
        AT CONSTANT P                                 1.0161

    D(LOG VOLUME)/D(LOG P)
        AT CONSTANT T                                -1.0008
```

** FROZEN SHOCK CALCULATION **

	INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE (ATM)	0.1227	1.6017	13.0535
VELOCITY (CM/SEC)	57875.77	18410.77	0.3181
DENSITY (GM/CM**3)	6.56092E-04	2.06248E-03	3.1436
TEMPERATURE (DEG K)	299.90	1245.31	4.1524
ENTROPY (CAL/GM/DEG K)	0.3421	0.3575	1.0449
MACH NUMBER	3.2646	0.5098	0.1562
GAMMA	1.6586	1.6577	0.9994
SONIC VELOCITY (CM/SEC)	17728.29	36115.83	2.0372

SPECIES	MOLE FRACTION
BR2	1.00000E-02
BR	0.00000
XE	9.90000E-01

MIXTURE MOLECULAR WEIGHT	131.58517
D(LOG VOLUME)/D(LOG T) AT CONSTANT P	1.0000
D(LOG VOLUME)/D(LOG P) AT CONSTANT T	-1.0000

DISTANCE-AREA VERSION

GENERAL CHEMICAL KINETICS PROGRAM

NASA LEWIS RESEARCH CENTER

GCKP84

BROMINE DISSOCIATION IN A SHOCK TUBE

CASE 1

REACTION NUMBER	REACTION	REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	M + 1.0*BR2 = 2.0*BR	6.99000E 11	0.5000	35500.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(BR2 , 1) = 3.80000

INTEGRATION CONTROLS

INITIAL STEP SIZE 0.10000E-05 CM

MAXIMUM RELATIVE ERROR 0.10000E-04

** ASSIGNED VARIABLE PROFILE **

THE AREA IS CALCULATED FROM THE FOLLOWING FUNCTION

1/AREA = 1 - (X/ 32200.000)**(0.50000)

** INITIAL CONDITIONS **

TIME 0.00000 SEC

AREA 1.00000E 00 SQ CM

AXIAL POSITION 0.00000 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.60166
VELOCITY (CM/SEC)	18410.77
DENSITY (GM/CM**3)	2.06248E-03
TEMPERATURE (DEG K)	1245.31
MASS FLOW RATE (GM/SEC)	3.79718E 01
ENTROPY (CAL/GM/DEG K)	0.3575
MACH NUMBER	0.5098
GAMMA	1.6577
ENTHALPY (CAL/GM)	3.66060E 01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
BR2	1.56741E-07	1.00000E-02	-5.66685E-05	1	1.4519E 07	8.62015E 00	1.00000
BR	0.00000	0.00000	7.33371E-05				
XE	1.55173E-05	9.90000E-01	0.00000				

MIXTURE MOLECULAR WEIGHT 131.58522 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) 3.97238E 05 MASS FRACTION SUM 0.99999994

TIME 2.71011E-05 SEC AREA 1.00396E 00 SQ CM AXIAL POSITION 5.00000E-01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.60569
VELOCITY (CM/SEC)	18303.13
DENSITY (GM/CM**3)	2.06647E-03
TEMPERATURE (DEG K)	1245.95
MASS FLOW RATE (GM/SEC)	3.79725E 01
ENTROPY CAL/GM/DEG K)	0.3575
MACH NUMBER	0.5066
GAMMA	1.6577
ENTHALPY (CAL/GM)	3.66533E 01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	4
AVERAGE STEP SIZE	0.75000E-01
TOTAL NUMBER OF STEPS	36
FUNCT EVALUATIONS	45
JACOBIAN EVALUATIONS	10

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
BR2	1.56039E-07	9.93535E-03	-3.68217E-05	1	1.4630E 07	8.62272E 00	0.99923
BR	2.01057E-09	1.28017E-04	7.36433E-05				
XE	1.55474E-05	9.89937E-01	0.00000				

MIXTURE MOLECULAR WEIGHT 131.57678 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) 3.97357E 05 MASS FRACTION SUM 0.99999994

TIME 1.09314E-04 SEC AREA 1.00794E 00 SQ CM AXIAL POSITION 2.00000E 00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.61048
VELOCITY (CM/SEC)	18174.59
DENSITY (GM/CM**3)	2.07277E-03
TEMPERATURE (DEG K)	1245.63
MASS FLOW RATE (GM/SEC)	3.79710E 01
ENTROPY CAL/GM/DEG K)	0.3575
MACH NUMBER	0.5031
GAMMA	1.6579
ENTHALPY (CAL/GM)	3.67093E 01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	6
AVERAGE STEP SIZE	0.25000E 00
TOTAL NUMBER OF STEPS	40
FUNCT EVALUATIONS	51
JACOBIAN EVALUATIONS	11

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
BR2	1.53520E-07	9.74337E-03	-5.57666E-05	1	1.4574E 07	8.32482E 00	0.98761
BR	8.00709E-09	5.08183E-04	7.15332E-05				
XE	1.55948E-05	9.89748E-01	0.00000				

MIXTURE MOLECULAR WEIGHT 131.55176 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) 3.83628E 05 MASS FRACTION SUM 0.99999994

TIME 2.18604E-04 SEC AREA 1.01127E 00 SQ CM AXIAL POSITION 4.00000E 00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.61485
VELOCITY (CM/SEC)	18056.59
DENSITY (GM/CM**3)	2.07948E-03
TEMPERATURE (DEG K)	1244.69
MASS FLOW RATE (GM/SEC)	3.79715E 01
ENTROPY CAL/GM/DEG K)	0.3575
MACH NUMBER	0.4999
GAMMA	1.6581
ENTHALPY (CAL/GM)	3.67604E 01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	4
AVERAGE STEP SIZE	0.50000E 00
TOTAL NUMBER OF STEPS	44
FUNCT EVALUATIONS	55
JACOBIAN EVALUATIONS	11

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
BR2	1.56184E-07	9.49862E-03	-5.33972E-05	1	1.4411E 07	7.72328E 00	0.95065
BR	1.56978E-08	9.92334E-04	6.67945E-05				
XE	1.56452E-35	9.89509E-01	0.00000				

MIXTURE MOLECULAR WEIGHT 131.51991 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) 3.55908E 05 MASS FRACTION SUM 0.99999994

(GCKP) END OF THIS CASE - READ DATA FOR NEXT CASE

DISTANCE-AREA VERSION GENERAL CHEMICAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

GCKP84 HYD - AIR TEST WITH HEAT TRANSFER STOICH CASE 2

REACTION NUMBER	REACTION						REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1.0*H	+ 1.0*O2	=	1.0*OH	+	1.0*O	2.20000E 14	0.0000	16790.00
2	1.0*O	+ 1.0*H2	=	1.0*OH	+	1.0*H	1.80000E 10	1.0000	8900.00
3	1.0*H2	+ 1.0*OH	=	1.0*H2O	+	1.0*H	5.20000E 13	0.0000	6580.00
4	1.0*OH	+ 1.0*OH	=	1.0*O	+	1.0*H2O	6.30000E 12	0.0000	1093.00
5	1.0*H	+ 1.0*O2	=	1.0*HO2	+	M	1.50000E 15	0.0000	-1000.00
6	1.0*O	+ 1.0*O	=	1.0*O2	+	M	5.70000E 13	0.0000	-1788.00
7	1.0*H	+ 1.0*H	=	1.0*H2	+	M	8.30000E 17	-1.0000	0.00
8	1.0*H	+ 1.0*OH	=	1.0*H2O	+	M	8.40000E 21	-2.0000	0.00
9	1.0*H2	+ 1.0*HO2	=	1.0*H2O	+	1.0*OH	7.20000E 11	0.0000	18700.00
10	M	+ 1.0*H2O2	=	2.0*OH			1.30000E 17	0.0000	45500.00
11	1.0*H2	+ 1.0*O2	=	2.0*OH			1.00000E 13	0.0000	43000.00
12	1.0*H	+ 1.0*HO2	=	1.0*OH	+	1.0*OH	2.50000E 14	0.0000	1900.00
13	1.0*O	+ 1.0*HO2	=	1.0*OH	+	1.0*O2	5.00000E 13	0.0000	1000.00
14	1.0*OH	+ 1.0*HO2	=	1.0*H2O	+	1.0*O2	5.00000E 13	0.0000	1000.00
15		2.0*HO2	=	1.0*H2O2	+	1.0*O2	1.00000E 12	0.0000	0.00
16	1.0*HO2	+ 1.0*NO	=	1.0*NO2	+	1.0*OH	1.20000E 13	0.0000	2380.00
17	1.0*O	+ 1.0*NO2	=	1.0*NO	+	1.0*O2	1.00000E 13	0.0000	596.00
18	1.0*HO	+ 1.0*O	=	1.0*NO2	+	M	5.62000E 15	0.0000	-1160.00
19	1.0*NO2	+ 1.0*H	=	1.0*NO	+	1.0*OH	2.90000E 14	0.0000	795.00
20	1.0*N	+ 1.0*O2	=	1.0*NO	+	1.0*O	6.40000E 09	1.0000	6250.00
21	1.0*O	+ 1.0*N2	=	1.0*NO	+	1.0*N	1.80000E 14	0.0000	76250.00
22	1.0*N	+ 1.0*OH	=	1.0*NO	+	1.0*H	4.00000E 13	0.0000	0.00
23	M	+ 1.0*N2O	=	1.0*N2	+	1.0*O	1.42000E 14	0.0000	51280.00
24	1.0*O	+ 1.0*N2O	=	1.0*N2	+	1.0*O2	6.23000E 13	0.0000	24520.00
25	1.0*O	+ 1.0*N2O	=	2.0*NO			3.10000E 13	0.0000	21800.00
26		2.0*NO2	=	2.0*NO	+	1.0*O2	4.00000E 12	0.0000	26900.00
27	1.0*N	+ 1.0*NO2	=	2.0*NO			5.60000E 12	0.0000	0.00
28	1.0*OH	+ 1.0*N2	=	1.0*N2O	+	1.0*H	3.20000E 12	0.0000	80280.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	, 5) = 5.00000	M(H2	, 7) = 5.00000	M(H2	, 8) = 4.00000	M(H2	, 10) = 2.30000
M(O2	, 5) = 2.00000	M(O2	, 7) = 2.00000	M(O2	, 8) = 1.60000	M(O2	, 10) = 0.78000
M(H2O	, 5) = 32.50000	M(H2O	, 7) = 15.00000	M(H2O	, 8) = 20.00000	M(H2O	, 10) = 6.00000
M(N2	, 5) = 2.00000	M(N2	, 7) = 2.00000	M(N2	, 8) = 1.60000	M(H2O2	, 10) = 6.60000

INTEGRATION CONTROLS

INITIAL STEP SIZE 0.10000E-05 CM MAXIMUM RELATIVE ERROR 0.10000E-03

** INITIAL CONDITIONS **

TIME 0.00000 SEC AREA 2.00000E 03 SQ CM AXIAL POSITION 0.00000 CM

FLOW PROPERTIES

PRESSURE (ATM)	0.95600
VELOCITY (CM/SEC)	450950.63
DENSITY (GM/CM**3)	1.56984E-04
TEMPERATURE (DEG K)	1559.00
MASS FLOW RATE (GM/SEC)	1.41584E 05
ENTROPY CAL/GM/DEG K)	2.6768
MACH NUMBER	5.0000
GAMMA	1.3183
ENTHALPY (CAL/GM)	4.54661E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

HEAT LOSS(QDOT/MDOT) = 6.4255E-02 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
H	0.00000	0.00000	4.73663E-10
O2	1.10332E-06	1.47635E-01	-2.28267E-05
OH	0.00000	0.00000	4.56534E-05
O	0.00000	0.00000	1.22591E-12
H2	2.20665E-06	2.95278E-01	-2.28269E-05
H2O	0.00000	0.00000	0.00000
HO2	0.00000	0.00000	0.00000
H2O2	0.00000	0.00000	0.00000
NO	0.00000	0.00000	0.00000
NO2	0.00000	0.00000	0.00000
N	0.00000	0.00000	0.00000
N2	4.11247E-06	5.50303E-01	-2.31940E-13
N2O	0.00000	0.00000	2.31940E-13
CO2	1.57996E-09	2.11419E-04	0.00000
AR	4.90836E-08	6.56802E-03	0.00000

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	9.7432E 11	0.00000	0.00000
2	1.5866E 12	0.00000	0.00000
3	6.3796E 12	0.00000	0.00000
4	4.4271E 12	0.00000	0.00000
5	2.0715E 15	0.00000	0.00000
6	1.0151E 14	-2.01666E-05	1.00000
7	5.3239E 14	-9.61006E-03	1.00000
8	3.4561E 15	0.00000	0.00000
9	1.7213E 09	0.00000	0.00000
10	5.4366E 10	0.00000	0.00000
11	9.3758E 06	9.26253E 02	1.00000
12	1.3539E 14	0.00000	0.00000
13	3.6206E 13	0.00000	0.00000
14	5.6206E 13	0.00000	0.00000
15	1.0000E 12	0.00000	0.00000
16	5.5659E 12	0.00000	0.00000
17	8.2499E 12	0.00000	0.00000
18	8.1724E 15	0.00000	0.00000
19	2.2436E 14	0.00000	0.00000
20	1.3270E 12	0.00000	0.00000
21	3.6821E 03	0.00000	0.00000
22	4.0000E 13	0.00000	0.00000
23	9.1952E 06	0.00000	0.00000
24	2.2758E 10	-9.41158E-06	1.00000
25	2.7246E 10	0.00000	0.00000
26	6.7773E 08	0.00000	0.00000
27	3.6000E 12	0.00000	0.00000
28	1.7825E 01	0.00000	0.00000

MIXTURE MOLECULAR WEIGHT 21.00656 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) 1.72621E 07 MASS FRACTION SUM 0.99999988

NEGATIVE CONCENTRATIONS-HALVE STEP SIZE -SAVE1(1) = -0.97233491D-06

PREDICTOR TROUBLE FOR Y10, VALUE = -0.16540184942951 61D-14, T= 0.267323973794948D 01, H= 0.16720320528520 14D 00

CUT STEP SIZE BY 0.10000004D 00

PREDICTOR TROUBLE FOR Y10, VALUE = -0.8110711496602457D-16, T= 0.2522756859172 45D 01, H= 0.16720326508172 73D-01

CUT STEP SIZE BY 0.10000004D 00

PREDICTOR TROUBLE FOR Y 7, VALUE = -0.4260212102642709D-05, T= 0.3014067935066 77D 01, H= 0.88133077565924 50D-01

CUT STEP SIZE BY 0.20000004D 00

PREDICTOR TROUBLE FOR Y10, VALUE = -0.1892096165937720D-14, T= 0.3049321188154 33D 01, H= 0.35253237330138 75D-01

CUT STEP SIZE BY 0.70000004D 00

TIME 6.75787E-06 SEC AREA 2.00000E 03 SQ CM AXIAL POSITION 3.04800E 00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.03443
VELOCITY (CM/SEC)	449828.11
DENSITY (GM/CM**3)	1.57376E-04
TEMPERATURE (DEG K)	1689.91
MASS FLOW RATE (GM/SEC)	1.41584E 05
ENTROPY CAL/GM/DEG K)	2.7378
MACH NUMBER	4.8140
GAMMA	1.3110
ENTHALPY (CAL/GM)	4.66542E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	43
AVERAGE STEP SIZE	0.70884E-01
TOTAL NUMBER OF STEPS	43
FUNCT EVALUATIONS	45
JACOBIAN EVALUATIONS	13

HEAT LOSS(QDOT/MDOT) = 6.9676E-02 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
H	5.53548E-07	7.42040E-02	3.97345E-01
O2	6.19606E-07	8.30592E-02	-3.84733E-01
OH	8.56676E-08	1.14839E-02	7.97796E-02
O	1.34743E-07	1.80626E-02	1.10187E-01
H2	1.14063E-06	1.52903E-01	-8.18645E-01
H2O	7.51634E-07	1.00758E-01	5.80141E-01
HO2	3.28954E-10	4.40969E-05	-5.26559E-04
H2O2	1.20376E-10	1.61366E-05	2.05118E-04
NO	1.04631E-14	1.40260E-09	2.48806E-08
NO2	7.96584E-19	1.06784E-13	1.96753E-12
N	2.11617E-15	2.83677E-10	4.31000E-09
N2	4.12274E-06	5.52660E-01	-1.55302E-07
N2O	1.31107E-13	1.75751E-08	1.48706E-07

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.4826E 12	1.45112E 07	0.78678
2	2.1485E 12	1.01151E 07	0.75878
3	7.5055E 12	2.31035E 07	0.78021
4	4.5497E 12	1.20228E 05	0.08918
5	2.0203E 15	1.13113E 06	0.99972
6	9.7076E 13	5.30853E 02	1.00000
7	4.9115E 14	1.65810E 05	1.00000
8	2.9414E 15	1.57736E 05	1.00000
9	2.7474E 09	4.16213E 01	0.99997
10	1.6966E 11	-8.27852E 03	0.44413
11	2.7476E 07	7.28561E 02	0.92924
12	1.4198E 14	1.04371E 06	0.99988
13	3.7123E 13	6.64093E 04	0.99959

CO2	1.58390E-09	2.12375E-04	0.00000	14	3.7123E 13	4.22235E 04	0.99962
AR	4.92060E-08	6.59616E-03	0.00000	15	1.000CE 12	3.30853E 00	0.75725
				16	5.9072E 12	7.99689E-04	0.97413
				17	8.373BE 12	5.57095E-05	0.98401
				18	7.938AE 15	3.37102E-03	0.99998
				19	2.2887E 14	4.05556E-03	0.99531
				20	1.6817E 12	8.90292E-02	0.99998
				21	2.4781E 04	5.5581?E-01	1.00000
				22	4.0000E 13	2.9276?E-01	0.99994
				23	3.3145E 07	-8.33143E 00	0.99984
				24	4.2015E 10	2.98933E-02	0.99751
				25	4.6994E 10	3.35194E-02	1.00000
				26	1.3279E 09	-2.21725E-17	0.99847

TIME 1.69746E-05 SEC AREA 2.00000E 03 SQ CM AXIAL POSITION 7.62000E 00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.43402
VELOCITY (CM/SEC)	444108.43
DENSITY (GM/CM**3)	1.59403E-04
TEMPERATURE (DEG K)	2418.13
MASS FLOW RATE (GM/SEC)	1.41584E 05
ENTROPY CAL/GM/DEG K)	2.7897
MACH NUMBER	4.1148
GAMMA	1.2779
ENTHALPY (CAL/GM)	5.27252E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	26
AVERAGE STEP SIZE	0.58615E-01
TOTAL NUMBER OF STEPS	101
FUNCT EVALUATIONS	108
JACOBIAN EVALUATIONS	30

HEAT LOSS(QDOT/MDOT) = 9.9832E-02 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RA?? (MOLE-CM**3/GM**2/SEC)	NET RATE/POSI-TIVE DIR RATE
H	4.84264E-07	6.70066E-02	-2.31366E-02	1	6.6827E 12	-1.33551E 05	0.00502
O2	2.07876E-07	2.87634E-02	-5.01287E-03	2	6.8293E 12	5.34288E 04	0.00234
OH	2.66808E-07	3.69177E-02	4.87359E-03	3	1.3444E 13	1.19693E 05	0.00175
O	1.75667E-07	2.43066E-02	-5.75456E-03	4	5.0183E 12	-8.32079E 03	0.00059
H2	4.82993E-07	6.68308E-02	-1.75482E-03	5	1.8470E 15	4.04643E 05	0.96883
H2O	1.32203E-06	1.91228E-01	1.08967E-02	6	8.2694E 13	7.23593E 02	0.99694
HO2	1.14723E-10	1.58740E-05	-2.88212E-06	7	3.4324E 14	1.03874E 05	0.99692
H2O2	2.92045E-11	4.04096E-06	-8.99411E-06	8	1.4365E 15	2.73559E 05	0.99692
NO	9.97963E-11	1.38086E-05	3.36740E-05	9	1.4697E 10	2.8A792E C1	0.90106
NO2	9.95284E-15	1.37715E-09	2.93106E-09	10	1.0039E 13	3.52836E 02	0.00208
N	1.46379E-12	2.02542E-07	3.08158E-07	11	1.2992E 09	-1.38642E 01	0.00269
N2	4.17578E-06	5.77794E-01	-1.70386E-05	12	1.6835E 14	3.31610E 05	0.98088
N2O	7.55518E-13	1.04539E-07	4.60507E-08	13	4.0606E 13	2.90299E 04	0.90138
CO2	1.60430E-09	2.21904E-04	0.00000	14	4.0606E 13	4.40886C 04	0.90132
AR	4.98397E-08	6.89622E-03	0.00000	15	1.0000E 12	-1.13263E 00	0.68619
				16	7.3127E 12	1.80670E 00	0.54832
				17	8.8335E 12	4.75112E-01	0.78166
				18	7.1545E 15	3.51743E 01	0.98599
				19	2.4578E 14	3.63906E 01	0.78056
				20	4.2149E 12	4.96827E 01	0.98429
				21	2.3111E 07	6.67020E 02	0.99972
				22	4.0000E 13	6.05209E 02	0.98437
				23	3.2932E 09	-4.06923E 01	0.98291
				24	3.?877E 11	1.62446E 00	0.82108
				25	3...96E 11	1.73391E 00	1.00000
				26	1.4?20E 10	-8.42817E-10	0.93585

TIME 3.40992E-05 SEC AREA 2.00000E 03 SQ CM AXIAL POSITION 1.52400E 01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.64871
VELOCITY (CM/SEC)	441035.34
DENSITY (GM/CM**3)	1.60514E-04
TEMPERATURE (DEG K)	2840.32
MASS FLOW RATE (GM/SEC)	1.41584E 05
ENTROPY CAL/GM/DEG K)	2.7986
MACH NUMBER	3.8464
GAMMA	1.2632
ENTHALPY (CAL/GM)	5.58925E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	12
AVERAGE STEP SIZE	0.63500E 00
TOTAL NUMBER OF STEPS	113
FUNCT EVALUATIONS	121
JACOBIAN EVALUATIONS	33

HEAT LOSS(QDOT/MDOT) = 1.1731E-01 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
H	2.80935E-07	3.97140E-02	-6.29677E-03
O2	1.59677E-07	2.25722E-02	-1.68085E-03
OH	2.90819E-07	4.11107E-02	2.93593E-04
O	1.14218E-07	1.61461E-02	-2.07111E-03
H2	4.41140E-07	6.23603E-02	-1.82955E-03
H2O	1.52917E-06	2.16166E-01	4.75567E-03
HO2	1.21528E-10	1.71794E-05	-4.41039E-07
H2O2	8.20276E-12	1.15956E-06	7.56868E-05
NO	2.43303E-09	3.43938E-04	2.32913E-04
NO2	4.06849E-13	5.75129E-08	2.62935E-09
N	1.05007E-11	1.48440E-06	4.96635E-07
N2	4.20370E-06	5.94243E-01	-1.16830E-04
N2O	2.51780E-12	3.55921E-07	1.24423E-07
CO2	1.61548E-09	2.28367E-04	0.00000
AR	5.01870E-08	7.09453E-03	0.00000

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.1233E 13	-2.82571E 04	0.00144
2	1.0564E 13	2.85460E 04	0.00138
3	1.6438E 13	6.69238E 04	0.00082
4	5.1909E 12	-9.62613E 03	0.00056
5	1.7908E 15	1.25009E 05	0.65330
6	7.8244E 13	2.21612E 02	0.79072
7	2.9222E 14	2.44802E 04	0.79013
8	1.0412E 15	1.04560E 05	0.79030
9	2.6209E 10	2.15487E 01	0.39513
10	4.1013E 13	-2.93804E 03	0.01453
11	4.9130E 09	-8.95976E-01	0.00007
12	1.7854E 14	9.33689E 04	0.39463
13	4.1882E 13	8.92418E 03	0.39551
14	4.1882E 13	2.27028E 04	0.39517
15	1.0000E 12	-4.13132E-01	0.41884
16	7.8714E 12	9.00765E 00	0.09971
17	8.9979E 12	5.33204E 00	0.32855
18	6.9023E 15	3.62502E 02	0.68832
19	2.5190E 14	3.66075E 02	0.32758
20	6.0067E 12	3.42950E 02	0.87732
21	2.4444E 08	4.52240E 03	0.99276
22	4.0000E 13	4.16025E 03	0.87749
23	1.6089E 10	-3.32227E 01	0.74953
24	8.0870E 11	1.48461E 00	0.16447
25	6.5155E 11	7.26711E 00	0.99926
26	3.4059E 10	-2.52571E-07	0.53581

DISTANCE-AREA VERSION GENERAL CHEMICAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

GCKP84 HYD - AIR TEST WITH HEAT TRANSFER FULL MECH CASE 3

REACTION NUMBER	REACTION	REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1.0*H + 1.0*O2 = 1.0*OH + 1.0*O	2.20000E 14	0.0000	16790.00
2	1.0*O + 1.0*H2 = 1.0*OH + 1.0*H	1.80000E 10	1.0000	8900.00
3	1.0*H2 + 1.0*OH = 1.0*H2O + 1.0*H	5.20000E 13	0.0000	6500.00
4	1.0*OH + 1.0*OH = 1.0*O + 1.0*H2O	6.30000E 12	0.0000	1093.00
5	1.0*H + 1.0*O2 = 1.0*HO2 + M	1.50000E 15	0.0000	-1000.00
6	1.0*O + 1.0*O = 1.0*O2 + M	5.70000E 13	0.0000	-1788.00
7	1.0*H + 1.0*H = 1.0*H2 + M	8.30000E 17	-1.0000	0.00
8	1.0*H + 1.0*OH = 1.0*H2O + M	8.40000E 21	-2.0000	0.00
9	1.0*H2 + 1.0*HO2 = 1.0*H2O + 1.0*OH	7.20000E 11	0.0000	18700.00
10	M + 1.0*H2O2 = 2.0*OH	1.30000E 17	0.0000	45500.00
11	1.0*H2 + 1.0*O2 = 2.0*OH	1.00000E 13	0.0000	43000.00
12	1.0*H + 1.0*HO2 = 1.0*OH + 1.0*OH	2.50000E 14	0.0000	1900.00
13	1.0*O + 1.0*HO2 = 1.0*OH + 1.0*O2	5.00000E 13	0.0000	1000.00
14	1.0*OH - 1.0*HO2 = 1.0*H2O + 1.0*O2	5.00000E 13	0.0000	1000.00
15	2.0*HO2 = 1.0*H2O2 + 1.0*O2	1.80000E 12	0.0000	0.00
16	1.0*HO2 + 1.0*NO = 1.0*NO2 + 1.0*OH	1.20000E 13	0.0000	2380.00
17	1.0*O + 1.0*NO2 = 1.0*NO + 1.0*O2	1.00000E 13	0.0000	596.00
18	1.0*NO + 1.0*O + M = 1.0*NO2	5.62000E 15	0.0000	-1160.00
19	1.0*NO2 + 1.0*H = 1.0*NO + 1.0*OH	2.90000E 14	0.0000	795.00
20	1.0*N + 1.0*O2 = 1.0*NO + 1.0*O	6.40000E 09	1.0000	6250.00
21	1.0*O + 1.0*N2 = 1.0*NO + 1.0*N	1.80000E 14	0.1300	76250.00
22	1.0*N + 1.0*OH = 1.0*NO + 1.0*H	4.00000E 13	0.0000	0.00
23	M + 1.0*N2O = 1.0*N2 + 1.0*O	1.42000E 14	0.0000	51280.00
24	1.0*O + 1.0*N2O = 1.0*N2 + 1.0*O2	6.23000E 13	0.0000	24520.00
25	1.0*O + 1.0*N2O = 2.0*NO	3.10000E 13	0.0000	21200.00
26	2.0*NO2 = 2.0*NO + 1.0*O2	4.00300E 12	0.0000	26900.00
27	1.0*N + 1.0*NO2 = 2.0*NO	3.60000E 12	0.0000	0.00
28	1.0*OH + 1.0*N2 = 1.0*N2O + 1.0*H	3.20000E 12	0.0000	80280.00
29	1.0*OH + 1.0*H2O2 = 1.0*H2O + 1.0*HO2	1.00000E 13	0.0000	1800.00
30	1.0*O + 1.0*H2O2 = 1.0*OH + 1.0*HO2	8.00000E 13	0.0000	1000.00
31	1.0*H + 1.0*H2O2 = 1.0*H2O + 1.0*OH	3.20000E 14	0.0000	9000.00

** ASSIGNED VARIABLE PROFILE **

THE AREA IS CALCULATED FROM THE FOLLOWING POLYNOMIAL

AREA (FT**2) = (0.00000)X**3 + (0.00000)X**2 + (0.00000)X + (2.15278E 00)

AIR - FUEL COMBUSTION, EQUIVALENCE RATIO = 1.0000 FUEL - AIR RATIO = 0.0292 OXYGEN FRACTION IN AIR = 0.2095

HEAT TRANSFER CASE QDOT (CAL/CM-SEC) =(0.00000)T**2 + (5.86300E 00)T + (-4.28800E 01)

** INITIAL CONDITIONS **

TIME 0.00000 SEC AREA 2.00000E 03 SQ CM AXIAL POSITION 0.00000 CM

FLOW PROPERTIES

PRESSURE (ATM)	0.95600
VELOCITY (CM/SEC)	450952.56
DENSITY (GM/CM**3)	1.56983E-04
TEMPERATURE (DEG K)	1559.00
MASS FLOW RATE (GM/SEC)	1.41584E 05
ENTROPY (CAL/GM/DEG K)	2.6768
MACH NUMBER	5.0000
GAMMA	1.3183
ENTHALPY (CAL/GM)	4.54665E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

HEAT LOSS(QDOT/MDOT) = 6.4255E-02 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
H	0.00000	0.00000	4.73677E-10
O2	1.10331E-06	1.47638E-01	-2.28271E-05
OH	0.00000	0.00000	4.56542E-05
O	0.00000	0.00000	1.22590E-12
H2	2.20670E-06	2.95285E-01	-2.28274E-05
H2O	0.00000	0.00000	0.00000
HO2	0.00000	0.00000	0.00000
H2O2	0.00000	0.00000	0.00000
NO	0.00000	0.00000	0.00000
NO2	0.00000	0.00000	0.00000
N	0.00000	0.00000	0.00000
N2	4.11244E-06	5.50298E-01	-2.31937E-13
N2O	0.00000	0.00000	2.31937E-13
CO2	1.57995E-09	2.11417E-04	0.00000
AR	4.90832E-08	6.56796E-03	0.00000

REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	9.7432E 11	0.00000	0.00000
2	1.5866E 12	0.00000	0.00000
3	6.3796E 12	0.00000	0.00000
4	4.4271E 12	0.00000	0.00000
5	2.0715E 15	0.00000	0.00000
6	1.0151E 14	2.40201E 00	1.00000
7	5.3239E 14	1.00146E 03	1.00000
8	3.4561E 15	0.00000	0.00000
9	1.7213E 09	0.00000	0.00000
10	5.4386E 10	0.00000	0.00000
11	9.3758E 06	1.72617E 07	1.00000
12	1.3539E 14	0.00000	0.00000
13	3.6206E 13	0.00000	0.00000
14	3.6206E 13	0.00000	0.00000
15	1.8000E 12	0.00000	0.00000
16	5.5659E 12	0.00000	0.00000
17	8.2499E 12	0.00000	0.00000
18	8.1724E 15	0.00000	0.00000
19	2.2436E 14	0.00000	0.00000
20	1.3270E 12	0.00000	0.00000
21	3.6822E 03	0.00000	0.00000
22	4.0000E 13	0.00000	0.00000
23	9.1952E 06	0.00000	0.00000
24	2.2758E 10	7.45054E-01	1.00000

TIME 6.75786E-06 SEC AREA 2.00000E 03 SQ CM AXIAL POSITION 3.04800E 00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.03463
VELOCITY (CM/SEC)	449827.12
DENSITY (GM/CM**3)	1.57376E-04
TEMPERATURE (DEG K)	1690.24
MASS FLOW RATE (GM/SEC)	1.41584E 05
ENTROPY (CAL/GM/DEG K)	2.7379
MACH NUMBER	4.8135
GAMMA	1.3110
ENTHALPY (CAL/GM)	4.66577E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	43
AVERAGE STEP SIZE	0.70884E-01
TOTAL NUMBER OF STEPS	43
FUNCT EVALUATIONS	45
JACOBIAN EVALUATIONS	13

HEAT LOSS(QDOT/MDOT) = 6.9698E-02 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
H	5.53541E-07	7.42032E-02	3.97200E-01
O2	6.19697E-07	8.30448E-02	-3.85002E-01
OH	8.57328E-08	1.14927E-02	7.99511E-02
O	1.34750E-07	1.80636E-02	1.10227E-01
H2	1.14042E-06	1.52876E-01	-8.19173E-01
H2O	7.51973E-07	1.00803E-01	5.80840E-01
HO2	3.30811E-10	4.43459E-05	-5.28237E-04

REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.4841E 12	2.43532E 11	0.70677
2	2.1500E 12	1.88866E 10	0.75851
3	7.5084E 12	-3.47048E 11	0.78005
4	4.5500E 12	-2.03339E 09	0.08923
5	2.0202E 15	-5.83695E 10	0.99972
6	9.7065E 13	-6.32286E 07	1.00000
7	4.9105E 14	-1.72769E 10	1.00000

H202	1.94366E-11	2.60552E-06	2.12009E-05	8	2.9402E 15	-1.88150E 10	1.00000
NO	1.04835E-14	1.40534E-09	2.49812E-08	9	2.7505E 09	-2.05190E 06	0.99997
NO2	7.99042E-19	1.07113E-13	1.96882E-12	10	1.7012E 11	-8.70082E 08	0.91012
N	2.12247E-15	2.84521E-10	4.33890E-09	11	2.7547E 07	1.36063E 07	0.92919
N2	4.12273E-06	5.52660E-01	-1.55487E-07	12	1.4199E 14	-3.56551E 10	0.99988
N20	1.31138E-13	1.75792E-08	1.40826E-07	13	3.7125E 13	-3.38872E 09	0.99959
CO2	1.58370E-09	2.12325E-04	0.00000	14	3.7125E 13	-2.87330E 09	0.99962
AR	4.92060E-08	6.59616E-03	0.00000	15	1.8000E 12	-2.56707E 05	0.96117
				16	5.9081E 12	-3.90968E 00	0.97422
				17	8.3741E 12	-1.64368E 00	0.98399
				18	7.9383E 15	-2.47315E 02	0.99998
				19	2.2888E 14	-1.18448E 02	0.99531
				20	1.6827E 12	-2.84448E 03	0.99998
				21	2.4894E 04	4.18782E 04	1.00000
				22	4.0000E 13	-1.42852E 04	0.99994
				23	3.3247E 07	-3.33106E 05	0.99984
				24	4.2076E 10	-2.37056E 03	0.99750
				25	4.7055E 10	-1.20884E 03	1.00000
				26	1.3301E 09	-6.08543E-13	0.99846

TIME 1.69608E-05 SEC AREA 2.00000E 03 SQ CM AXIAL POSITION 7.62000E 00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.44304
VELOCITY (CM/SEC)	443981.37
DENSITY (GM/CM**3)	1.59448E-04
TEMPERATURE (DEG K)	2435.41
MASS FLOW RATE (GM/SEC)	1.41584E 05
ENTROPY CAL/GM/DEG K)	2.7903
MACH NUMBER	4.1023
GAMMA	1.2773
ENTHALPY (CAL/GM)	5.28610E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	9
AVERAGE STEP SIZE	0.16933E 00
TOTAL NUMBER OF STEPS	76
FUNCT EVALUATIONS	82
JACOBIAN EVALUATIONS	22

HEAT LOSS(QDOT/MDOT) = 1.0055E-01 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
H	4.75068E-07	6.57898E-02	-2.38144E-02	1	6.8503E 12	-1.78921E 09	0.00403
02	2.05951E-07	2.85211E-02	-5.35927E-03	2	6.9690E 12	1.08905E 08	0.00255
OH	2.68623E-07	3.72003E-02	5.13112E-03	3	1.3574E 13	-1.55554E 09	0.00150
O	1.73267E-07	2.39949E-02	-5.59682E-03	4	5.0264E 12	2.53171E 08	0.00105
H2	4.82322E-07	6.67943E-02	-1.59358E-03	5	1.8443E 15	-2.02234E 10	0.96487
H20	1.38710E-06	1.92093E-01	1.07126E-02	6	8.2476E 13	-8.34537E 07	0.99630
H02	1.16707E-10	1.61622E-05	-1.07206E-05	7	3.4081E 14	-1.03499E 10	0.99627
H202	2.12837E-11	2.94748E-06	2.27913E-04	8	1.4162E 15	-3.17910E 10	0.99628
NO	1.09236E-10	1.51276E-05	3.71506E-05	9	1.5109E 10	-1.46644E 06	0.89385
NO2	1.10822E-14	1.53472E-09	3.51003E-09	10	1.0736E 13	-2.00659E 09	0.22826
N	1.60426E-12	2.22167E-07	3.64371E-07	11	1.3843E 09	-1.51335E 05	0.00150
N2	4.17696E-06	5.78446E-01	-1.88116E-05	12	1.6882E 14	-1.11761E 10	0.89369
N20	7.73879E-13	1.07171E-07	5.23272E-08	13	4.0666E 13	-1.46729E 09	0.89412
CO2	1.60475E-09	2.22235E-04	0.00000	14	4.0666E 13	-3.03110E 09	0.89401
AR	4.98538E-08	6.9040.E-03	0.00000	15	1.8000E 12	4.32413E 04	0.57179
				16	7.3384E 12	-9.67850E 03	0.54219
				17	8.8413E 12	-2.35536E 04	0.76873
				18	7.1422E 15	-2.76637E 06	0.98398
				19	2.4607E 14	-1.13912E 06	0.76779
				20	4.2844E 1?	-1.74390E 06	0.98362
				21	2.5065E 02	5.52037E 07	0.99970
				22	4.0000E 13	-3.24218E 07	0.98369
				23	3.5522E 09	-1.63843E 06	0.98132
				24	3.9273E 11	-1.31452E 05	0.80167
				25	3.4282E 11	-6.51019E 04	1.00000
				26	1.5420E 10	-2.73661E-05	0.93074

TIME 3.41266E-05 SEC AREA 2.00000E 03 SQ CM AXIAL POSITION 1.52400E 01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.65671
VELOCITY (CM/SEC)	440920.94
DENSITY (GM/CM**3)	.60555E-04
TEMPERATURE (DEG K)	2856.43
MASS FLOW RATE (GM/SEC)	1.41584E 05
ENTROPY CAL/GM/DEG K)	2.7988
MACH NUMBER	3.8374

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	27
AVERAGE STEP SIZE	0.28222E 00
TOTAL NUMBER OF STEPS	103
FUNCT EVALUATIONS	109
JACOBIAN EVALUATIONS	28

GAMMA 1.2627

ENTHALPY (CAL/GM) 5.60169E 02

HEAT LOSS(QDOT/MDOT) = 1.1798E-01 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
H	2.74154E-07	3.87866E-02	-4.40748E-03
O2	1.57884E-07	2.23370E-02	-1.56905E-03
OH	2.90762E-07	4.11363E-02	-1.62945E-03
O	1.11867E-07	1.58267E-02	-2.09798E-03
H2	4.38730E-07	6.20705E-02	-3.18984E-03
H2O	1.53564E-06	2.17259E-01	5.80489E-03
HO2	1.23302E-10	1.74444E-05	7.73952E-06
H2O2	7.13903E-12	1.01001E-06	3.99542E-04
NO	2.52575E-09	3.57337E-04	2.45798E-04
NO2	4.30934E-13	6.09675E-08	6.37471E-08
N	1.10819E-11	1.56783E-06	8.36049E-07
N2	4.20673E-06	5.94875E-01	-1.23504E-04
N2O	2.66736E-12	3.77371E-07	1.55492E-07
CO2	1.61589E-09	2.26612E-04	0.00000
AR	5.01998E-08	7.10215E-03	0.00000

REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/CM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.1423E 13	-3.99432E 08	0.00124
2	1.0719E 13	6.69686E 07	0.00176
3	1.6545E 13	-1.65224E 09	0.00134
4	5.1965E 12	1.19203E 08	0.00041
5	1.7890E 15	-5.88711E 09	0.61695
6	7.8105E 13	-2.41823E 07	0.75754
7	2.9057E 14	-2.31748E 09	0.75681
8	1.0295E 15	-1.15459E 10	0.75714
9	2.6703E 10	-1.00538E 06	0.36632
10	4.2921E 13	-1.05812E 09	0.10212
11	5.1286E 09	1.32660E 05	0.00052
12	1.7888E 14	-2.91194E 09	0.36546
13	4.1924E 13	-4.16847E 08	0.36625
14	4.1924E 13	-1.44281E 09	0.36599
15	1.8000E 12	1.73740E 04	0.32767
16	7.8901E 12	-4.18384E 04	0.09048
17	9.0032E 12	-2.34246E 05	0.30321
18	6.8943E 15	-2.55018E 07	0.65204
19	2.5210E 14	-1.01708E 07	0.30234
20	6.0786E 12	-1.15155E 07	0.87653
21	2.6379E 08	3.58297E 08	0.99249
22	4.0000E 13	-2.13081E 08	0.87668
23	1.6935E 10	-1.27166E 06	0.71992
24	8.2875E 11	-1.02020E 05	0.13434
25	6.6590E 11	-2.77321E 05	0.99920
26	3.4986E 10	-6.90774E-03	0.50063

DISTANCE-PRESSURE VERSION GENERAL CHEMICAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

GCKP84 HYD - OXYGEN CASE WITH HEAT TRANSFER CASE 6

REACTION NUMBER	REACTION	A	N	ACTIVATION ENERGY
1	1.0*H + 1.0*O2 = 1.0*OH + 1.0*O	2.20000E 14	0.0000	16790.00
2	1.0*O + 1.0*H2 = 1.0*OH + 1.0*H	1.80000E 10	1.0000	8900.00
3	1.0*H2 + 1.0*OH = 1.0*H2O + 1.0*H	5.20000E 13	0.0000	6500.00
4	1.0*OH + 1.0*OH = 1.0*O + 1.0*H2O	6.30000E 12	0.0000	1093.00
5	1.0*H + 1.0*O2 = 1.0*HO2 + M	1.50000E 15	0.0000	-1000.00
6	1.0*O + 1.0*O + M	5.70000E 13	0.0000	-1788.00
7	1.0*H + 1.0*H + M	8.30000E 17	-1.0000	0.00
8	1.0*H + 1.0*OH + M	8.40000E 21	-2.0000	0.00
9	1.0*H2 + 1.0*HO2 = 1.0*H2O + 1.0*OH	7.20000E 11	0.0000	18700.00
10	M + 1.0*H2O2 = 2.0*OH	1.30000E 17	0.0000	45500.00
11	1.0*H2 + 1.0*O2 = 2.0*OH	1.00000E 13	0.0000	43000.00
12	1.0*H + 1.0*HO2 = 1.0*OH + 1.0*OH	2.50000E 14	0.0000	1900.00
13	1.0*O + 1.0*HO2 = 1.0*OH + 1.0*O2	5.00000E 13	0.0000	1000.00
14	1.0*OH + 1.0*HO2 = 1.0*H2O + 1.0*O2	5.00000E 13	0.0000	1000.00
15	2.0*HO2 = 1.0*H2O2 + 1.0*O2	1.80000E 12	0.0000	0.00
16	1.0*OH + 1.0*H2O2 = 1.0*H2O + 1.0*HO2	1.00000E 13	0.0000	1800.00
17	1.0*O + 1.0*H2O2 = 1.0*OH + 1.0*HO2	8.00000E 13	0.0000	1000.00
18	1.0*H + 1.0*H2O2 = 1.0*H2O + 1.0*OH	3.20000E 14	0.0000	9000.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2 , 5) =	5.00000	M(H2 , 7) =	5.00000	M(H2 , 8) =	4.00000	M(H2 , 10) =	2.30000
M(O2 , 5) =	2.00000	M(O2 , 7) =	2.00000	M(O2 , 8) =	1.60000	M(O2 , 10) =	0.78000
M(H2O , 5) =	32.50000	M(H2O , 7) =	15.00000	M(H2O , 8) =	20.00000	M(H2O , 10) =	6.00000
M(H2O2 , 10) =	6.60000						

INTEGRATION CONTROLS

INITIAL STEP SIZE 0.10000E-05 CM MAXIMUM RELATIVE ERROR 0.10000E-05

** ASSIGNED VARIABLE PROFILE **

THE PRESSURE IS CALCULATED FROM THE FOLLOWING POLYNOMIAL

PRESSURE (ATM) = (0.00000)X**3 + (0.00000)X**2 + (1.00000E-02)X + (5.00000E 00)

AIR - FUEL COMBUSTION, EQUIVALENCE RATIO = 1.0000 OXYGEN FRACTION IN AIR = 1.0000

HEAT TRANSFER CASE QDOT (CAL/CM-SEC) =(0.00000)T**2 + (5.86300E 00)T + (-4.28800E 01)

** INITIAL CONDITIONS **

TIME 0.00000 SEC AREA 2.15278E 00 SQ FT AXIAL POSITION 0.00000 FT

FLOW PROPERTIES

PRESSURE (LB/FT**2)	1.05810E 04
VELOCITY (FT/SEC)	1.64424E 03
DENSITY (LB/FT**3)	4.24984E-02
TEMPERATURE (DEG R)	1.93500E 03
MASS FLOW RATE (LB/SEC)	1.50427E 02
ENTROPY BTU/LB/DEG R)	3.70382E 00
MACH NUMBER	5.00000E-01
GAMMA	1.34995E 00
ENTHALPY (BTU/LB)	8.50740E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

HEAT LOSS(QDOT/MDOT) = 5.0334E 00 BTU/(LB-FT)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/FT**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/FT**3/SEC)
H	0.00000	0.00000	1.99062E-12
O2	1.17957E-03	3.33333E-01	-8.07404E-04
OH	0.00000	0.00000	1.61481E-03
O	0.00000	0.00000	3.38739E-16
H2	2.35914E-03	6.66667E-01	-8.07404E-04
H2O	0.00000	0.00000	0.00000
HO2	0.00000	0.00000	0.00000
H2O2	0.00000	0.00000	0.00000

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-FT**3/LB**2/SEC)	NET RATE/POSITIVE DIR RATE
1	8.4914E 10	0.00000	0.00000
2	3.0012E 11	0.00000	0.00000
3	2.4805E 12	0.00000	0.00000
4	3.7769E 12	0.00000	0.00000
5	2.3955E 15	0.00000	0.00000
6	1.3164E 14	-9.37754E-14	1.00000
7	7.7209E 14	-5.51077E-10	1.00000
8	7.2688E 15	0.00000	0.00000
9	1.1365E 08	0.00000	0.00000
10	7.3064E 07	0.00000	0.00000
11	1.8114E 06	4.47038E-01	1.00000
12	1.0272E 14	0.00000	0.00000
13	3.1309E 13	0.00000	0.00000
14	3.1309E 13	0.00000	0.00000
15	1.8000E 12	0.00000	0.00000
16	4.3058E 12	0.00000	0.00000
17	5.0096E 13	0.00000	0.00000
18	4.7362E 12	0.00000	0.00000

MIXTURE MOLECULAR WEIGHT 12.00960 TOTAL ENERGY EXCHANGE RATE (BTU-FT**3/LB**2/SEC) 1.49962E 04 MASS FRACTION SUM 0.99999994

NEGATIVE CONCENTRATIONS-HALVE STEP SIZE -SAVE1(8) = -0.39213875D-14
NEGATIVE CONCENTRATIONS-HALVE STEP SIZE -SAVE1(8) = -0.43733928D-15
NEGATIVE CONCENTRATIONS-HALVE STEP SIZE -SAVE1(8) = -0.42137914D-16

TIME 4.90488E-04 SEC AREA 2.71149E 00 SQ FT AXIAL POSITION 7.48368E-01 FT

FLOW PROPERTIES

PRESSURE (LB/FT**2)	1.10637E 04
VELOCITY (FT/SEC)	1.40721E 03
DENSITY (LB/FT**3)	3.94251E-02
TEMPERATURE (DEG R)	2.20339E 03
MASS FLOW RATE (LB/SEC)	1.50427E 02
ENTROPY BTU/LB/DEG R)	3.77720E 00
MACH NUMBER	4.04876E-01
GAMMA	1.33789E 00
ENTHALPY (BTU/LB)	8.61375E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	71
AVERAGE STEP SIZE	0.39577E-01
TOTAL NUMBER OF STEPS	114
FUNCT EVALUATIONS	126
JACOBIAN EVALUATIONS	35

HEAT LOSS(QDOT/MDOT) = 5.7363E 00 BTU/(LB-FT)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/FT**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/FT**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-FT**3/LB**2/SEC)	NET RATE/POSITIVE DIR RATE
H	5.96086E-06	1.21892E-03	1.49841E 01	1	2.2119E 11	9.48486E 03	0.99498
O2	1.05585E-03	3.24930E-01	-4.70496E 01	2	5.6767E 11	6.68943E 03	0.99757
OH	7.24939E-07	2.23094E-04	2.76186E 00	3	3.5934E 12	5.68052E 04	0.99848
O	5.40886E-07	1.66453E-04	2.17610E 00	4	4.0197E 12	8.20010E 00	0.37667
H2	2.11924E-03	6.52179E-01	-9.87117E 01	5	2.2627E 15	2.30527E 04	0.99994
H2O	6.27524E-05	1.93116E-02	9.12121E 01	6	1.1888E 14	1.86550E-02	1.00000
HO2	4.41892E-06	1.35989E-03	6.15606E-01	7	6.7805E 14	2.39874E 01	1.00000
H2O2	1.98698E-06	6.11479E-04	-1.64121E 00	8	5.6059E 15	3.03782E 01	1.00000
				9	3.3011E 08	3.18582E 01	1.00000
				10	9.7824E 08	1.18098E 02	0.96699
				11	2.1031E 05	4.84940E 00	0.99999
				12	1.1448E 14	2.06483E 04	1.00000
				13	3.3146E 13	8.16423E 02	1.00000
				14	3.3146E 13	1.09424E 03	1.00000
				15	1.8000E 12	3.61895E 02	0.99912
				16	4.7712E 12	7.08088E 01	0.99977
				17	5.3034E 13	5.87152E 02	0.99962
				18	7.9123E 12	6.41726E 02	1.00000

MIXTURE MOLECULAR WEIGHT 12.13275 TOTAL ENERGY EXCHANGE RATE (BTU-FT**3/LB**2/SEC) -4.96293E 09 MASS FRACTION SUM 0.99999923

TIME 4.91182E-04 SEC AREA 5.32857E 00 SQ FT AXIAL POSITION 7.49344E-01 FT

FLOW PROPERTIES

PRESSURE (LB/FT**2)	1.10643E 04
VELOCITY (FT/SEC)	1.40675E 03
DENSITY (LB/FT**3)	2.00683E-02
TEMPERATURE (DEG R)	4.82030E 03
MASS FLOW RATE (LB/SEC)	1.50427E 02
ENTROPY BTU/LB/DEG R)	4.25434E 00
MACH NUMBER	2.98812E-01
GAMMA	1.24937E 00
ENTHALPY (BTU/LB)	8.61386E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	61
AVERAGE STEP SIZE	8.16409E-03
TOTAL NUMBER OF STEPS	199
FUNCT EVALUATIONS	253
JACOBIAN EVALUATIONS	48

HEAT LOSS(QDOT/MDOT) = 1.2590E 01 BTU/(LB-FT)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/FT**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/FT**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-FT**3/LB**2/SEC)	NET RATE/POSITIVE DIR RATE
H	2.19428E-04	7.67717E-01	-5.01000E 02	1	9.3794E 12	1.72522E 04	0.00216
O2	9.74220E-05	6.55836E-02	-1.80957E 02	2	9.0519E 12	1.84872E 05	0.02358
OH	1.53992E-04	1.03666E-01	2.25529E 02	3	1.5330E 13	2.23126E 05	0.00951
O	8.71616E-05	5.86764E-02	-1.17606E 02	4	5.1303E 12	-6.97266E 04	0.01421
H2	2.49808E-04	1.68169E-01	-1.18363E 02	5	1.8101E 15	5.49307E 05	0.93169
H2O	6.77286E-04	4.55943E-01	2.57061E 02	6	7.9762E 13	5.71224E 02	0.99611
HO2	3.11634E-07	2.09789E-04	-1.14544E 00	7	3.0994E 14	1.14240E 05	0.99602
H2O2	5.33938E-08	3.59442E-05	-3.89319E-01	8	1.1713E 15	3.80796E 05	0.99686
				9	2.1439E 10	6.26534E 01	0.94384
				10	2.5156E 13	-3.98442E 04	0.12596
				11	3.0955E 09	7.69931E 01	0.02570
				12	1.7494E 14	4.48797E 05	0.94330
				13	4.1434E 13	4.22189E 04	0.94317
				14	4.1434E 13	7.45250E 04	0.94255
				15	1.8000E 12	1.90814E 00	0.27445
				16	7.1302E 12	2.14646E 03	0.92055
				17	6.6295E 13	1.13899E 04	0.92168
				18	5.8973E 13	2.73564E 04	0.99549

MIXTURE MOLECULAR WEIGHT 13.50979 TOTAL ENERGY EXCHANGE RATE (BTU-FT**3/LB**2/SEC) -2.04909E 11 MASS FRACTION SUM 0.99999446

TIME 4.91295E-04 SEC AREA 5.74169E 00 SQ FT AXIAL POSITION 7.49507E-01 FT

FLOW PROPERTIES

PRESSURE (LB/FT**2)	1.10644E 04
VELOCITY (FT/SEC)	1.40663E 03
DENSITY (LB/FT**3)	1.86260E-02
TEMPERATURE (DEG R)	5.32857E 03
MASS FLOW RATE (LB/SEC)	1.50427E 02
ENTROPY BTU/LB/DEG R)	4.27053E 00
MACH NUMBER	2.89213E-01
GAMMA	1.23759E 00
ENTHALPY (BTU/LB)	8.61390E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	16
AVERAGE STEP SIZE	8.31185E-03
TOTAL NUMBER OF STEPS	215
FUNCT EVALUATIONS	278
JACOBIAN EVALUATIONS	50

HEAT LOSS(QDOT/MDOT) = 1.3921E 01 BTU/(LB-FT)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/FT**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/FT**3/SEC)
H	1.64226E-04	1.22211E-01	-2.39616E 02
O2	7.98408E-05	5.94148E-02	-5.97115E 01
OH	1.56151E-04	1.16203E-01	6.34101E 01
O	6.96923E-05	5.18627E-02	-7.61195E 01
H2	2.25701E-04	1.67959E-01	-4.45877E 01
H2O	6.47924E-04	4.82163E-01	1.32966E 02
HO2	2.25030E-07	1.67460E-04	-2.82974E-01
H2O2	2.43051E-08	1.95754E-05	-1.33918E-01

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-FT**3/LB**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.2673E 13	-6.47036E 04	0.00836
2	1.1737E 13	8.66527E 04	0.01017
3	1.7224E 13	1.02902E 05	0.00367
4	5.2318E 12	-3.86431E 04	0.00652
5	1.7779E 15	3.15323E 05	0.80442
6	7.7246E 13	3.57713E 02	0.95937
7	2.8037E 14	6.10996E 04	0.95861
8	9.5852E 14	2.50616E 05	0.95576
9	2.9976E 10	5.54981E 01	0.78951
10	5.6865E 13	-1.84871E 04	0.05221
11	6.6906E 09	1.00731E 01	0.00181
12	1.8108E 14	2.43584E 05	0.78873
13	4.2184E 13	2.41456E 04	0.79050
14	4.2184E 13	5.40062E 04	0.78913
15	1.8000E 12	-1.00266E-01	0.02327
16	7.3640E 12	1.10893E 03	0.79603
17	6.7494E 13	4.54389E 03	0.79538
18	6.9297E 13	1.32202E 04	0.95649

MIXTURE MOLECULAR WEIGHT 13.86086 TOTAL ENERGY EXCHANGE RATE (BTU-FT**3/LB**2/SEC) -1.25069E 11 MASS FRACTION SUM 0.99999374

(GCKP) END OF THIS CASE - READ DATA FOR NEXT CASE

TIME-PRESSURE VERSION GENERAL CHEMICAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

GCKP84 CH4 - AIR RICH MECH. BATCH RXN WITH OTTO CYCLE HEAT LOSS - CASE 5

REACTION NUMBER	REACTION	REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1.0*CH4 = 1.0*CH3 + 1.0*H	2.00000E 15	0.0000	104000.00
2	1.0*H + 1.0*CH4 = 1.0*CH3 + 1.0*H2	1.26000E 14	0.0000	11900.00
3	1.0*O + 1.0*CH4 = 1.0*CH3 + 1.0*OH	2.00000E 13	0.0000	9200.00
4	1.0*OH + 1.0*CH4 = 1.0*CH3 + 1.0*H2O	3.00000E 13	0.0000	6000.00
5	1.0*CH + 1.0*O2 = 1.0*HCO + 1.0*O	1.00000E 13	0.0000	0.00
6	1.0*CH2 + 1.0*O2 = 1.0*CH2O + 1.0*O	1.00000E 14	0.0000	3700.00
7	1.0*CH3 + 1.0*O2 = 1.0*CH2O + 1.0*OH	1.70000E 12	0.0000	14000.00
8	1.0*CH3 + 1.0*O = 1.0*CH2O + 1.0*H	6.80000E 13	0.0000	0.00
9	1.0*CH2G + 1.0*H = 1.0*HCO + 1.0*H2	2.00000E 13	0.0000	3300.00
10	1.0*CH2O + 1.0*O = 1.0*HCO + 1.0*OH	5.00000E 13	0.0000	4570.00
11	1.0*CH2O + 1.0*OH = 1.0*HCO + 1.0*H2O	5.00000E 15	0.0000	13000.00
12	M + 1.0*CH2O = 1.0*HCO + 1.0*H	5.00000E 16	0.0000	72000.00
13	1.0*O + 1.0*HCO = 1.0*H + 1.0*CO2	5.30000E 13	0.0000	0.00
14	1.0*HCO + 1.0*O = 1.0*CO + 1.0*OH	3.00000E 13	0.0000	0.00
15	1.0*HCO + 1.0*H = 1.0*CO + 1.0*H2	2.00000E 13	0.0000	0.00
16	1.0*HCO + 1.0*OH = 1.0*CO + 1.0*H2O	3.00000E 13	0.0000	0.00
17	M + 1.0*HCO = 1.0*H + 1.0*CO	3.00000E 14	0.0000	14700.00
18	1.0*CO + 1.0*OH = 1.0*CO2 + 1.0*H	4.00000E 12	0.0000	8000.00
19	1.0*CO + 1.0*O = 1.0*CO2 + M	2.80000E 13	0.0000	-4540.00
20	1.0*CO + 1.0*O2 = 1.0*CO2 + 1.0*O	1.20000E 11	0.0000	35000.00
21	1.0*H + 1.0*O2 = 1.0*OH + 1.0*O	2.20000E 14	0.0000	16790.00
22	1.0*O + 1.0*H2 = 1.0*OH + 1.0*H	1.80000E 10	1.0000	8900.00
23	1.0*H2 + 1.0*OH = 1.0*H2O + 1.0*H	5.20000E 13	0.0000	6500.00
24	1.0*OH + 1.0*OH = 1.0*O + 1.0*H2O	6.30000E 12	0.0000	1093.00
25	1.0*H + 1.0*O2 = 1.0*HO2 + M	1.50000E 15	0.0000	-1000.00
26	1.0*O + 1.0*O = 1.0*O2 + M	5.70000E 13	0.0000	-1788.00
27	1.0*H + 1.0*H = 1.0*H2 + M	8.30000E 17	-1.0000	0.00
28	1.0*H + 1.0*OH = 1.0*H2O + M	8.40000E 21	-2.0000	0.00
29	1.0*O + 1.0*H = 1.0*OH + M	6.20000E 16	-0.6000	0.00
30	1.0*H + 1.0*CH3 = 1.0*H2 + 1.0*CH2	2.70000E 11	0.6700	25700.00
31	1.0*O + 1.0*CH3 = 1.0*OH + 1.0*CH2	1.90000E 11	0.6800	25700.00
32	1.0*OH + 1.0*CH3 = 1.0*H2O + 1.0*CH2	2.70000E 11	0.6700	25700.00
33	1.0*HO2 + 1.0*NO = 1.0*NO2 + 1.0*OH	1.20000E 13	0.0000	2380.00
34	1.0*O + 1.0*NO2 = 1.0*NO + 1.0*O2	1.00000E 13	0.0000	596.00
35	1.0*NO + 1.0*O + M = 1.0*NO2 + M	5.62000E 15	0.0000	-1160.00
36	1.0*NO2 + 1.0*H = 1.0*NO + 1.0*OH	2.90000E 14	0.0000	795.00
37	1.0*H + 1.0*O2 = 1.0*NO + 1.0*O	6.40000E 09	1.0000	6250.00
38	1.0*O + 1.0*N2 = 1.0*NO + 1.0*N	1.80000E 14	0.0000	76250.00
39	1.0*N + 1.0*OH = 1.0*NO + 1.0*H	4.00000E 13	0.0000	0.00
40	1.0*CH + 1.0*N2 = 1.0*HCN + 1.0*N	1.50000E 11	0.0000	19000.00
41	1.0*CN + 1.0*H2 = 1.0*HCN + 1.0*H	6.00000E 13	0.0000	5300.00
42	1.0*O + 1.0*HCN = 1.0*H + 1.0*NCO	5.20000E 12	0.6800	8100.00
43	1.0*OH + 1.0*HCN = 1.0*HNCO + 1.0*H	4.00000E 11	0.0000	2800.00
44	1.0*CN + 1.0*O = 1.0*CO + 1.0*N	1.20000E 13	0.0000	0.00
45	1.0*CN + 1.0*OH = 1.0*NCO + 1.0*H	2.50000E 14	0.0000	6000.00
46	1.0*CN + 1.0*O2 = 1.0*NCO + 1.0*O	3.20000E 13	0.0000	1000.00
47	1.0*CN + 1.0*CO2 = 1.0*NCO + 1.0*CO	3.70000E 12	0.0000	0.00
48	1.0*O + 1.0*NCO = 1.0*NO + 1.0*CO	2.00000E 13	0.0000	0.00
49	1.0*N + 1.0*NCO = 1.0*N2 + 1.0*CO	1.00000E 13	0.0000	0.00
50	1.0*H + 1.0*NCO = 1.0*NH + 1.0*CO	2.00000E 13	0.0000	0.00
51	1.0*H2 + 1.0*NCO = 1.0*HNCO + 1.0*H	1.00000E 14	0.0000	9000.00
52	1.0*HNCO + 1.0*H = 1.0*NH2 + 1.0*CO	1.00000E 14	0.0000	8500.00
53	1.0*NH + 1.0*OH = 1.0*N + 1.0*H2O	5.00000E 11	0.5000	1999.00
54	1.0*CH + 1.0*CO2 = 1.0*HCO + 1.0*CO	3.70000E 12	0.0000	0.00
55	1.0*CH + 1.0*NO = 1.0*N + 1.0*HCO	1.00000E 14	0.0000	0.00
56	1.0*CH + 1.0*NO = 1.0*O + 1.0*HCN	1.00000E 13	0.0000	0.00
57	1.0*H + 1.0*CH2 = 1.0*H2 + 1.0*CH	2.90000E 11	0.7000	26000.00
58	1.0*O + 1.0*CH2 = 1.0*H + 1.0*CH	3.20000E 11	0.5000	26000.00
59	1.0*OH + 1.0*CH2 = 1.0*H2O + 1.0*CH	5.00000E 11	0.5000	6000.00
60	1.0*H + 1.0*HO2 = 1.0*OH + 1.0*OH	1.40000E 14	0.0000	1070.00
61	1.0*H + 1.0*HO2 = 1.0*O + 1.0*H2O	1.00000E 13	0.0000	1000.00
62	1.0*O + 1.0*HO2 = 1.0*OH + 1.0*O2	1.60000E 13	0.0000	1070.00

63	1.0*OH	+ 1.0*HO2	= 1.0*H2O	+ 1.0*O2	7.90000E 12	0.0000	0.00
64	1.0*CH3	+ 1.0*OH	= 1.0*CH2O	+ 1.0*H2	7.44000E 12	0.0000	0.00
65	1.0*H2	+ 1.0*HO2	= 1.0*H2O	+ 1.0*OH	7.20000E 11	0.0000	18700.00
66	1.0*HCO	+ 1.0*O2	= 1.0*CO	+ 1.0*HO2	3.00000E 13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(O2	, 25) = 2.00000	M(O2	, 28) = 1.60000	M(N2	, 25) = 2.00000	M(N2	, 28) = 1.60000
M(H2O	, 25) = 32.50000	M(H2O	, 28) = 20.00000	M(CO2	, 25) = 7.50000	M(CO2	, 28) = 7.50000
M(CO	, 25) = 2.00000	M(CO	, 28) = 1.60000	M(CH4	, 25) = 5.00000	M(H2	, 25) = 5.00000

INTEGRATION CONTROLS

INITIAL STEP SIZE 0.10000E-09 SEC

MAXIMUM RELATIVE ERROR 0.50000E-04

** ASSIGNED VARIABLE PROFILE **

THE PRESSU' IS CALCULATED FROM THE FOLLOWING POLYNOMIAL

PRESSURE (ATM) = (0.00000)T**3 + (0.00000)T**2 + (7.00000E 02)T + (2.00000E 00)

HEAT TRANSFER CASE WALL TEMPERATURE = 1000.00 QDOT COMPUTED FROM TRANSPORT PROP. DATA

** INITIAL CONDITIONS **

TIME 0.00000 SEC AREA 0.00000 SQ CM AXIAL POSITION 0.00000 CM

FLOW PROPERTIES

PRESSURE (ATM)	2.00000
VELOCITY (CM/SEC)	0.00
DENSITY (GM/CM**3)	4.29913E-04
TEMPERATURE (DEG K)	1510.00
MASS FLOW RATE (GM/SEC)	0.00000
ENTROPY CAL/GM/DEG K)	2.2698
MACH NUMBER	0.0000
GAMMA	1.2327
ENTHALPY (CAL/GM)	2.97501E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

HEAT LOSS(QDOT/TOTMAS) = 7.0612E 01 CAL/(G-SEC)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	2.78440E-06	1.72503E-01	-4.93543E-06
CH3	0.00000	0.00000	4.93543E-06
H	0.00000	0.00000	4.93543E-06
H2	0.00000	0.00000	0.00000
O	0.00000	0.00000	3.74268E-02
OH	0.00000	0.00000	0.00000
H2O	0.00000	0.00000	0.00000
CH	4.84244E-10	3.00006E-05	-1.34844E-02
O2	2.78440E-06	1.72503E-01	-3.74268E-02
HCO	0.00000	0.00000	1.34833E-02
CH2	1.61415E-10	1.00002E-05	-1.30965E-02
CH2O	0.00000	0.00000	1.30965E-02
CO2	0.00000	0.00000	0.00000
CO	0.00000	0.00000	0.00000
HO2	0.00000	0.00000	0.00000
NO	0.00000	0.00000	5.41051E-04
NO2	0.00000	0.00000	0.00000
N	1.61415E-10	1.00002E-05	-5.39685E-04
N2	1.05714E-05	6.54933E-01	-1.36560E-06
HCN	0.00000	0.00000	1.36560E-06
CN	1.61415E-10	1.00002E-05	-1.03060E-02
NCO	0.00000	0.00000	1.03060E-02
HNCO	0.00000	0.00000	0.00000
NH	0.00000	0.00000	0.00000
NH2	0.00000	0.00000	0.00000

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.7725E 00	2.67032E 01	1.00000
2	2.3879E 12	0.00000	0.00000
3	9.3211E 11	0.00000	0.00000
4	4.0617E 12	0.00000	0.00000
5	1.0000E 13	7.29515E 04	1.00000
6	2.9139E 13	7.08588E 04	1.00000
7	1.6001E 10	0.00000	0.00000
8	6.8000E 13	0.00000	0.00000
9	6.6589E 12	0.00000	0.00000
10	1.0903E 13	0.00000	0.00000
11	6.5677E 13	0.00000	0.00000
12	1.8970E 06	0.00000	0.00000
13	5.3000E 13	0.00000	0.00000
14	3.0000E 13	0.00000	0.00000
15	2.0000E 13	0.00000	0.00000
16	3.0000E 13	0.00000	0.00000
17	2.2362E 12	0.00000	0.00000
18	2.7809E 11	0.00000	0.00000
19	1.2713E 14	0.00000	0.00000
20	1.0315E 06	0.00000	0.00000
21	8.1719E 11	0.00000	0.00000
22	1.3999E 12	0.00000	0.00000
23	5.9597E 12	0.00000	0.00000
24	4.3767E 12	0.00000	0.00000
25	2.0933E 15	0.00000	0.00000
26	1.0343E 14	-4.31634E-06	0.00000
27	5.4967E 14	0.00000	1.00000
28	3.6849E 15	0.00000	0.00000
29	7.6737E 14	0.00000	0.00000
30	6.9437E 09	0.00000	0.00000
31	5.2574E 09	0.00000	0.00000
32	6.9437E 09	0.00000	0.00000
33	5.4289E 12	0.00000	0.00000
34	8.1986E 12	0.00000	0.00000
35	8.2723E 15	0.00000	0.00000

36	2.2250E 14	0.00000	0.00000
37	1.2038E 12	2.92737E 03	1.00000
38	1.6567E 03	0.00000	0.00000
39	4.0000E 13	0.00000	0.00000
40	2.6676E 08	7.38858E 00	1.00000
41	1.0258E 13	0.00000	0.00000
42	5.0740E 13	0.00000	0.00000
43	1.5733E 11	0.00000	0.00000
44	1.2000E 13	0.00000	0.00000
45	3.3848E 13	0.00000	0.00000
46	2.2931E 13	5.57607E 04	1.00000
47	3.7000E 12	0.00000	0.00000
48	2.0000E 13	0.00000	0.00000
49	1.0000E 13	0.00000	0.00000
50	2.0000E 13	0.00000	0.00000
51	4.9818E 12	0.00000	0.00000
52	5.8851E 12	0.00000	0.00000
53	9.9801E 12	0.00000	0.00000
54	3.7000E 12	0.00000	0.00000
55	1.0000E 14	0.00000	0.00000
56	1.0000E 13	0.00000	0.00000
57	8.4057E 09	0.00000	0.00000
58	2.1455E 09	0.00000	0.00000
59	2.6306E 12	0.00000	0.00000
60	9.8008E 13	0.00000	0.00000
61	7.1658E 12	0.00000	0.00000
62	1.1201E 13	0.00000	0.00000
63	7.9000E 12	0.00000	0.00000
64	7.6000E 12	0.00000	0.00000
65	1.6151E 09	0.00000	0.00000
66	3.0000E 13	0.00000	0.00000

MIXTURE MOLECULAR WEIGHT 26.63463 TOTAL ENERGY EXCHANGE RATE -9.98687E 09 (CAL-CM**3/GM**2/SEC) MASS FRACTION SUM 0.99999982

NEGATIVE CONCENTRATIONS-HALVE STEP SIZE -SAVE1(25) = -0.12544309D-26
REYNOLDS NUMBER =4.5118E 03 PRANDTL NUMBER = 0.744 HEAT TRANSFER COEFF = 5.05942E-04
REYNOLDS NUMBER =4.5113E 03 PRANDTL NUMBER = 0.744 HEAT TRANSFER COEFF = 5.05919E-04
REYNOLDS NUMBER =4.5109E 03 PRANDTL NUMBER = 0.744 HEAT TRANSFER COEFF = 5.05905E-04
NEGATIVE CONCENTRATIONS-HALVE STEP SIZE -SAVE1(11) = -0.3443530ZD-12
REYNOLDS NUMBER =4.5108E 03 PRANDTL NUMBER = 0.744 HEAT TRANSFER COEFF = 5.05903E-04

PREDICTOR TROUBLE FOR Y11, VALUE = -0.13979163026021O6D-12, T= 0.220506037152793D-06, H= 0.1418886923900657D-07

CUT STEP SIZE BY 0.600000040 00
REYNOLDS NUMBER =4.5108E 03 PRANDTL NUMBER = 0.744 HEAT TRANSFER COEFF = 5.05908E-04

TIME 5.00000E-04 SEC AREA 0.00000 SQ CM AXIAL POSITION 0.00000 CM

FLOW PROPERTIES

PRESSURE (ATM)	2.35000
VELOCITY (CM/SEC)	0.00
DENSITY (GM/CM**3)	4.48773E-04
TEMPERATURE (DEG K)	1687.05
MASS FLOW RATE (GM/SEC)	0.00000
ENTROPY (CAL/GM/DEG K)	2.3277
MACH NUMBER	0.0000
GAMMA	1.2293
ENTHALPY (CAL/GM)	3.16291E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	29
AVERAGE STEP SIZE	0.15517E-04
TOTAL NUMBER OF STEPS	155
FUNCT EVALUATIONS	275
JACOBIAN EVALUATIONS	45

HEAT LOSS(QDOT/TOTMAS) = 9.6645E 01 CAL/(G-SEC)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	2.56877E-06	1.51321E-01	-3.54537E-03
CH3	4.05068E-08	2.38617E-03	5.86365E-04
H	1.72309E-10	1.01504E-05	6.62502E-07
H2	8.09474E-08	4.76844E-03	1.26350E-03
O	8.12279E-11	4.78497E-06	1.92748E-06
OH	1.78792E-10	1.05323E-05	2.91970E-06
H2O	3.89164E-07	2.29248E-02	4.71867E-03
CH	9.06528E-20	5.32839E-15	-2.38835E-14
O2	2.53523E-06	1.49345E-01	-3.99597E-03
HCO	1.99950E-11	1.17786E-06	5.34602E-07
CH2	3.67055E-15	2.16225E-10	-1.41580E-09
CH2O	1.31262E-07	7.73236E-03	1.72563E-06
CO2	5.17715E-10	3.04976E-05	1.25226E-05
CO	1.66160E-07	9.78818E-03	2.77357E-03
HO2	2.71427E-08	1.59892E-03	1.48667E-04
NO	3.64580E-11	2.14767E-06	4.78925E-07
NO2	1.34065E-10	7.89752E-06	-4.76895E-07
N	4.47839E-16	2.63813E-11	8.01511E-12
N2	1.10351E-05	6.50057E-01	-2.08886E-11
HCN	5.24166E-12	3.08775E-07	-2.68385E-08
CN	2.04252E-16	1.20320E-11	-1.54467E-09
NCO	6.52115E-14	3.84148E-09	2.12189E-08
HNCO	1.49042E-10	8.77979E-06	-1.69135E-07
NH	9.34344E-13	5.50403E-08	-1.72661E-09
NH2	1.09009E-11	6.42152E-07	1.76030E-07

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	6.7363E 01	8.17290E 01	0.09515
2	3.6206E 12	5.57720E 03	0.70890
3	1.2859E 12	1.33080E 03	0.97890
4	5.0101E 12	1.06141E 04	0.92900
5	1.0000E 13	1.13863E-05	1.00000
6	3.3165E 13	1.53208E 00	0.99978
7	2.6110E 10	1.33138E 04	1.00000
8	6.8000E 13	1.11093E 03	1.00000
9	7.4736E 12	8.39253E 02	0.99993
10	1.2792E 13	6.77230E 02	1.00000
11	1.0349E 14	1.20588E 04	0.99998
12	2.3534E 07	2.60324E 02	0.99980
13	5.3000E 13	4.27414E-01	1.00000
14	3.0000E 13	2.41932E-01	1.00000
15	2.0000E 13	3.42123E-01	0.99995
16	3.0000E 13	5.32513E-01	0.99999
17	3.7394E 12	6.30124E 03	0.99984
18	3.6787E 11	5.42367E 01	0.99949
19	1.0847E 14	1.23396E-01	1.00000
20	3.5082E 06	7.33799E 00	1.00000
21	1.4701E 12	3.18785E 03	0.99971
22	2.1352E 12	6.94550E 01	0.99633
23	7.4810E 12	4.09987E 02	0.76263
24	4.5472E 12	-4.59852E 01	0.98455
25	2.0213E 15	-3.88229E 03	0.94295
26	9.7163E 13	-1.70362E-04	0.75920
27	4.9198E 14	8.24245E-04	0.66945
28	2.9514E 15	1.35693E-02	0.92154
29	7.1798E 14	8.46007E-04	0.99879
30	1.8375E 10	6.36774E-01	0.99997
31	1.3928E 10	2.27540E-01	1.00000

32	1.8375E 10	6.60748E-01	0.99999
33	5.9001E 12	2.80763E 01	0.96847
34	8.3713E 12	4.51653E-01	0.99781
35	7.9434E 15	-3.75159E 00	0.99947
36	2.2878E 14	2.62410E 01	1.00000
37	1.6736E 12	9.43445E-03	0.99996
38	2.3867E 04	1.83718E-04	0.97723
39	4.0000E 13	1.37585E-05	0.86516
40	5.1867E 08	2.45232E-09	0.95434
41	1.2347E 13	2.11524E-06	0.20868
42	7.2632E 13	1.43504E-01	0.93457
43	1.7351E 11	-1.00389E-02	0.92550
44	1.2000E 13	9.88547E-07	1.00000
45	4.1751E 13	-9.92898E-05	0.92915
46	2.3747E 13	6.08051E-02	0.99588
47	3.7000E 12	-5.32486E-02	0.99996
48	2.0000E 13	5.26024E-04	1.00000
49	1.0000E 13	1.45008E-09	1.00000
50	2.0000E 13	8.10166E-04	0.72605
51	6.8248E 12	4.42668E-02	0.24747
52	7.9225E 12	8.74043E-01	0.86518
53	1.1313E 13	9.38330E-03	0.99996
54	3.7000E 12	-2.50165E-08	0.96675
55	1.0000E 14	1.44934E-09	0.88513
56	1.0000E 13	-1.64600E-10	0.50131
57	2.2553E 10	7.05996E-08	0.99681
58	5.6303E 09	8.33503E-09	0.99999
59	3.4297E 12	1.11675E-05	0.99924
60	1.0175E 14	2.36277E 03	1.00000
61	7.4209E 12	1.72330E 02	1.00000
62	1.1628E 13	1.27286E 02	0.99993
63	7.9000E 12	1.89507E 02	0.99552
64	7.4000E 12	2.66098E 02	0.99998
65	2.7216E 09	2.96915E 01	1.00000
66	5.0000E 13	7.53013E 03	0.99723

MIXTURE MOLECULAR WEIGHT 26.43633 TOTAL ENERGY EXCHANGE RATE -1.32969E 09 (CAL-CM**3/GM**2/SEC) MASS FRACTION SUM 0.99999946

REYNOLDS NUMBER =4.3404E 03 PRANDTL NUMBER = 0.748 HEAT TRANSFER COEFF = 5.29748E-04

NEGATIVE CONCENTRATIONS-HALVE STEP SIZE -SAVE1(22) = -0.52349265D-09

PREDICTOR TROUBLE FOR Y22, VALUE = -0.10792186684412940-09, T= 0.5446190425367490-03, H= 0.5413326398601751D-05

CUT STEP SIZE BY 0.70000004D 00

TIME 5.58000E-04 SEC AREA 0.00000 SQ CM AXIAL POSITION 0.00000 CM

FLOW PROPERTIES

PRESSURE (ATM)	2.38500
VELOCITY (CM/SEC)	0.00
DENSITY (GM/CM**3)	4.12732E-04
TEMPERATURE (DEG K)	1836.57
MASS FLOW RATE (GM/SEC)	0.00000
ENTROPY CAL/GM/DEG K)	2.3890
MACH NUMBER	0.0000
GAMMA	1.2301
ENTHALPY (CAL/GM)	3.18235E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	7
AVERAGE STEP SIZE	0.71429E-05
TOTAL NUMBER OF STEPS	162
FUNCT EVALUATIONS	291
JACOBIAN EVALUATIONS	46

HEAT LOSS(QDOT/TOTMAS) = 1.2216E 02 CAL/(G-SEC)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	2.04758E-06	1.29375E-01	-1.23162E-02
CH3	9.76333E-03	6.16891E-03	2.56683E-03
H	8.93043E-10	5.64264E-05	4.77694E-05
H2	1.99517E-07	1.26063E-02	5.38070E-03
O	3.23668E-10	2.04508E-05	1.38310E-05
OH	6.50919E-10	4.11280E-05	2.70814E-05
H2O	7.90905E-07	4.99729E-02	1.67298E-02
CH	1.19378E-17	7.54203E-13	1.90276E-12
O2	1.98909E-06	1.25679E-01	-1.29062E-02
HCO	7.57368E-11	4.78539E-06	2.04395E-06
CH2	8.77610E-14	5.54513E-09	9.63102E-09
CH2O	1.02560E-07	6.48019E-03	-1.15816E-03
CO2	2.65960E-09	1.68046E-06	1.31257E-06
CO	4.23272E-07	2.67442E-02	1.07749E-02
HO2	2.23139E-08	1.40989E-03	-4.18240E-04
NO	9.35493E-11	5.91086E-06	2.54923E-06
NO2	6.36676E-11	4.01016E-06	-2.54143E-06
N	1.51087E-15	9.54635E-11	5.35154E-11
N2	1.01489E-05	6.41252E-01	-4.94815E-10
HCN	5.01933E-12	1.90775E-07	-4.71264E-08
CN	1.11397E-15	7.03855E-11	1.06436E-09
NCO	1.41781E-13	8.95839E-09	-5.00092E-09
HNCO	1.20967E-10	7.64326E-06	-7.06726E-07
NH	7.38661E-13	4.66719E-08	-3.68229E-09
NH2	2.77926E-11	1.75606E-06	7.54594E-07

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	8.4167E 02	-1.17736E 03	0.10425
2	4.8337E 12	2.96556E 04	0.57154
3	1.6078E 12	6.23721E 03	0.99712
4	5.7960E 12	3.75847E 04	0.82881
5	1.0000E 13	1.39393E-03	1.00000
6	3.6283E 13	3.71754E 01	0.99984
7	3.6683E 10	4.18196E 04	1.00000
8	6.8000E 13	1.26145E 04	1.00000
9	8.0972E 12	4.35262E 03	0.99978
10	1.4294E 13	2.78538E 03	1.00000
11	1.4190E 14	5.56050E 04	0.99991
12	1.3522E 08	1.28775E 03	0.99943
13	5.3000E 13	7.62687E 00	1.00000
14	3.0000E 13	4.31709E 00	1.00000
15	2.0000E 13	7.93976E 00	0.99985
16	3.0000E 13	8.68454E 00	0.99994
17	5.3436E 12	3.75862E 04	0.99961
18	4.4675E 11	7.20745E 02	0.99750
19	9.7143E 13	1.23647E 00	0.99999
20	8.2076E 06	4.05653E 01	1.00000
21	2.2102E 12	2.30309E 04	0.99929
22	2.8853E 12	1.08643E 03	0.99328
23	8.7601E 12	4.01005E 03	0.60044
24	4.6695E 12	-6.78871E 02	0.98318
25	1.9728E 15	-1.43969E 04	0.91825
26	9.3035E 13	-2.38160E-03	0.72453
27	4.5193E 14	2.06345E-02	0.61621
28	2.4904E 15	2.76345E-01	0.84665
29	6.8232E 14	1.82764E-02	0.99742
30	3.6336E 10	1.85802E 01	0.99986
31	2.7543E 10	5.10936E 00	1.00000
32	3.6306E 10	1.35438E 01	0.99994

33	6.2512E 12	7.44056E 01	0.97132
34	8.4933E 12	1.01669E 00	0.99265
35	7.7228E 15	-1.07049E 01	0.99797
36	2.3324E 14	7.76031E 01	0.99999
37	2.1205E 12	3.73977E-02	0.99967
38	1.5192E 05	2.90416E-03	0.99136
39	4.0000E 13	1.23362E-04	0.53620
40	8.2266E 08	5.86569E-07	0.99935
41	1.4043E 13	1.36079E-02	0.73179
42	9.3678E 13	3.64592E-01	0.67842
43	1.8572E 11	-7.45356E-02	0.97206
44	1.2000E 13	2.53989E-05	0.99999
45	4.8300E 13	-2.43290E-03	0.99208
46	2.4330E 13	3.13590E-01	0.59088
47	3.7000E 12	-3.30839E-01	0.09981
48	2.0000E 13	5.38781E-03	0.00000
49	1.0000E 13	1.25747E-08	0.00997
50	2.0000E 13	1.33668E-02	0.07783
51	8.4920E 12	3.55533E-01	0.00212
52	9.7389E 12	4.42972E 00	0.00724
53	1.2391E 13	3.49631E-02	0.00172
54	3.7000E 12	-7.79497E-07	0.00059
55	1.0000E 14	6.48100E-07	0.00259
56	1.0000E 13	6.06307E-08	0.00264
57	4.5002E 10	2.05175E-05	0.99996
58	1.1045E 10	1.84170E-06	0.99994
59	4.1398E 12	1.38325E-03	0.99639
60	1.0442E 14	1.22155E 04	0.00000
61	7.6033E 12	8.89424E 02	0.99995
62	1.1936E 13	5.05870E 02	0.99997
63	7.9000E 12	6.65143E 02	0.99874
64	7.4000E 12	2.76062E 03	0.99999
65	4.2860E 09	1.12014E 02	0.00000
66	3.0000E 13	2.64040E 04	0.00793

MIXTURE MOLECULAR WEIGHT 26.07826 TOTAL ENERGY EXCHANGE RATE -5.39206E 09 (CAL-CM**3/GM**2/SEC) MASS FRACTION SUM 1.00000000

REYNOLDS NUMBER =3.8115E 03 PRANDTL NUMBER = 0.744 HEAT TRANSFER COEFF = 5.03061E-04

PREDICTOR TROUBLE FOR Y22, VALUE = -0.6108586336670109D-09, T= 0.5715686683978410-03, H= 0.2105600805852992D-05

CUT STEP SIZE BY 0.50000004D 00
REYNOLDS NUMBER =3.1400E 03 PRANDTL NUMBER = 0.731 HEAT TRANSFER COEFF = 4.64693E-04
REYNOLDS NUMBER =2.9364E 03 PRANDTL NUMBER = 0.723 HEAT TRANSFER COEFF = 4.52526E-04
REYNOLDS NUMBER =2.6134E 03 PRANDTL NUMBER = 0.707 HEAT TRANSFER COEFF = 4.34565E-04
REYNOLDS NUMBER =2.3102E 03 PRANDTL NUMBER = 0.676 HEAT TRANSFER COEFF = 4.17070E-04

TIME 5.85000E-04 SEC AREA 0.00000 SQ CM AXIAL POSITION 0.00000 CM

FLOW PROPERTIES

PRESSURE (ATM)	2.40950
VELOCITY (CM/SEC)	0.00
DENSITY (GM/CM**3)	2.74460E-04
TEMPERATURE (DEG K)	2529.42
MASS FLOW RATE (GM/SEC)	0.00000
ENTROPY (CAL/GM/DEG K)	2.6657
MACH NUMBER	0.0000
GAMMA	1.2542
ENTHALPY (CAL/GM)	3.19861E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	36
AVERAGE STEP SIZE	0.97222E-06
TOTAL NUMBER OF STEPS	198
FUNCT EVALUATIONS	382
JACOBIAN EVALUATIONS	54

HEAT LOSS(QDOT/TOTMAS) = 2.7197E 02 CAL/(G-SEC)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
CH4	1.63436E-07	1.40765E-02	-5.68816E-02	1	2.0658E 06	1.01913E 05	0.02274
CH3	1.97708E-07	1.70283E-02	-3.04038E-02	2	1.1808E 13	5.43189E 05	0.28297
H	7.49297E-08	6.45359E-03	1.27737E-02	3	3.2072E 12	1.64191E 04	0.74417
H2	1.05982E-06	9.12809E-02	1.20732E-01	4	9.0929E 12	9.35930E 04	0.19071
O	3.17079E-09	2.73095E-04	-7.96664E-04	5	1.0000E 13	8.54765E 02	1.00000
OH	2.48765E-08	2.14258E-03	2.87300E-03	6	4.7897E 13	6.94745E 04	0.99998
H2O	1.81226E-06	1.56087E-01	3.37379E-02	7	1.9491E 11	2.97804E 04	1.00000
CH	5.95296E-11	5.12720E-06	5.85835E-05	8	6.8000E 13	5.65894E 05	0.99999
O2	1.08159E-07	9.31557E-03	-7.10768E-02	9	1.0373E 13	8.79607E 04	0.99664
HCO	4.70513E-10	4.05246E-05	-1.28410E-04	10	2.0142E 13	7.24354E 03	0.99880
CH2	1.01023E-09	8.70100E-05	6.43696E-04	11	3.7647E 14	1.05941E 06	0.99621
CH2O	8.55375E-09	7.36722E-04	-3.44808E-03	12	3.0056E 10	3.94451E 04	0.99542
CO2	8.21861E-08	7.07857E-03	2.00980E-02	13	5.3000E 13	1.04926E 03	0.99961
CO	1.32466E-06	1.14091E-01	7.00605E-02	14	3.0000E 13	5.93235E 02	0.99845
HO2	1.85978E-10	1.60180E-05	-1.70710E-04	15	2.0000E 13	9.31973E 03	0.99565
NO	1.11528E-10	9.60574E-06	2.44723E-06	16	3.0000E 13	4.63859E 03	0.99589
NO2	1.01692E-14	8.75862E-10	-8.06606E-09	17	1.6106E 13	1.16112E 06	0.99407
N	1.48935E-12	1.28276E-07	1.85895E-06	18	8.1439E 11	2.65736E 05	0.74590
N2	6.74885E-06	5.81268E-01	-2.36394E-06	19	6.9092E 13	4.17542E 01	0.93348
HCN	9.80409E-12	8.44412E-07	2.90709E-06	20	1.1352E 08	2.14908E 02	0.99536
CN	6.32198E-14	5.44503E-09	2.11835E-08	21	7.7931E 12	8.23113E 05	0.98172
NCO	1.95812E-13	1.68650E-08	-2.23294E-08	22	7.7500E 12	2.22383E 05	0.64322
HNCO	1.01114E 11	8.70884E-07	-1.69583E-06	23	1.4269E 13	-6.42577E 05	0.11400
NH	7.99239E-13	6.88373E-08	8.72417E-08	24	5.0688E 12	-9.08886E 04	0.68389
NH2	8.05055E-11	6.93382E-06	-6.75803E-08	25	1.8302E 15	1.13623E 02	0.00701
				26	8.1351E 13	-1.67951E 00	0.93018
				27	3.2814E 14	7.56145E 01	0.26628
				28	1.3129E 15	2.87497E 02	0.17188
				29	5.6309E 14	1.52224E 01	0.73822
				30	3.0962E 11	5.86205E 04	0.96273

31	2.3564E 11	1.93492E 03	0.98670
32	3.0962E 11	1.93649E 04	0.95794
33	7.4738E 12	2.00694E 00	0.97523
34	8.8819E 12	-3.66576E-02	0.90603
35	7.0789E 15	-1.33449E-01	0.25698
36	2.4758E 14	2.01722E 00	0.80549
37	4.6685E 12	9.97543E 00	0.99920
38	4.6454E 07	1.31247E 01	0.99454
39	4.0000E 13	1.88085E 01	0.95602
40	3.4232E 09	1.d2572E 01	1.00000
41	2.0903E 13	2.74550E 00	0.14767
42	2.1359E 14	-1.39593E 01	0.13655
43	2.2916E 11	-2.74885E 00	0.78746
44	1.2000E 13	3.15756E-02	0.98880
45	7.5774E 13	-2.79496E 00	0.63856
46	2.6227E 13	2.26030E 00	0.94943
47	3.7000E 12	-2.52363E 00	0.90816
48	2.0000E 13	1.64816E-01	0.99982
49	1.0000E 13	3.74515E-05	0.96737
50	2.0000E 13	3.77479E 00	0.96901
51	1.6687E 13	-2.06608E 01	0.31007
52	1.8432E 13	-8.97143E-01	0.00482
53	1.6895E 13	2.61664E 00	0.58678
54	3.7030E 12	2.40332E 02	0.99996
55	1.0000E 14	8.81153E 00	0.99977
56	1.0000E 13	8.8134 1E-01	0.99992
57	3.9630E 11	2.71054E 02	0.68063
58	9.1232E 10	3.43769E 00	0.88605
59	7.6219E 12	1.62621E 03	0.63953
60	1.1316E 14	2.08322E 04	0.99518
61	8.1959E 12	1.49308E 03	0.98476
62	1.2932E 13	7.45481E 01	0.73637
63	7.9000E 12	2.05571E 01	0.16603
64	7.4000E 12	4.83136E 05	0.99996
65	1.7442E 10	4.53899E 01	0.99456
66	3.0000E 13	2.61480E 04	0.99411

MIXTURE MOLECULAR WEIGHT 23.63887 TOTAL ENERGY EXCHANGE RATE -6.53716E 10 (CAL-CM**3/GM**2/SEC) MASS FRACTION SUM 1.00000286

(GCKP) END OF THIS CASE - READ DATA FOR NEXT CASE

DISTANCE-PRESSURE VERSION GENERAL CHEMICAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

GCKP84 METHANE - AIR LEAN MECH - NO CH REACTIONS CASE 6

REACTION NUMBER	REACTION	REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1.0*CH4 = 1.0*CH3 + 1.0*H	2.00000E 15	0.0000	104000.00
2	1.0*H + 1.0*CH4 = 1.0*CH3 + 1.0*H2	1.26000E 14	0.0000	11900.00
3	1.0*O + 1.0*CH4 = 1.0*CH3 + 1.0*OH	2.00000E 13	0.0000	9200.00
4	1.0*OH + 1.0*CH4 = 1.0*CH3 + 1.0*H2O	3.00000E 13	0.0000	6000.00
5	1.0*CH2 + 1.0*O2 = 1.0*CH2O + 1.0*O	1.00000E 14	0.0000	3700.00
6	1.0*CH3 + 1.0*O2 = 1.0*CH2O + 1.0*OH	1.70000E 12	0.0000	14000.00
7	1.0*CH3 + 1.0*O = 1.0*CH2O + 1.0*H	6.80000E 13	0.0000	0.00
8	1.0*CH2O + 1.0*H = 1.0*HCO + 1.0*H2	2.00000E 13	0.0000	3300.00
9	1.0*CH2O + 1.0*O = 1.0*HCO + 1.0*OH	5.00000E 13	0.0000	4570.00
10	1.0*CH2O + 1.0*OH = 1.0*HCO + 1.0*H2O	5.00000E 15	0.0000	13000.00
11	M + 1.0*CH2O = 1.0*HCO + 1.0*H	5.00000E 16	0.0000	72000.00
12	1.0*O + 1.0*HCO = 1.0*H + 1.0*CO2	5.30000E 13	0.0000	0.00
13	1.0*HCO + 1.0*O = 1.0*CO + 1.0*OH	3.00000E 13	0.0000	0.00
14	1.0*HCO + 1.0*H = 1.0*CO + 1.0*H2	2.00000E 13	0.0000	0.00
15	1.0*HCO + 1.0*OH = 1.0*CO + 1.0*H2O	3.00000E 13	0.0000	0.00
16	M + 1.0*HCO = 1.0*H + 1.0*CO	3.00000E 14	0.0000	14700.00
17	1.0*CO + 1.0*OH = 1.0*CO2 + 1.0*H	4.00000E 12	0.0000	8000.00
18	1.0*CO + 1.0*O = 1.0*CO2 + M	2.80000E 13	0.0000	-4540.00
19	1.0*CO - 1.0*O2 = 1.0*CO2 + 1.0*O	1.20000E 11	0.0000	35000.00
20	1.0*H + 1.0*O2 = 1.0*OH + 1.0*O	2.20000E 14	0.0000	16790.00
21	1.0*O + 1.0*H2 = 1.0*OH + 1.0*H	1.80000E 10	1.0000	8900.00
22	1.0*H2 + 1 0*OH = 1.0*H2O + 1.0*H	5.20000E 13	0.0000	6500.00
23	1.0*OH + 1.0*OH = 1.0*O + 1.0*H2O	6.30000E 12	0.0000	1093.00
24	1.0*H + 1.0*O2 = 1.0*HO2 + M	1.50000E 15	0.0000	-1000.00
25	1.0*O + 1.0*O = 1.0*O2 + M	5.70000E 13	0.0000	-1788.00
26	1.0*H + 1.0*H = 1.0*H2 + M	8.30000E 17	-1.0000	0.00
27	1.0*H + 1.0*OH = 1.0*H2O + M	8.40000E 21	-2.0000	0.00
28	1.0*O + 1.0*H = 1.0*OH + M	6.20000E 16	-0.6000	0.00
29	1.0*H + 1.0*CH3 = 1.0*H2 + 1.0*CH2	2.70000E 11	0.6700	25700.00
30	1.0*O + 1.0*CH3 = 1.0*OH + 1.0*CH2	1.90000E 11	0.6800	25700.00
31	1.0*OH + 1.0*CH3 = 1.0*H2O + 1.0*CH2	2.70000E 11	0.6700	25700.00
32	1.0*HO2 + 1.0*NO = 1.0*NO2 + 1.0*OH	1.20000E 13	0.0000	2380.00
33	1 0*O + 1.0*NO2 = 1.0*NO + 1.0*O2	1.00000E 13	0.0000	596.00
34	1.0*NO + 1.0*O = 1.0*NO2 + M	5.62000E 15	0.0000	-1160.00
35	1.0*NO2 + 1.0*H = 1.0*NO + 1.0*OH	2.90000E 14	0.0000	795.00
36	1.0*N + 1.0*O2 = 1.0*NO + 1.0*O	6.40000E 09	1.0000	6250.00
37	1.0*O + 1.0*N2 = 1.0*NO + 1.0*N	1.80000E 14	0.0000	76250.00
38	1.0*N + 1.0*OH = 1.0*NO + 1.0*H	4.00000E 13	0.0000	0.00
39	1.0*CN + 1.0*H2 = 1.0*HCN + 1.0*H	6.00000E 13	0.0000	5300.00
40	1.0*O + 1.0*HCN = 1.0*NH + 1.0*NCO	5.20000E 12	0.6800	8100.00
41	1.0*OH + 1.0*HCN = 1.0*HNCO + 1.0*H	4.00000E 11	0.0000	2800.00
42	1.0*CN + 1.0*O = 1.0*CO + 1.0*N	1.20000E 13	0.0000	0.00
43	1.0*CN + 1.0*OH = 1.0*NCO + 1.0*H	2.50000E 14	0.0000	6000.00
44	1.0*CN + 1.0*O2 = 1.0*NCO + 1.0*O	3.20000E 13	0.0000	1000.00
45	1.0*CN + 1.0*CO2 = 1.0*NCO + 1.0*CO	3.70000E 12	0.0000	0.00
46	1.0*O + 1.0*NCO = 1.0*NO + 1.0*CO	2.00000E 13	0.0000	0.00
47	1.0*N + 1.0*NCO = 1.0*N2 + 1.0*CO	2.00000E 13	0.0000	0.00
48	1.0*H + 1.0*NCO = 1.0*NH + 1.0*CO	2.00300E 13	0.0000	0.00
49	1.0*H2 + 1.0*NCO = 1.0*HNCO + 1.0*H	1.00000E 14	0.0000	9000.00
50	1.0*HNCO + 1.0*H = 1.0*NH2 + 1.0*CO	1.00000E 14	0.0000	8500.00
51	1.0*NH + 1.0*OH = 1.0*N + 1.0*H2O	5.00000E 11	0.5000	1999.00
52	1.0*H + 1.0*HO2 = 1.0*OH + 1.0*OH	1.40000E 14	0.0000	1070.00
53	1.0*H + 1.0*HO2 = 1.0*O + 1.0*H2O	1.00000E 13	0.0000	1000.00
54	1.0*O + 1.0*HO2 = 1.0*OH + 1.0*O2	1.60000E 13	0.0000	1070.00

55	1.0*OH	+ 1.0*HO2	= 1.0*H2O	+ 1.0*O2		7.90000E 12	0.0000	0.00
56	1.0*CH3	+ 1.0*OH	= 1.0*CH2O	+ 1.0*H2		7.40000E 12	0.0000	0.00
57	1.0*H2	+ 1.0*HO2	= 1.0*H2O	+ 1.0*OH		7.20000E 11	0.0000	18700.00
58	1.0*HCO	+ 1.0*O2	= 1.0*CO	+ 1.0*HO2		3.00000E 13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(O2	, 24) = 2.00000	M(O2	, 27) = 1.60000	M(N2	, 24) = 2.00000	M(H2	, 27) = 1.60000
M(H2O	, 24) = 32.50000	M(H2O	, 27) = 20.00000	M(CO2	, 24) = 7.50000	M(CO2	, 27) = 7.50000
M(CO	, 24) = 2.00000	M(CO	, 27) = 1.60000	M(CH4	, 24) = 5.00000	M(N2	, 24) = 5.00000

INTEGRATION CONTROLS

INITIAL STEP SIZE 0.10000E-05 CM

MAXIMUM RELATIVE ERROR 0.10000E-05

** ASSIGNED VARIABLE PROFILE **

THE PRESSURE IS CALCULATED FROM THE FOLLOWING POLYNOMIAL

PRESSURE (ATM) = (0.00000)X**3 + (0.00000)X**2 + (0.00000)X + (1.73000E 00)

** EQUILIBRIUM COMBUSTION **

	INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE (ATM)	1.7300	1.7300	1.0000
VELOCITY (CM/SEC)	0.00	0.00	0.0000
DENSITY (GM/CM**3)	3.61558E-04	2.34368E-04	0.6482
TEMPERATURE (DEG K)	1645.00	2517.41	1.5303
ENTROPY (CAL/GM/DEG K)	2.1308	2.3026	1.0806
MACH NUMBER	0.0000	0.0000	0.0000
GAMMA	1.2777	1.187[illegible]	0.9298
SONIC VELOCITY (CM/SEC)	0.00	0.00	0.0000

SPECIES	MOLE FRACTION
CH4	2.79844E-10
CH3	2.79844E-10
H	7.94669E-04
H2	1.50221E-03
O	3.57186E-03
OH	1.04750E-02
H2O	9.15948E-02
CH2	2.79844E-10
O2	8.96812E-02
CH2O	2.79844E-10
HCO	2.79844E-10
CO2	4.48322E-02
CO	4.53881E-03
HO2	1.44643E-05
NO	1.57034E-02
NO2	1.07225E-05
N	2.22075E-07
N2	7.37294E-01
CN	2.79844E-10
HCN	2.79844E-10
NCO	2.79844E-10
HNCO	2.79844E-10
NH	5.66927E-09
NH2	1.61065E-09

MIXTURE MOLECULAR WEIGHT	27.98444
D(LOG VOLUME)/D(LOG T) AT CONSTANT P	1.0871
D(LOG VOLUME)/D(LOG P) AT CONSTANT T	-1.0033

** INITIAL CONDITIONS **

TIME 0.00000 SEC AREA 1.00000E 03 SQ CM AXIAL POSITION 0.00000 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.73000
VELOCITY (CM/SEC)	157410.31
DENSITY (GM/CM**3)	3.61558E-04
TEMPERATURE (DEG K)	1645.00
MASS FLOW RATE (GM/SEC)	5.69130E 04

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000
TOTAL NUMBER OF STEPS	0

ENTROPY (CAL/GM/DEG K)	2.1308	FUNCT EVALUATIONS	0
MACH NUMBER	2.0000	JACOBIAN EVALUATIONS	0
GAMMA	1.2777		
ENTHALPY (CAL/GM)	3.60714E 02		

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
CH4	6.37852E-07	4.97680E-02	-1.94367E-05	1	3.0472E 01	1.55849E 07	1.00000
CH3	0.00000	0.00000	1.94367E-05	2	3.3065E 12	0.00000	0.00000
H	0.00000	0.00000	1.94367E-05	3	1.1988E 12	0.00000	0.00000
H2	0.00000	0.00000	0.00000	4	4.7861E 12	0.00000	0.00000
O	0.00000	0.00000	7.70623E-05	5	3.2243E 13	0.00000	0.00000
OH	0.00000	0.00000	0.00000	6	2.3467E 10	0.00000	0.00000
H2O	0.00000	0.00000	0.00000	7	6.8000E 13	0.00000	0.00000
CH2	0.00000	0.00000	0.00000	8	7.2879E 12	0.00000	0.00000
O2	2.55141E-06	1.99072E-01	-7.70623E-05	9	1.2354E 13	0.00000	0.00000
CH2O	0.00000	0.00000	0.00000	10	9.3719E 13	0.00000	0.00000
HCO	0.00000	0.00000	0.00000	11	1.3591E 07	0.00000	0.00000
CO2	0.00000	0.00000	0.00000	12	5.3000E 13	0.00000	0.00000
CO	0.00000	0.00000	0.00000	13	3.0000E 13	0.00000	0.00000
HO2	0.00000	0.00000	0.00000	14	2.0000E 13	0.00000	0.00000
NO	0.00000	0.00000	0.00000	15	3.6000E 13	0.00000	0.00000
NO2	0.00000	0.00000	0.00000	16	3.3429E 12	0.00000	0.00000
N	0.00000	0.00000	0.00000	17	3.4610E 11	0.00000	0.00000
N2	9.62725E-06	7.51160E-01	0.00000	18	1.1229E 14	0.00000	0.00000
CN	1.28165E-12	9.99999E-05	-7.70623E-05	19	2.6865E 06	0.00000	0.00000
HCN	0.00000	0.00000	0.00000	20	1.2935E 12	0.00000	0.00000
NCO	0.00000	0.00000	7.70623E-05	21	1.9454E 12	0.00000	0.00000
HNCO	0.00000	0.00000	0.00000	22	7.1192E 12	0.00000	0.00000
NH	0.00000	0.00000	0.00000	23	4.5095E 12	0.00000	0.00000
NH2	0.00000	0.00000	0.00000	24	2.0368E 15	0.00000	0.00000
				25	9.8497E 13	1.28597E 01	1.00000
				26	5.0456E 14	0.00000	0.00000
				27	3.1042E 15	0.00000	0.00000
				28	7.2894E 14	0.00000	0.00000
				29	1.4851E 10	0.00000	0.00000
				30	1.1254E 10	0.00000	0.00000
				31	1.4851E 10	0.00000	0.00000
				32	5.7960E 12	0.00000	0.00000
				33	8.3333E 12	0.00000	0.00000
				34	8.0140E 15	0.00000	0.00000
				35	2.2739E 14	0.00000	0.00000
				36	1.5559E 12	0.00000	0.00000
				37	1.3333E 04	0.00000	0.00000
				38	4.0000E 13	0.00000	0.00000
				39	1.1858E 13	0.00000	0.00000
				40	6.7120E 13	0.00000	0.00000
				41	1.6985E 11	0.00040	0.00000
				42	1.2000E 13	0.00000	0.00000
				43	3.9884E 13	0.00000	0.00000
				44	2.3566E 13	-3.74062E 06	1.00000
				45	3.7000E 12	0.00000	0.00000
				46	2.0000E 13	0.00000	0.00000
				47	1.0000E 13	0.00000	0.00000
				48	2.0000E 13	0.00000	0.00000
				49	6.3722E 12	0.00000	0.00000
				50	7.4253E 12	0.00000	0.00000
				51	1.1002E 13	0.00000	0.00000
				52	1.0092E 14	0.00000	0.00000
				53	7.3645E 12	0.00000	0.00000
				54	1.1534E 13	0.00000	0.00000
				55	7.9000E 12	0.00000	0.00000
				56	7.4000E 12	0.00000	0.00000
				57	2.3600E 09	0.00000	0.00000
				58	3.0000E 13	0.00000	0.00000

MIXTURE MOLECULAR WEIGHT 28.21036 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) 1.18443E 07 MASS FRACTION SUM 0.99999988

NEGATIVE CONCENTRATIONS-HALVE STEP SIZE -SAVE1(19) = -0.12223875D-14

TIME 2.22158E-04 SEC AREA 1.07332E 03 SQ CM AXIAL POSITION 3.50000E 01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.73000
VELOCITY (CM/SEC)	157410.31
DENSITY (GM/CM**3)	3.36861E-04
TEMPERATURE (DEG K)	1755.78
MASS FLOW RATE (GM/SEC)	5.69130E 04
ENTROPY CAL/GM/DEG K)	2.1689
MACH NUMBER	1.9307
GAMMA	1.2774
ENTHALPY (CAL/GM)	3.60714E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	17
AVERAGE STEP SIZE	0.58824E 00
TOTAL NUMBER OF STEPS	128
FUNCT EVALUATIONS	142
JACOBIAN EVALUATIONS	28

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
CH4	4.44451E-07	3.70132E-02	-2.59831E-03	1	2.2684E 02	-5.07117E 07	0.35250
CH3	2.16817E-08	1.80562E-03	3.12196E-04	2	4.1603E 12	2.71858E 06	0.84205
H	5.23018E-10	2.69004E-05	4.18038E-05	3	1.4317E 12	6.55316E 06	0.99744

H2	2.59722E-08	2.16292E-03	5.24383E-04	4	5.3737E 12	-2.34761E 08	0.96875
O	4.72431E-10	3.93434E-05	3.27901E-07	5	5.4629E 13	-4.37557E 05	0.99982
OH	7.99754E-10	6.66023E-05	-1.17961E-05	6	5.0748E 10	-6.84736E 08	1.00000
H2O	2.08781E-07	1.73869E-02	4.34991E-03	7	6.8000E 13	-4.29502E 08	1.00000
CH2	1.05206E-14	9.01119E-10	-2.60439E-09	8	7.7672E 12	-7.22324E 06	0.99992
O2	2.19069E-06	1.82438E-01	-3.38100E-03	9	1.3493E 13	-1.59075E 07	1.00000
CH2O	2.33344E-08	1.94326E-03	-1.84218E-04	10	1.2065E 14	-5.74676E 08	0.99998
HCO	2.08021E-11	1.73237E-06	-4.53132E-06	11	5.4554E 07	1.21418E 07	0.99923
CO2	7.47732E-10	6.22700E-05	3.52727E-05	12	5.3000E 13	-5.13625E 05	1.00000
CO	1.04045E-07	8.66471E-03	2.43949E-03	13	3.0000E 13	-2.26174E 05	1.00000
HO2	1.69532E-08	1.41184E-03	5.10315E-05	14	2.0000E 13	-1.05304E 05	0.99998
NO	5.30233E-14	4.41578E-09	1.07972E-09	15	3.0000E 13	-4.57104E 05	1.00000
NO2	6.04379E-14	5.03318E-09	-2.40958E-10	16	4.4397E 12	1.49379E 08	0.99985
N	1.14257E-16	9.51516E-12	6.39032E-12	17	4.0389E 11	-7.35431E 06	0.99936
N2	8.96962E-06	7.46976E-01	-2.46164E-10	18	1.2287E 14	-6.80513E 04	1.00000
CN	2.42071E-17	2.01593E-12	6.84311E-11	19	5.2794E 06	-8.56643E 04	1.00000
HCN	7.51056E-14	6.25463E-09	-2.05499E-09	20	1.7885E 12	1.86302E 08	0.99610
NCO	1.26972E-14	1.05740E-09	-3.16083E-10	21	2.4656E 12	4.89602E 05	0.98389
HNCO	8.94719E-13	7.45109E-08	-2.52257E-10	22	8.0209E 12	-1.77871E 07	0.80212
NH	2.46335E-14	2.05144E-09	-1.52136E-10	23	4.6056E 12	4.94258E 06	0.91858
NH2	8.65966E-14	7.21164E-09	2.35421E-09	24	1.9979E 15	2.29902E 08	0.91849
				25	9.5156E 13	-1.54596E 02	0.57754
				26	4.7272E 14	-4.88277E 02	0.89774
				27	2.7248E 15	-1.64751E 04	0.97976
				28	7.0099E 14	-1.15655E 03	0.99835
				29	2.5478E 10	8.53471E 03	0.99997
				30	1.9320E 10	1.27207E 04	1.00000
				31	2.5478E 10	-3.73068E 04	0.99999
				32	6.8664E 12	-2.15938E 02	0.92630
				33	8.4297E 12	-9.71486E 01	0.99818
				34	7.8366E 15	3.51110E 02	0.99569
				35	2.3091E 14	-1.15665E 03	0.99999
				36	1.8736E 12	-1.31601E 02	1.00000
				37	5.8092E 04	1.62698E 02	1.00000
				38	4.0000E 13	-1.56492E 00	0.99944
				39	1.3135E 13	-4.48459E-01	0.31445
				40	8.2036E 13	-3.02101E 01	0.71318
				41	1.7928E 11	2.23398E 00	0.63018
				42	1.2000E 13	-9.31156E-02	1.00000
				43	4.4781E 13	1.97854E 00	0.91806
				44	2.4026E 13	-6.78546E 01	0.95240
				45	3.7000E 12	-1.94685E 01	0.99995
				46	2.0000E 13	-1.08359E 02	1.00000
				47	1.0000E 13	-2.26898E-05	0.99992
				48	2.0000E 13	-1.89034E 01	0.98237
				49	7.5811E 12	-1.92399E 02	0.84818
				50	8.7492E 12	-1.80917E 02	0.93103
				51	1.1814E 13	-9.05183E 01	0.99992
				52	1.0302E 14	-1.68277E 08	1.00000
				53	7.5080E 12	-1.84219E 07	0.99999
				54	1.1774E 13	-4.21578E 07	0.99987
				55	7.9000E 12	-6.37152E 07	0.99835
				56	7.4000E 12	-8.12342E 07	1.00000
				57	3.3858E 09	-6.43449E 05	1.00000
				58	3.0000E 13	-4.36719E 08	0.99815

MIXTURE MOLECULAR WEIGHT 28.05325 TOTAL ENERGY EXCHANGE RATE -2.24392E 09 (CAL-CM**3/GM**2/SEC) MASS FRACTION SUM 0.99999988

TIME 2.66793E-04 SEC AREA 1.36120E 03 SQ CM AXIAL POSITION 4.20000E 01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.73000
VELOCITY (CM/SEC)	157410.31
DENSITY (GM/CM**3)	2.65617E-04
TEMPERATURE (DEG K)	2177.13
MASS FLOW RATE (GM/SEC)	5.69130E 04
ENTROPY CAL/GM/DEG K)	2.2803
MACH NUMBER	1.7129
GAMMA	1.2797
ENTHALPY (CAL/GM)	3.68714E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	28
AVERAGE STEP SIZE	0.71429E-01
TOTAL NUMBER OF STEPS	180
FUNCT EVALUATIONS	198
JACOBIAN EVALUATIONS	36

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
CH4	3.42259E-08	3.53426E-03	-2.46060E-02	1	7.2620E 04	-1.76280E 09	0.32313
CH3	8.73206E-09	9.01695E-04	-5.98879E-03	2	8.0590E 12	4.49037E 07	0.97516
H	1.92240E-08	1.98512E-03	4.98698E-03	3	2.3850E 12	1.21191E 08	0.98865
H2	4.59989E-08	4.74996E-03	-8.21047E-03	4	7.4958E 12	-3.50558E 09	0.98397
O	4.27231E-08	4.41169E-03	1.75648E-02	5	4.2518E 13	-1.10113E 08	0.99973
OH	6.80552E-08	7.02756E-03	2.53021E-02	6	6.6845E 10	-5.28751E 08	1.00000
H2O	7.62632E-07	7.87513E-02	5.33521E-02	7	6.8000E 13	-2.51594E 10	1.00000
CH2	2.51485E-12	2.59689E-07	-4.37765E-07	8	9.3274E 12	-6.34258E 07	0.99920
O2	1.20127E-06	1.24046E-01	-7.01015E-02	9	1.7387E 13	-2.27819E 08	0.99964
CH2O	1.78378E-09	1.84197E-04	-1.15501E-03	10	2.4773E 14	-1.23598E 10	0.99949
HCO	2.30627E-10	2.37944E-05	-2.77148E-04	11	2.9600E 09	6.22775E 07	0.95263
CO2	4.12978E-08	4.26451E-03	1.65744E-02	12	5.3000E 13	-8.27529E 08	1.00000
CO	3.82323E-07	3.94797E-02	1.54531E-02	13	3.0000E 13	-3.64398E 08	0.99999
HO2	2.93528E-09	3.03105E-04	-1.59396E-03	14	2.0000E 13	-1.11654E 08	0.99998
NO	3.39492E-12	3.50568E-07	2.32498E-06	15	3.0000E 13	-6.92993E 08	0.99999
NO2	1.30304E-14	1.34555E-09	-2.35580E-11	16	1.0034E 13	4.84488E 09	0.99862
N	1.66402E-13	1.71831E-08	1.00454E-07	17	6.2948E 11	-5.64305E 09	0.97830
N2	7.07261E-06	7.30336E-01	-1.20559E-06	18	7.9966E 13	-2.27986E 07	0.99983
CN	3.40222E-16	3.51322E-11	1.13868E-10	19	3.6790E 07	-1.91840E 06	0.99160
HCN	1.30451E-14	1.34707E-09	-1.53257E-09	20	4.5391E 12	1.52711E 10	0.61294
HCO	1.13662E-14	1.17370E-09	1.14226E-10	21	5.0008E 12	1.41489E 08	0.54333
HNCO	2.62107E-13	2.70659E-08	-7.09590E-08	22	1.1575E 13	-2.73459E 09	0.35474

NH	5.71692E-15	5.90344E-10	2.17213E-11	23	4.8935E 12	2.23882E 09	0.29227
NH2	5.16094E-13	5.32932E-08	5.80138E-08	24	1.8901E 15	1.22815E 08	0.08220
				25	8.6171E 13	-2.52039E 06	0.98016
				26	3.8124E 14	-1.98131E 06	0.98318
				27	1.7722E 15	-1.14847E 08	0.98915
				28	6.1611E 14	-7.05351E 06	0.99232
				29	1.2242E 11	1.58035E 06	0.99960
				30	9.3033E 10	3.58755E 06	0.99982
				31	1.2242E 11	-9.87851E 06	0.99974
				32	6.9226E 12	-4.00267E 03	0.84390
				33	8.7131E 12	-3.01217E 03	0.95485
				34	7.3482E 15	-6.00484E 03	0.56058
				35	2.4132E 14	-2.45104E 04	0.98252
				36	3.2860E 12	-2.96426E 05	0.99991
				37	3.9899E 06	1.28158E 06	0.99999
				38	4.0000E 13	-3.12034E 05	0.99976
				39	1.7624E 13	-2.04059E 01	0.26636
				40	1.4882E 14	-5.94639E 01	0.03863
				41	2.0940E 11	1.82993E 02	0.83408
				42	1.2000E 13	-1.90272E 02	0.99959
				43	6.2465E 13	2.64062E 02	0.35786
				44	2.5396E 13	-3.70827E 02	0.39724
				45	3.7000E 12	-9.03545E 01	0.98607
				46	2.0000E 13	-1.41086E 04	1.00000
				47	1.0000E 13	-4.73755E-02	0.99567
				48	2.0000E 13	-1.64628E 03	0.99845
				49	1.2489E 13	1.75292E 03	0.64781
				50	1.4020E 13	-7.17056E 03	0.82125
				51	1.4698E 13	-2.71607E 03	0.75924
				52	1.0932E 14	-2.96186E 09	0.99727
				53	7.9363E 12	-3.21478E 08	0.99615
				54	1.2494E 13	-1.11879E 09	0.99295
				55	7.9000E 12	-1.49728E 09	0.99004
				56	7.4000E 12	-4.47770E 09	1.00000
				57	9.5531E 09	-8.93825E 05	0.99824
				58	3.0000E 13	-4.26803E 09	0.99850

MIXTURE MOLECULAR WEIGHT 27.42831 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) -4.60456E 10 MASS FRACTION SUM 1.00000000

(GCKP) END OF THIS CASE - READ DATA FOR NEXT CASE

DISTANCE-AREA VERSION GENERAL CHEMICAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

GCKP84 CH4 - AIR WITH AREA PROFILE OF CASE 6 CASE 7

REACTION NUMBER	REACTION						REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1		1.0*CH4	=	1.0*CH3	+	1.0*H	2.00000E 15	0.0000	104000.00
2	1.0*H	+ 1.0*CH4	=	1.0*CH3	+	1.0*H2	1.26000E 14	0.0000	11900.00
3	1.0*O	+ 1.0*CH4	=	1.0*CH3	+	1.0*OH	2.00000E 13	0.0000	9200.00
4	1.0*OH	+ 1.0*CH4	=	1.0*CH3	+	1.0*H2O	3.00000E 13	0.0000	6000.00
5	1.0*CH2	+ 1.0*O2	=	1.0*CH2O	+	1.0*O	1.00000E 14	0.0000	3700.00
6	1.0*CH3	+ 1.0*O2	=	1.0*CH2O	+	1.0*OH	1.70000E 12	0.0000	14000.00
7	1.0*CH3	+ 1.0*O	=	1.0*CH2O	+	1.0*H	6.80000E 13	0.0000	0.00
8	1.0*CH2O	+ 1.0*H	=	1.0*HCO	+	1.0*H2	2.00000E 13	0.0000	3300.00
9	1.0*CH2O	+ 1.0*O	=	1.0*HCO	+	1.0*OH	5.00000E 13	0.0000	4570.00
10	1.0*CH2O	+ 1.0*OH	=	1.0*HCO	+	1.0*H2O	5.00000E 15	0.0000	13000.00
11	M	+ 1.0*CH2O	=	1.0*HCO	+	1.0*H	5.00000E 16	0.0000	72000.00
12	1.0*O	+ 1.0*HCO	=	1.0*H	+	1.0*CO2	5.30000E 13	0.0000	0.00
13	1.0*HCO	+ 1.0*O	=	1.0*CO	+	1.0*OH	3.00000E 13	0.0000	0.00
14	1.0*HCO	+ 1.0*H	=	1.0*CO	+	1.0*H2	2.00000E 13	0.0000	0.00
15	1.0*HCO	+ 1.0*OH	=	1.0*CO	+	1.0*H2O	3.00000E 13	0.0000	0.00
16	M	+ 1.0*HCO	=	1.0*H	+	1.0*CO	3.00000E 14	0.0000	14700.00
17	1.0*CO	+ 1.0*OH	=	1.0*CO2	+	1.0*H	4.00000E 12	0.0000	8000.00
18	1.0*CO	+ 1.0*O	=	1.0*CO2	+	M	2.80000E 13	0.0000	-4540.00
19	1.0*CO	+ 1.0*O2	=	1.0*CO2	+	1.0*O	1.20000E 11	0.0000	35000.00
20	1.0*H	+ 1.0*O2	=	1.0*OH	+	1.0*O	2.20000E 14	0.0000	16790.00
21	1.0*O	+ 1.0*H2	=	1.0*OH	+	1.0*H	1.80000E 10	1.0000	8900.00
22	1.0*H2	+ 1.0*OH	=	1.0*H2O	+	1.0*H	5.20000E 13	0.0000	6500.00
23	1.0*OH	+ 1.0*OH	=	1.0*O	+	1.0*H2O	6.30000E 12	0.0000	1093.00
24	1.0*H	+ 1.0*O2	=	1.0*HO2	+	M	1.50000E 15	0.0000	-1000.00
25	1.0*O	+ 1.0*O	=	1.0*O2	+	M	5.70000E 13	0.0000	-1788.00
26	1.0*H	+ 1.0*H	=	1.0*H2	+	M	8.30000E 17	-1.0000	0.00
27	1.0*H	+ 1.0*OH	=	1.0*H2O	+	M	8.40000E 21	-2.0000	0.00
28	1.0*O	+ 1.0*H	=	1.0*OH	+	M	6.20000E 16	-0.6000	0.00
29	1.0*H	+ 1.0*CH3	=	1.0*H2	+	1.0*CH2	2.70000E 11	0.6700	25700.00
30	1.0*O	+ 1.0*CH3	=	1.0*OH	+	1.0*CH2	1.90000E 11	0.6800	25700.00
31	1.0*OH	+ 1.0*CH3	=	1.0*H2O	+	1.0*CH2	2.70000E 11	0.6700	25700.00
32	1.0*HO2	+ 1.0*NO	=	1.0*NO2	+	1.0*OH	1.20000E 13	0.0000	2380.00
33	1.0*O	+ 1.0*NO2	=	1.0*NO	+	1.0*O2	1.00000E 13	0.0000	596.00
34	1.0*NO	+ 1.0*O	=	1.0*NO2	+	M	5.62000E 15	0.0000	-1160.00
35	1.0*NO2	+ 1.0*H	=	1.0*NO	+	1.0*OH	2.90000E 14	0.0000	795.00
36	1.0*N	+ 1.0*O2	=	1.0*NO	+	1.0*O	6.40000E 09	1.0000	6250.00
37	1.0*O	+ 1.0*N2	=	1.0*NO	+	1.0*N	1.80000E 14	0.0000	76250.00
38	1.0*N	+ 1.0*OH	=	1.0*NO	+	1.0*H	4.00000E 13	0.0000	0.00
39	1.0*CN	+ 1.0*H2	=	1.0*HCN	+	1.0*H	6.00000E 13	0.0000	5300.00
40	1.0*O	+ 1.0*HCN	=	1.0*NH	+	1.0*HCO	5.20000E 12	0.6800	8100.00
41	1.0*OH	+ 1.0*HCN	=	1.0*HNCO	+	1.0*H	4.00000E 11	0.0000	2800.00
42	1.0*CN	+ 1.0*O	=	1.0*CO	+	1.0*N	1.20000E 13	0.0000	0.00
43	1.0*CN	+ 1.0*OH	=	1.0*NCO	+	1.0*H	2.50000E 14	0.0000	6000.00
44	1.0*CN	+ 1.0*O2	=	1.0*NCO	+	1.0*O	3.20000E 13	0.0000	1000.00
45	1.0*CN	+ 1.0*CO2	=	1.0*NCO	+	1.0*CO	3.70000E 12	0.0000	0.00
46	1.0*C	+ 1.0*NCO	=	1.0*NO	+	1.0*CO	2.00000E 13	0.0000	0.00
47	1.0*N	+ 1.0*NCO	=	1.0*N2	+	1.0*CO	1.00000E 13	0.0000	0.00
48	1.0*H	+ 1.0*NCO	=	1.0*NH	+	1.0*CO	2.00000E 13	0.0000	0.00
49	1.0*H2	+ 1.0*NCO	=	1.0*HNCO	+	1.0*H	1.00000E 14	0.0000	9000.00
50	1.0*HNCO	+ 1.0*H	=	1.0*NH2	+	1.0*CO	1.00000E 14	0.0000	8500.00
51	1.0*NH	+ 1.0*OH	=	1.0*N	+	1.0*H2O	5.00000E 11	0.5000	1999.00
52	1.0*H	+ 1.0*HO2	=	1.0*OH	+	1.0*OH	1.40000E 14	0.0000	1070.00
53	1.0*H	+ 1.0*HO2	=	1.0*O	+	1.0*H2O	1.00000E 13	0.0000	1000.00

54	1.0*O	+ 1.0*HO2	= 1.0*OH	+ 1.0*O2	1.60000E 13	0.0000	1070.00
55	1.0*OH	+ 1.0*HO2	= 1.0*H2O	+ 1.0*O2	7.90000E 12	0.0000	0.00
56	1.0*CH3	+ 1.0*OH	= 1.0*CH2O	+ 1.0*H2	7.40000E 12	0.0000	0.00
57	1.0*H2	+ 1.0*HO2	= 1.0*H2O	+ 1.0*OH	7.20000E 11	0.0000	18700.00
58	1.0*HCO	+ 1.0*O2	= 1.0*CO	+ 1.0*HO2	3.00000E 13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(O2 , 24) = 2.00000	M(O2 , 27) = 1.60000	M(N2 , 24) = 2.00000	M(N2 , 27) = 1.60000
M(H2O , 24) = 32.50000	M(H2O , 27) = 20.00000	M(CO2 , 24) = 7.50000	M(CO2 , 27) = 7.50000
M(CO , 24) = 2.00000	M(CO , 27) = 1.60000	M(CH4 , 24) = 5.00000	M(H2 , 24) = 5.00000

INTEGRATION CONTROLS

INITIAL STEP SIZE 0.50000E-04 CM MAXIMUM RELATIVE ERROR 0.12400E-05

** ASSIGNED VARIABLE PROFILE **

THE AREA IS CALCULATED BY INTERPOLATION FROM THE FOLLOWING TABLE

STATION	AXIAL DISTANCE (CM)	AREA (CM**2)
1	0.00000	1.00000E 03
2	5.00000E 00	1.00036E 03
3	1.00000E 01	1.00212E 03
4	1.50000E 01	1.00561E 03
5	2.00000E 01	1.01148E 03
6	2.50000E 01	1.02136E 03
7	3.00000E 01	1.03885E 03
8	3.50000E 01	1.07332E 03
9	3.70000E 01	1.09749E 03
10	3.80000E 01	1.11404E 03
11	3.85000E 01	1.12404E 03
12	3.90000E 01	1.13566E 03
13	3.95000E 01	1.14948E 03
14	4.00000E 01	1.16651E 03
15	4.05000E 01	1.18872E 03
16	4.10000E 01	1.22048E 03
17	4.15000E 01	1.27343E 03
18	4.20000E 01	1.36117E 03
19	4.25000E 01	1.40117E 03
20	4.30000E 01	1.41170E 03

TIME 2.22063E-04 SEC AREA 1.07332E 03 SQ CM AXIAL POSITION 3.50000E 01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.72981
VELOCITY (CM/SEC)	157414.17
DENSITY (GM/CM**3)	3.36833E-04
TEMPERATURE (DEG K)	1755.72
MASS FLOW RATE (GM/SEC)	5.69098E 04
ENTROPY CAL/GM/DEG K)	2.1689
MACH NUMBER	1.9308
GAMMA	1.2774
ENTHALPY (CAL/GM)	3.60699E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	13
AVERAGE STEP SIZE	0.76923E 00
TOTAL NUMBER OF STEPS	132
FUNCT EVALUATIONS	146
JACOBIAN EVALUATIONS	32

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	4.44416E-07	3.70134E-02	-2.59382E-03
CH3	2.16753E-08	1.80524E-03	3.10482E-04
H	3.26016E-10	2.71524E-05	8.45046E-06
H2	2.59847E-08	2.16414E-03	5.30766E-04
O	4.71562E-10	3.92742E-05	1.47299E-05
OH	7.96583E-10	6.63438E-05	2.63089E-05
H2O	2.08735E-07	1.73846E-02	4.33334E-03
CH2	1.07700E-14	8.96985E-10	4.04043E-10
O2	2.19052E-06	1.82438E-01	-3.32635E-03
CH2O	2.33675E-08	1.94651E-03	-1.79435E-04
HCO	2.07047E-11	1.72440E-06	-1.37783E-07
CO2	7.47021E-10	6.22160E-05	3.52261E-05
CO	1.04025E-07	8.66378E-03	2.42769E-03
HO2	1.69579E-08	1.41234E-03	3.98757E-05
NO	5.28902E-14	4.40498E-09	1.11553E-09
NO2	6.02671E-14	5.01937E-09	-2.76418E-10
N	1.14529E-16	9.53857E-12	4.08529E-12
N2	8.96887E-06	7.46976E-01	-2.45511E-10
CN	2.52450E-17	2.10254E-12	1.55509E-11
HCN	7.55631E-14	6.29331E-09	-2.05751E-09
NCO	1.27178E-14	1.05921E-09	-2.63030E-10
HNCO	8.94411E-13	7.44914E-08	-2.73204E-10
NH	2.46655E-14	2.05428E-09	-1.50611E-10
NH2	8.66135E-14	7.21364E-09	2.37663E-09

REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	2.2661E 02	-5.21158E 07	0.35903
2	4.1599E 12	2.74832E 06	0.84346
3	1.4316E 12	6.54112E 06	0.99746
4	5.3734E 12	-2.33811E 08	0.96864
5	3.4628E 13	-4.35536E 05	0.99982
6	3.0743E 10	-6.84503E 08	1.00000
7	6.8000E 13	-4.28658E 08	1.00000
8	7.7670E 12	-7.29538E 06	0.99992
9	1.3493E 13	-1.58891E 07	1.00000
10	1.2043E 14	-5.72742E 08	0.99998
11	5.4517E 07	1.21412E 07	0.99923
12	5.3000E 13	-5.10366E 05	1.00000
13	3.0000E 13	-2.24739E 05	1.00000
14	2.0000E 13	-1.05802E 05	0.99998
15	3.0000E 13	-4.53236E 05	1.00000
16	4.4390E 12	1.48671E 08	0.99985
17	4.0386E 11	-7.32436E 06	0.99935
18	1.0287E 14	-6.79217E 04	1.00000
19	5.2776E 06	-8.56269E 04	1.00000
20	1.7883E 12	1.88029E 08	0.99616
21	2.4653E 12	4.88907E 05	0.98378
22	8.0704E 12	-1.76725E 07	0.79966
23	4.6056E 12	4.93499E 06	0.91904
24	1.9979E 15	2.29673E 08	0.91772
25	9.5157E 13	-1.53763E 02	0.57649
26	4.7274E 14	-4.98508E 02	0.89966
27	2.7250E 15	-1.65665E 04	0.97990
28	7.0100E 14	-1.16528E 03	0.99837
29	2.5472E 10	8.61054E 03	0.99997

30	1.9315E 10	1.26923E 04	1.00000
31	2.5472E 10	-3.71442E 04	0.99999
32	6.0663E 12	-2.15565E 02	0.92664
33	3.4297E 12	-9.67111E 01	0.99817
34	7.8367E 15	3.49914E 02	0.99569
35	2.3091E 14	-1.16427E 03	0.99999
36	1.8735E 12	-1.31913E 02	1.00000
37	5.8049E 04	1.62293E 02	1.00000
38	4.0000E 13	-1.56268E 00	0.99943
39	1.3135E 13	-4.95462E-01	0.33293
40	8.2027E 13	-3.02593E 01	0.71128
41	1.7928E 11	2.26288E 00	0.63265
42	1.2000E 13	-9.69456E-02	1.00000
43	4.4779E 13	1.99505E 00	0.91579
44	2.4025E 13	-7.09155E 01	0.95437
45	3.7000E 12	-1.94999E 01	0.99995
46	2.0000E 13	-1.08353E 02	1.00000
47	1.0000E 13	-2.27845E-05	0.99992
48	2.0000E 13	-1.91165E 01	0.98255
49	7.5804E 12	-1.92587E 02	0.84708
50	8.7485E 12	-1.82670E 02	0.93165
51	1.1813E 13	-9.02882E 01	0.99992
52	1.0302E 14	-1.70518E 08	1.00000
53	7.5080E 12	-1.86009E 07	0.99999
54	1.1774E 13	-4.20986E 07	0.99987
55	7.9000E 12	-6.34902E 07	0.99835
56	7.4000E 12	-8.09018E 07	1.00000
57	3.3852E 09	-6.63926E 05	1.00000
58	3.0000E 13	-4.34710E 08	0.99814

MIXTURE MOLECULAR WEIGHT 28.05325 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) -2.23966E 09 MASS FRACTION SUM 0.99999982

TIME 2.66793E-04 SEC AREA 1.36117E 03 SQ CM AXIAL POSITION 4.20000E 01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.72718
VELOCITY (CM/SEC)	157467.79
DENSITY (GM/CM**3)	2.65509E-04
TEMPERATURE (DEG K)	2174.66
MASS FLOW RATE (GM/SEC)	5.69093E 04
ENTROPY (CAL/GM/DEG K)	2.2798
MACH NUMBER	1.7146
GAMMA	1.2797
ENTHALPY (CAL/GM)	3.60498E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	37
AVERAGE STEP SIZE	0.54054E-01
TOTAL NUMBER OF STEPS	192
FUNCT EVALUATIONS	211
JACOBIAN EVALUATIONS	39

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	3.56304E-08	3.68133E-03	-2.49495E-02
CH3	9.05969E-09	9.36046E-04	-5.98289E-03
H	1.88634E-08	1.94897E-03	4.92247E-03
H2	4.63778E-03	4.79175E-03	-8.07126E-03
O	4.15916E-08	4.29724E-03	1.72413E-02
OH	6.64351E-06	6.86407E-03	2.49831E-02
H2O	7.59440E-07	7.84653E-02	5.41216E-02
CH2	2.52160E-12	2.60532E-07	-3.54994E-07
O2	1.20480E-06	1.24480E-01	-7.00889E-02
CH2O	1.86028E-09	1.92204E-04	-1.28336E-03
HCO	2.33173E-10	2.40914E-05	-8.39324E-05
CO2	4.03958E-08	4.17368E-03	1.61136E-02
CO	3.81223E-07	3.93879E-02	1.61865E-02
HO2	3.02132E-09	3.12163E-04	-1.60833E-03
NO	3.23634E-12	3.34378E-07	2.21324E-06
NO2	1.29587E-14	1.33889E-09	-1.30417E-10
N	1.59559E-13	1.64856E-08	1.00554E-07
N2	7.06973E-06	7.30444E-01	-1.14991E-06
CN	3.32494E-16	3.43533E-11	1.09353E-10
HCN	1.30911E-14	1.35257E-09	-1.48754E-09
NCO	1.13138E-14	1.16894E-09	3.06226E-10
HNCO	2.66012E-13	2.74843E-08	-7.05188E-08
NH	5.69501E-15	5.88408E-10	4.95243E-12
NH2	5.12828E-13	5.29853E-08	5.77521E-08

REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	7.0661E 04	-1.81480E 09	0.32650
2	8.0249E 12	4.57356E 07	0.97456
3	2.3793E 12	1.22626E 08	0.98866
4	7.4839E 12	-3.55911E 09	0.98377
5	4.2477E 13	-1.10716E 08	0.99973
6	6.6599E 10	-5.48630E 08	1.00000
7	6.8000E 13	-2.54328E 10	1.00000
8	9.3193E 12	-6.49023E 07	0.99921
9	1.7366E 13	-2.31212E 08	0.99965
10	2.4628E 14	-1.25505E 10	0.99950
11	2.9046E 09	6.38285E 07	0.95384
12	5.3000E 13	-8.15879E 08	1.00000
13	3.0000E 13	-3.59267E 08	0.99999
14	2.0000E 13	-1.10956E 08	0.99998
15	3.0000E 13	-6.85116E 08	0.99999
16	9.9952E 12	4.88518E 09	0.99866
17	6.2616E 11	-5.48814E 09	0.97872
18	8.0061E 13	-2.21632E 07	0.99984
19	3.6453E 07	-1.90328E 06	0.99201
20	4.5191E 12	1.52621E 10	0.62471
21	4.9914E 12	1.41253E 08	0.55410
22	1.1555E 13	-2.74289E 09	0.36184
23	4.8921E 12	2.22871E 09	0.30127
24	1.8906E 15	1.67874E 08	0.11077
25	8.6212E 13	-2.38915E 06	0.97964
26	3.8167E 14	-1.90972E 06	0.93287
27	1.7762E 15	-1.10072E 08	0.98907
28	6.1653E 14	-6.74451E 06	0.99236
29	1.2151E 11	1.59815E 06	0.99960
30	9.2335E 10	3.59934E 06	0.99982
31	1.2151E 11	-9.93837E 06	0.99975
32	6.9182E 12	-3.93683E 03	0.84573
33	8.7117E 12	-2.92159E 03	0.95597
34	7.3505E 15	-5.34873E 03	0.53774
35	2.4127E 14	-2.39560E 04	0.98367
36	3.2768E 12	-2.84513E 05	0.99991
37	3.9108E 06	1.22339E 06	0.99999
38	4.0000E 13	-2.92317E 05	0.99976
39	1.7600E 13	-2.03731E 01	0.27004
40	1.4639E 14	-5.83414E 01	0.03083
41	2.0925E 11	1.82196E 02	0.83630
42	1.2000E 13	-1.81175E 02	0.99959
43	6.2366E 13	2.64954E 02	0.36971
44	2.5389E 13	-3.70384E 02	0.40458
45	3.7000E 12	-8.98503E 01	0.98659

46	2.0000E 13	-1.36878E 04	1.00000
47	1.0000E 13	-4.52552E-02	0.99569
48	2.0000E 13	-..609?4E 03	0.99843
49	1.2460E 13	1.72898E 03	0.64420
50	1.3980E 13	-7.144?4E 03	0.82278
51	1.4681E 13	-2.66513E 03	0.76632
52	1.0929E 14	-2.99363E 09	0.99745
53	7.9342E 12	-3.24941E 08	0.99635
54	1.2491E 13	-1.12198E 09	0.99321
55	7.9000E 12	-1.50607E 09	0.99028
56	7.4000E 12	-4.53881E 09	1.00000
57	9.5063E 09	-9.23933E 05	0.99837
58	3.0000E 13	-4.33512E 09	0.99850

MIXTURE MOLECULAR WEIGHT 27.43237 TOTAL ENERGY EXCHANGE RATE -4.65682E 10 (CAL-CM**3/GM**2/SEC) MASS FRACTION SUM 1.00000095

(GCKP) END OF THIS CASE - READ DATA FOR NEXT CASE

TIME-AREA VERSION GENERAL CHEMICAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

GCKP84 METHANOL - AIR COMBUSTION CASE 8

REACTION NUMBER	REACTION					REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	M	+ 1.0*CH3OH	= 1.0*CH3	+ 1.0*OH		3.20000E 18	0.0000	80000.00
2	1.0*O2	+ 1.0*CH3OH	= 1.0*CH2OH	+ 1.0*HO2		4.00000E 13	0.0000	50900.00
3	1.0*OH	+ 1.0*CH3OH	= 1.0*CH2OH	+ 1.0*H2O		4.00000E 12	0.0000	2000.00
4	1.0*O	+ 1.0*CH3OH	= 1.0*CH2OH	+ 1.0*OH		1.60000E 12	0.0300	2300.00
5	1.0*H	+ 1.0*CH3OH	= 1.0*CH2OH	+ 1.0*H2		3.20000E 13	0.0000	7000.00
6	1.0*H	+ 1.0*CH3OH	= 1.0*CH3	+ 1.0*H2O		5.00000E 12	0.0000	5300.00
7	1.0*CH3	+ 1.0*CH3OH	= 1.0*CH2OH	+ 1.0*CH4		2.00000E 11	0.0000	9800.00
8	1.0*HO2	+ 1.0*CH3OH	= 1.0*CH2OH	+ 1.0*H2O2		6.30000E 12	0.0000	19400.00
9	M	+ 1.0*CH2OH	= 1.0*CH2O	+ 1.0*H		2.50000E 13	0.0000	29000.00
10	1.0*O2	+ 1.0*CH2OH	= 1.0*CH2O	+ 1.0*HO2		1.00000E 12	0.0000	6000.00
11		1.0*CH4	= 1.0*CH3	+ 1.0*H		2.00000E 15	0.0000	104000.00
12	1.0*H	+ 1.0*CH4	= 1.0*CH3	+ 1.0*H2		1.26000E 14	0.0000	11900.00
13	1.0*O	+ 1.0*CH4	= 1.0*CH3	+ 1.0*OH		2.00000E 13	0.0000	9200.00
14	1.0*OH	+ 1.0*CH4	= 1.0*CH3	+ 1.0*H2O		5.00000E 13	0.0000	6900.00
15	1.0*CH	+ 1.0*O2	= 1.0*HCO	+ 1.0*O		1.00000E 13	0.0000	0.00
16	1.0*CH2	+ 1.0*O2	= 1.0*CH2O	+ 1.0*O		1.00000E 14	0.0000	3700.00
17	1.0*CH3	+ 1.0*O2	= 1.0*CH2O	+ 1.0*OH		1.70000E 12	0.0000	14000.00
18	1.0*CH3	+ 1.0*O	= 1.0*CH2O	+ 1.0*H		6.80000E 13	0.0000	0.00
19	1.0*CH2O	+ 1.0*H	= 1.0*HCO	+ 1.0*H2		2.00000E 13	0.0000	3300.00
20	1.0*CH2O	+ 1.0*O	= 1.0*HCO	+ 1.0*OH		5.00000E 13	0.0000	4570.00
21	1.0*CH2O	+ 1.0*OH	= 1.0*HCO	+ 1.0*H2O		5.00000E 15	0.0000	13000.00
22	1.0*HCO	+ 1.0*O	= 1.0*CO	+ 1.0*OH		3.00000E 13	0.0000	0.00
23	1.0*HCO	+ 1.0*H	= 1.0*CO	+ 1.0*H2		2.00000E 13	0.0000	0.00
24	1.0*HCO	+ 1.0*OH	= 1.0*CO	+ 1.0*H2O		3.00000E 13	0.0000	0.00
25	M	+ 1.0*HCO	= 1.0*H	+ 1.0*CO		3.00000E 14	0.0000	14700.00
26	1.0*CO	+ 1.0*OH	= 1.0*CO2	+ 1.0*H		4.00000E 12	0.0000	8000.00
27	1.0*CO	+ 1.0*O	= 1.0*CO2	+ M		2.80000E 13	0.0000	-4540.00
28	1.0*CO	+ 1.0*O2	= 1.0*CO2	+ 1.0*O		1.20000E 11	0.0000	35000.00
29	1.0*H	+ 1.0*O2	= 1.0*OH	+ 1.0*O		2.20000E 14	0.0000	16790.00
30	1.0*O	+ 1.0*H2	= 1.0*OH	+ 1.0*H		1.80000E 10	1.0000	8900.00
31	1.0*H2	+ 1.0*OH	= 1.0*H2O	+ 1.0*H		5.20000E 13	0.0000	6500.00
32	1.0*OH	+ 1.0*OH	= 1.0*O	+ 1.0*H2O		6.30000E 12	0.0000	1093.00
33	1.0*H	+ 1.0*O2	= 1.0*HO2	+ M		1.50000E 15	0.0000	-1000.00
34	1.0*O	+ 1.0*O	= 1.0*O2	+ M		5.70000E 13	0.0000	-1788.00
35	1.0*H	+ 1.0*H	= 1.0*H2	+ M		8.30000E 17	-1.0000	0.00
36	1.0*H	+ 1.0*OH	= 1.0*H2O	+ M		8.40000E 21	-2.0000	0.00
37	1.0*H	+ 1.0*CH3	= 1.0*H2	+ 1.0*CH2		2.70000E 11	0.6700	25700.00
38	1.0*O	+ 1.0*CH3	= 1.0*OH	+ 1.0*CH2		1.90000E 11	0.6800	25700.00
39	1.0*OH	+ 1.0*CH3	= 1.0*H2O	+ 1.0*CH2		2.70000E 11	0.6700	25700.00
40	1.0*H	+ 1.0*CH2	= 1.0*H2	+ 1.0*CH		2.90000E 11	0.7000	26000.00
41	1.0*O	+ 1.0*CH2	= 1.0*OH	+ 1.0*CH		3.20000E 11	0.5000	26000.00
42	1.0*OH	+ 1.0*CH2	= 1.0*H2O	+ 1.0*CH		5.00000E 11	0.5000	6000.00
43	1.0*HO2	+ 1.0*NO	= 1.0*NO2	+ 1.0*OH		1.20000E 13	0.0000	2380.00
44	1.0*O	+ 1.0*NO2	= 1.0*NO	+ 1.0*O2		1.00000E 13	0.0000	596.00
45	1.0*NO	+ 1.0*O	= 1.0*NO2	+ M		5.62000E 15	0.0000	-1160.00
46	1.0*NO2	+ 1.0*H	= 1.0*NO	+ 1.0*OH		2.90000E 14	0.0000	795.00
47	1.0*N	+ 1.0*O2	= 1.0*NO	+ 1.0*O		6.40000E 09	1.0000	6250.00
48	1.0*O	+ 1.0*N2	= 1.0*NO	+ 1.0*N		1.80000E 14	0.0000	76250.00
49	1.0*N	+ 1.0*OH	= 1.0*NO	+ 1.0*H		4.00000E 13	0.0000	0.00
50	1.0*HCN	+ 1.0*H2	= 1.0*HCN	+ 1.0*H		6.00000E 13	0.0000	5300.00
51	1.0*O	+ 1.0*HCN	= 1.0*H	+ 1.0*NCO		5.20000E 12	0.6800	8100.00
52	1.0*OH	+ 1.0*HCN	= 1.0*HNCO	+ 1.0*H		4.00000E 11	0.0000	2800.00
53	1.0*CN	+ 1.0*O	= 1.0*CO	+ 1.0*N		1.20000E 13	0.0000	0.00
54	1.0*CN	+ 1.0*OH	= 1.0*NCO	+ 1.0*H		2.50000E 14	0.0000	6000.00
55	1.0*CN	+ 1.0*O2	= 1.0*NCO	+ 1.0*O		3.20000E 13	0.0000	1000.00
56	1.0*CN	+ 1.0*CO2	= 1.0*NCO	+ 1.0*CO		3.70000E 12	0.0000	0.00
57	1.0*O	+ 1.0*NCO	= 1.0*NO	+ 1.0*CO		2.00000E 13	0.0000	0.00
58	1.0*N	+ 1.0*NCO	= 1.0*N2	+ 1.0*CO		1.00000E 13	0.0000	0.00
59	1.0*H	+ 1.0*NCO	= 1.0*NH	+ 1.0*CO		2.00000E 13	0.0000	0.00
60	1.0*H2	+ 1.0*NCO	= 1.0*HNCO	+ 1.0*H		1.00000E 14	0.0000	9800.00
61	1.0*HNCO	+ 1.0*H	= 1.0*NH2	+ 1.0*CO		1.00000E 14	0.0000	8500.00
62	1.0*NH	+ 1.0*OH	= 1.0*N	+ 1.0*H2O		5.00000E 11	0.5000	1999.00
63	1.0*H	+ 1.0*HO2	= 1.0*OH	+ 1.0*OH		1.40000E 14	0.0000	1078.00
64	1.0*H	+ 1.0*HO2	= 1.0*O	+ 1.0*H2O		1.00000E 13	0.0000	1000.00
65	1.0*O	+ 1.0*HO2	= 1.0*OH	+ 1.0*O2		1.60000E 13	0.0000	1078.00
66	1.0*OH	+ 1.0*HO2	= 1.0*H2O	+ 1.0*O2		7.90000E 12	0.0000	0.00
67	1.0*CH3	+ 1.0*OH	= 1.0*CH2O	+ 1.0*H2		7.40000E 12	0.0000	0.00
68	1.0*H2	+ 1.0*HO2	= 1.0*H2O	+ 1.0*OH		7.20000E 11	0.0000	18700.00
69	1.0*HCO	+ 1.0*O2	= 1.0*CO	+ 1.0*HO2		3.00000E 13	0.0000	0.00
70	1.0*OH	+ 1.0*H2O2	= 1.0*H2O	+ 1.0*HO2		1.00000E 13	0.0000	1800.00
71	1.0*O2	+ 1.0*H2O2	= 2.0*HO2			4.00000E 13	0.0000	42600.00
72	1.0*H	+ 1.0*H2O2	= 1.0*HO2	+ 1.0*H2		1.60000E 12	0.0000	3800.00
73	M	+ 1.0*H2O2	= 2.0*OH			1.30000E 17	0.0000	45500.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(O2 , 33) = 2.00000	M(O2 , 36) = 1.60000	M(N2 , 33) = 2.00000	M(N2 , 36) = 1.60000
M(H2O , 33) = 32.50000	M(H2O , 36) = 20.00000	M(CO2 , 33) = 7.50000	M(CO2 , 36) = 7.50000
M(CO , 33) = 2.00000	M(CO , 36) = 1.60000		

INTEGRATION CONTROLS

INITIAL STEP SIZE 0.10000E-09 SEC

MAXIMUM RELATIVE ERROR 0.50000E-05

** ASSIGNED VARIABLE PROFILE **

THIS IS A V=0 PROBLEM - AN ASSIGNED VARIABLE IS NOT REQUIRED

THE VOLUME (DENSITY) WILL BE HELD CONSTANT FOR THIS CASE

AIR - FUEL COMBUSTION, EQUIVALENCE RATIO = 2.0000 OXYGEN FRACTION IN AIR = 0.2095

TIME 6.00000E-04 SEC AREA 1.00000E 00 SQ CM AXIAL POSITION 0.00000 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.25714
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	2.77821E-04
TEMPERATURE (DEG K)	1576.02
MASS FLOW RATE (GM/SEC)	0.00000
ENTROPY (CAL/GM/DEG K)	2.3087
MACH NUMBER	0.0000
GAMMA	1.2064
ENTHALPY (CAL/GM)	3.41167E 00

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	22
AVERAGE STEP SIZE	0.18182E-05
TOTAL NUMBER OF STEPS	241
FUNCT EVALUATIONS	431
JACOBIAN EVALUATIONS	61

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH3OH	1.62118E-06	1.66771E-01	-1.05615E-02
CH3	6.89624E-09	7.09418E-04	4.03594E-04
OH	1.67395E-09	1.72197E-04	8.31330E-05
O2	1.13915E-06	1.17185E-01	-8.57976E-03
CH2OH	4.20428E-03	4.32495E-03	1.63544E-03
HO2	9.26919E-08	9.53524E-03	1.20835E-04
H2O	5.98042E-07	6.15202E-02	1.81066E-02
O	1.72541E-10	1.77493E-05	1.37557E-05
H	3.59721E-10	3.70046E-05	2.58391E-05
H2	4.17864E-08	4.29853E-03	1.80249E-03
CH4	3.96287E-09	4.07661E-04	1.81562E-04
H2O2	7.66043E-09	7.88030E-04	-4.27404E-04
CH2O	7.51084E-03	7.72642E-03	-1.89854E-03
CH	1.82751E-18	1.87976E-13	4.40617E-13
HCO	1.68152E-10	1.72978E-05	6.62802E-06
CH2	4.34773E-15	4.47252E-10	7.16569E-10
CO	2.95472E-07	3.01953E-02	1.00785E-02
CO2	4.31030E-09	4.43410E-04	1.54376E-04
NO	1.34051E-12	1.37890E-07	7.37667E-08
NO2	8.16427E-12	8.39360E-07	-7.20460E-08
N	1.00029E-15	1.02933E-10	3.02948E-11
N2	5.72199E-06	5.88622E-01	-4.70291E-12
CN	2.86858E-16	2.95092E-11	1.14873E-11
HCN	5.61270E-13	5.77380E-08	-4.21597E-09
NCO	2.51435E-14	2.58653E-09	1.40767E-10
HNCO	8.22234E-12	8.45836E-07	-1.48263E-08
NH	9.42595E-14	9.69654E-09	-1.47920E-09
NH2	3.36235E-13	3.45937E-08	1.86277E-08
AR	6.82936E-03	7.02538E-03	0.00000

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	2.5788E 07	4.76416E 03	0.90483
2	3.4968E 06	-3.59054E 03	0.97723
3	2.1121E 12	7.41856E 04	0.99899
4	7.6767E 11	2.78040E 03	0.99940
5	3.4233E 12	2.56380E 04	0.99122
6	9.2047E 11	6.95433E 03	0.99995
7	8.7508E 09	1.26618E 03	0.99893
8	1.2856E 10	2.48368E 04	0.99230
9	2.3794E 09	1.25987E 04	0.99999
10	1.4722E 11	9.13290E 04	0.99976
11	7.5712E 00	-7.33924E 02	0.99947
12	2.8195E 12	-3.76372E 02	0.87846
13	1.0599E 12	4.12867E 00	0.43973
14	4.4166E 12	2.00405E 01	0.05280
15	1.0000E 13	2.69718E-04	1.00000
16	3.0684E 13	1.96364E 00	0.99986
17	1.9456E 10	1.98020E 03	1.00000
18	6.8000E 13	1.04829E 03	1.00000
19	6.9729E 12	2.40040E 03	0.99982
20	1.1621E 13	1.95112E 03	0.99999
21	7.8748E 13	1.23271E 05	0.99998
22	3.0000E 13	1.12767E 01	1.00000
23	2.0000E 13	1.56735E 01	1.00000
24	3.0000E 13	1.09404E 02	1.00000
25	2.7457E 12	5.81415E 04	0.99991
26	3.1095E 11	1.99189E 03	0.99966
27	1.1932E 14	7.66153E-01	1.00000
28	1.6814E 06	7.33223E 00	1.00000
29	1.0331E 12	5.43718E 03	0.99136
30	1.6545E 12	1.44021E 02	0.93190
31	6.5258E 12	5.23317E 03	0.88487
32	4.4440E 12	-1.11422E 02	0.40850
33	2.0643E 15	-8.14349E 03	0.95410
34	1.0088E 14	3.65265E-04	0.96566
35	5.2664E 14	8.54538E-03	0.99564
36	3.3818E 15	6.69955E-01	0.99950
37	1.0230E 10	3.28766E-01	0.99994
38	7.7487E 09	1.19455E-01	1.00000
39	1.0230E 10	1.52998E 00	0.99999
40	1.2452E 10	2.49129E-07	0.98742
41	3.1511E 09	3.05997E-08	0.99914
42	2.9223E 12	2.75147E-04	0.99855
43	5.6123E 12	7.85590E 00	0.86950
44	8.2671E 12	1.50864E-01	0.99990
45	8.1395E 15	-7.78161E-02	0.99696
46	2.2499E 14	8.56064E 00	1.00000

47	1.3710E 12	2.02494E-02	1.00000
48	4.8034E 03	6.09339E-05	0.99174
49	4.0000E 13	8.67595E-04	0.99982
50	1.1046E 13	1.42654E-03	0.83162
51	5.8493E 13	5.64488E-02	0.76916
52	1.6360E 11	-4.00322E-04	0.16738
53	1.2000E 13	7.69502E-06	1.00000
54	3.6805E 13	9.82722E-05	0.42919
55	2.3253E 13	9.79602E-02	0.99507
56	3.7000E 12	-9.96415E-02	0.99941
57	2.0000E 13	1.12413E-03	1.00000
58	1.0000E 13	3.25853E-09	1.00000
59	2.0000E 13	2.26742E-03	0.96748
60	5.6488E 12	4.96504E-02	0.66571
61	6.6266E 12	2.41339E-01	0.95040
62	1.0484E 13	2.14319E-02	0.99994
63	9.9683E 13	4.29761E 04	1.00000
64	7.2665E 12	3.13910E 03	1.00000
65	1.1369E 13	2.35580E 03	0.99999
66	7.9000E 12	1.58807E 04	0.99998
67	7.4000E 12	1.10676E 03	1.00000
68	1.8373E 09	9.21972E 01	1.00000
69	3.0000E 13	7.62986E 04	0.99795
70	5.6235E 12	8.12325E 02	0.86871
71	4.9504E 07	-3.19247E 04	0.99982
72	4.7552E 11	-2.38381E 00	0.12313
73	6.3735E 10	6.14890E 04	0.99997

MIXTURE MOLECULAR WEIGHT 28.57954 TOTAL ENERGY EXCHANGE RATE -9.66158E 09 (CAL-CM**3/GM**2/SEC) MASS FRACTION SUM 0.99999923

TIME 6.20000E-04 SEC AREA 1.00000E 00 SQ CM AXIAL POSITION 0.00000 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.60309
VELOCITY (CM/SEC)	0.00
DENSITY (GM/CM**3)	2.77821E-04
TEMPERATURE (DEG K)	1900.68
MASS FLOW RATE (GM/SEC)	0.00000
ENTROPY (CAL/GM/DEG K)	2.4485
MACH NUMBER	0.0000
GAMMA	1.2142
ENTHALPY (CAL/GM)	3.35672E 01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	26
AVERAGE STEP SIZE	0.76923E-06
TOTAL NUMBER OF STEPS	267
FUNCT EVALUATIONS	476
JACOBIAN EVALUATIONS	65

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH3OH	1.05995E-06	1.03122E-01	-8.74267E-02
CH3	5.07595E-08	4.93832E-03	8.23407E-03
OH	1.03763E-08	1.00955E-03	2.05463E-03
O2	8.20173E-07	7.97935E-02	-3.85605E-02
CH2OH	1.44850E-07	1.40922E-02	1.75986E-02
HO2	4.64320E-08	4.51731E-03	-7.58079E-03
H2O	1.38725E-06	1.34964E-01	1.02120E-01
O	2.05565E-09	2.00011E-04	4.82950E-04
H	5.65500E-09	5.50157E-04	1.79312E-03
H2	1.66902E-07	1.62377E-02	2.31166E-02
CH4	3.10126E-08	3.01713E-03	7.33274E-03
H2O2	3.94868E-10	3.84162E-05	-1.67815E-04
CH2O	3.22703E-08	3.13954E-03	-1.81633E-03
CH	6.77563E-15	6.59192E-10	5.66791E-09
HCO	6.57388E-10	6.20107E-05	1.03154E-04
CH2	1.33909E-12	1.30279E-07	7.62756E-07
CO	7.09204E-07	6.89975E-02	5.24455E-02
CO2	2.04436E-08	1.98835E-03	3.52853E-03
NO	7.57309E-12	7.36776E-07	7.51991E-07
NO2	2.01431E-12	1.95970E-07	-7.36766E-07
N	4.16701E-15	4.05403E-10	1.10973E-09
N2	5.72199E-06	5.56635E-01	-3.61490E-09
CN	1.45773E-15	1.41821E-10	2.14962E-10
HCN	3.75010E-13	3.64842E-08	-3.62916E-09
NCO	4.74343E-14	4.61422E-09	2.13176E-09
HNCO	6.67898E-12	6.49730E-07	-3.59962E-07
NH	5.35195E-14	5.20688E-09	-1.79542E-09
NH2	2.01169E-12	1.95714E-07	3.53941E-07
AR	6.82936E-08	6.64419E-03	0.00000

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	2.0247E 09	2.71777E 05	0.95095
2	5.6147E 07	-8.22225E 03	0.92858
3	2.3555E 12	3.33255E 05	0.99280
4	8.7027E 11	2.45119E 04	0.99763
5	5.0148E 12	3.82096E 05	0.98113
6	1.2290E 12	9.54051E 04	0.99961
7	1.4934E 10	1.03090E 04	0.99029
8	3.7037E 10	2.35640E 04	0.99779
9	1.1571E 10	2.23203E 05	1.00000
10	2.0422E 11	3.14304E 05	0.99992
11	2.2009E 03	-8.08258E 04	0.98918
12	5.3957E 12	-1.15683E 04	0.48548
13	1.7505E 12	1.09361E 03	0.75630
14	6.1265E 12	6.60679E 03	0.25865
15	1.0000E 13	7.19986E-01	1.00000
16	3.7545E 13	5.34200E 02	0.99991
17	4.1750E 10	2.25192E 04	1.00000
18	6.8000E 13	9.19364E 04	1.00000
19	8.3479E 12	1.97196E 04	0.99911
20	1.4910E 13	1.28146E 04	0.99989
21	1.6002E 14	6.93934E 05	0.99966
22	3.0000E 13	5.09315E 02	1.00000
23	2.0000E 13	9.33967E 02	0.99999
24	3.0000E 13	2.57074E 03	1.00000
25	6.1213E 12	5.19358E 05	0.99957
26	4.8104E 11	4.56115E 04	0.99446
27	9.3151E 13	1.80864E 01	0.99999
28	1.1343E 07	8.54469E 01	0.99987
29	2.5812E 12	1.51410E 05	0.97616
30	3.2420E 12	1.26054E 04	0.87461
31	9.3025E 12	1.29116E 05	0.61856
32	4.7170E 12	-1.34379E 04	0.67128
33	1.9547E 15	-1.05258E 05	0.93591
34	9.1510E 13	4.58083E-02	0.88937
35	4.3668E 14	1.82057E 00	0.97897
36	2.3252E 15	7.21078E 01	0.99198
37	4.7111E 10	1.75112E 02	0.99948
38	3.5752E 10	4.83337E 01	0.99994
39	4.7111E 10	3.21430E 02	0.99980
40	5.8617E 10	5.48766E-03	0.95422
41	1.4289E 10	5.06721E-04	0.99426
42	4.4516E 12	7.87425E-01	0.98256
43	6.3902E 12	2.64996E 01	0.91025
44	8.5402E 12	4.57339E-01	0.99812
45	7.6404E 15	-9.14636E-01	0.98298
46	2.3496E 14	3.46732E 01	0.99996

47	2.3251E 12	1.02931E-01	0.99980
48	3.0738E 05	4.68345E-02	0.99973
49	4.0000E 13	2.22197E-02	0.99156
50	1.4748E 13	3.59857E-02	0.77409
51	1.0334E 14	1.40971E-01	0.13657
52	1.9059E 11	-5.79663E-02	0.85780
53	1.2000E 13	4.65927E-04	0.99999
54	5.1054E 13	-5.55980E-03	0.35718
55	2.4556E 13	3.66272E-01	0.96291
56	3.7000E 12	-3.99949E-01	0.99644
57	2.0000E 13	2.52688E-02	1.00000
58	1.0000E 13	2.56051E-08	0.99986
59	2.0000E 13	6.89665E-02	0.99223
60	9.2286E 12	-2.01198E-02	0.02081
61	1.0535E 13	4.58564E 00	0.88953
62	1.2840E 13	9.22279E-02	0.99826
63	1.0546E 14	3.56766E 05	1.00000
64	7.6739E 12	2.61053E 04	0.99999
65	1.2053E 13	1.49036E 04	0.99983
66	7.9000E 12	4.92896E 04	0.99949
67	7.4000E 12	5.04989E 04	1.00000
68	5.0947E 09	5.11520E 02	1.00000
69	3.0000E 13	2.01820E 05	0.99326
70	6.2091E 12	-7.42330E 02	0.69250
71	5.0543E 08	-1.34122E 04	0.99984
72	5.8503E 11	-1.27375E 02	0.88271
73	7.6231E 11	4.00201E 04	0.99837

MIXTURE MOLECULAR WEIGHT 27.02887 TOTAL ENERGY EXCHANGE RATE -4.06502E 10 (CAL-CM**3/GM**2/SEC) MASS FRACTION SUM 0.99999923

(GCKP) END OF THIS CASE - READ DATA FOR NEXT CASE

DISTANCE-AREA VERSION GENERAL CHEMICAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

C3H8 - AIR WELL-STIRRED REACTOR + ROCKET EXPANSION PROB. GCKP84 CASE 9

REACTION NUMBER	REACTION							REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1			1.0*C3H8	=	1.0*C2H5	+	1.0*CH3	4.50000E 16	0.0000	84900.00
2			1.0*C2H5	=	1.0*C2H4	+	1.0*H	3.16000E 13	0.0000	40700.00
3	1.0*O	+	1.0*C2H4	=	1.0*CH2O	+	1.0*CH2	2.50000E 13	0.0000	5000.00
4	1.0*O	+	1.0*C2H4	=	1.0*CH3	+	1.0*HCO	2.26000E 13	0.0000	2700.00
5	1.0*CH3	+	1.0*C3H8	=	1.0*CH4	+	1.0*C3H7	2.00000E 13	0.0000	10300.00
6			1.0*C3H7	=	1.0*C2H4	+	1.0*CH3	4.00000E 13	0.0000	33100.00
7	1.0*H	+	1.0*CH4	=	1.0*CH3	+	1.0*H2	1.26000E 14	0.0000	11900.00
8	1.0*O	+	1.0*CH4	=	1.0*CH3	+	1.0*OH	2.00000E 13	0.0000	9200.00
9	1.0*OH	+	1.0*CH4	=	1.0*CH3	+	1.0*H2O	3.00000E 13	0.0000	6000.00
10	1.0*CH	+	1.0*O2	=	1.0*HCO	+	1.0*O	1.00000E 13	0.0000	0.00
11	1.0*CH2	+	1.0*O2	=	1.0*CH2O	+	1.0*O	1.00000E 14	0.0000	3700.00
12	1.0*CH3	+	1.0*O2	=	1.0*CH2O	+	1.0*OH	1.70000E 12	0.0000	14000.00
13	1.0*CH3	+	1.0*O	=	1.0*CH2O	+	1.0*H	6.80000E 13	0.0000	0.00
14	1.0*CH2O	+	1.0*H	=	1.0*HCO	+	1.0*H2	2.00000E 13	0.0000	3300.00
15	1.0*CH2O	+	1.0*O	=	1.0*HCO	+	1.0*OH	5.00000E 13	0.0000	4570.00
16	1.0*CH2O	+	1.0*OH	=	1.0*HCO	+	1.0*H2O	5.00000E 15	0.0000	13000.00
17	1.0*HCO	+	1.0*O	=	1.0*CO	+	1.0*OH	3.00000E 13	0.0000	0.00
18	1.0*HCO	+	1.0*H	=	1.0*CO	+	1.0*H2	2.00000E 13	0.0000	0.00
19	1.0*HCO	+	1.0*OH	=	1.0*CO	+	1.0*H2O	3.00000E 13	0.0000	0.00
20	M	+	1.0*HCO	=	1.0*H	+	1.0*CO	3.00000E 14	0.0000	14700.00
21	1.0*CO	+	1.0*OH	=	1.0*CO2	+	1.0*H	4.00000E 12	0.0000	8000.00
22	1.0*CO	+	1.0*O	=	1.0*CO2	+	M	2.80000E 13	0.0000	-4540.00
23	1.0*CO	+	1.0*O2	=	1.0*CO2	+	1.0*O	1.20000E 11	0.0000	35000.00
24	1.0*H	+	1.0*O2	=	1.0*OH	+	1.0*O	2.20000E 14	0.0000	16790.00
25	1.0*O	+	1.0*H2	=	1.0*OH	+	1.0*H	1.80000E 10	1.0000	8900.00
26	1.0*H2	+	1.0*OH	=	1.0*H2O	+	1.0*H	5.20000E 13	0.0000	6500.00
27	1.0*OH	+	1.0*OH	=	1.0*O	+	1.0*H2O	6.30000E 12	0.0000	1093.00
28	1.0*H	+	1.0*O2	=	1.0*HO2	+	M	1.50000E 15	0.0000	-1000.00
29	1.0*O	+	1.0*O	=	1.0*O2	+	M	5.70000E 13	0.0000	-1788.00
30	1.0*H	+	1.0*H	=	1.0*H2	+	M	8.30000E 17	-1.0000	0.00
31	1.0*H	+	1.0*OH	=	1.0*H2O	+	M	8.40000E 21	-2.0000	0.00
32	1.0*H	+	1.0*CH3	=	1.0*H2	+	1.0*CH2	2.70000E 11	0.6700	25700.00
33	1.0*O	+	1.0*CH3	=	1.0*OH	+	1.0*CH2	1.90000E 11	0.6800	25700.00
34	1.0*OH	+	1.0*CH3	=	1.0*H2O	+	1.0*CH2	2.70000E 11	0.6700	25700.00
35	1.0*HO2	+	1.0*NO	=	1.0*NO2	+	1.0*OH	1.20000E 13	0.0000	2380.00
36	1.0*O	+	1.0*NO2	=	1.0*NO	+	1.0*O2	1.00000E 13	0.0000	596.00
37	1.0*NO	+	1.0*O	=	1.0*NO2	+	M	5.62000E 15	0.0000	-1160.00
38	1.0*NO2	+	1.0*H	=	1.0*NO	+	1.0*OH	2.90000E 14	0.0000	795.00
39	1.0*H	+	1.0*O2	=	1.0*NO	+	1.0*O	6.40000E 09	1.0000	6250.00
40	1.0*O	+	1.0*N2	=	1.0*NO	+	1.0*N	1.80000E 14	0.0000	76250.00
41	1.0*N	+	1.0*OH	=	1.0*NO	+	1.0*H	4.00000E 13	0.0000	0.00
42	1.0*CH	+	1.0*N2	=	1.0*HCN	+	1.0*N	1.50000E 11	0.0000	19000.00
43	1.0*CN	+	1.0*H2	=	1.0*HCN	+	1.0*H	6.00000E 13	0.0000	5300.00
44	1.0*O	+	1.0*HCN	=	1.0*OH	+	1.0*CN	1.40000E 11	0.6800	16900.00
45	1.0*OH	+	1.0*HCN	=	1.0*H2CO	+	1.0*H	4.00000E 11	0.0000	2800.00
46	1.0*CH	+	1.0*O	=	1.0*CO	+	1.0*N	1.20000E 13	0.0000	0.00
47	1.0*CH	+	1.0*OH	=	1.0*HCO	+	1.0*H	2.50000E 14	0.0000	6000.00
48	1.0*H2	+	1.0*HCO	=	1.0*H2CO	+	1.0*H	1.00000E 14	0.0000	9000.00
49	1.0*H2CO	+	1.0*H	=	1.0*HCO	+	1.0*CO	1.00000E 14	0.0000	8500.00
50	1.0*CN	+	1.0*O2	=	1.0*NCO	+	1.0*O	3.20000E 13	0.0000	1000.00
51	1.0*CN	+	1.0*CO2	=	1.0*NCO	+	1.0*CO	3.70000E 12	0.0000	0.00
52	1.0*O	+	1.0*NCO	=	1.0*NO	+	1.0*CO	2.00000E 13	0.0000	0.00
53	1.0*N	+	1.0*NCO	=	1.0*N2	+	1.0*CO	1.00000E 13	0.0000	0.00
54	1.0*H	+	1.0*HCO	=	1.0*NH	+	1.0*CO	2.00000E 13	0.0000	0.00
55	1.0*NH	+	1.0*OH	=	1.0*N	+	1.0*H2O	5.00000E 11	0.5000	2000.00
56	1.0*CH	+	1.0*CO2	=	1.0*HCO	+	1.0*CO	3.70000E 12	0.0000	0.00
57	1.0*H	+	1.0*C2H4	=	1.0*H2	+	1.0*C2H3	1.10000E 14	0.0000	8500.00
58	1.0*OH	+	1.0*C2H4	=	1.0*H2O	+	1.0*C2H3	1.00000E 14	0.0000	3500.00
59	M	+	1.0*C2H3	=	1.0*C2H2	+	1.0*H	3.00000E 16	0.0000	40500.00
60	1.0*O	+	1.0*C2H2	=	1.0*CH2	+	1.0*CO	5.20000E 13	0.0000	3700.00
61	1.0*H	+	1.0*CH2	=	1.0*H2	+	1.0*CH	2.90000E 11	0.7000	26000.00
62	1.0*O	+	1.0*CH2	=	1.0*OH	+	1.0*CH	3.20000E 11	0.5000	26000.00
63	1.0*OH	+	1.0*CH2	=	1.0*H2O	+	1.0*CH	5.00000E 11	0.5000	6000.00

64	1.0*CH	+ 1.0*NO	=	1.0*N	+ 1.0*HCO	1.00000E 14	0.0000	0.00
65	1.0*CH	+ 1.0*NO	=	1.0*O	+ 1.0*HCN	1.00000E 13	0.0000	0.00
66	1.0*CH3	+ 1.0*OH	=	1.0*CH2O	+ 1.0*H2	7.40000E 12	0.0000	0.00
67	1.0*H2	+ 1.0*HO2	=	1.0*H2O	+ 1.0*OH	7.20000E 11	0.0000	18700.00
68	1.0*HCO	+ 1.0*O2	=	1.0*CO	+ 1.0*HO2	3.00000E 13	0.0000	0.00
69	1.0*C2H5	+ 1.0*O2	=	1.0*C2H4	+ 1.0*HO2	1.50000E 12	0.0000	4860.00
70	1.0*H	+ 1.0*C2H5	=	1.0*C2H6	+ 1.0*H2	4.80000E 13	0.0000	0.00
71	1.0*CH3	+ 1.0*CH2	=	1.0*C2H4	+ 1.0*H	2.00000E 13	0.0000	0.00
72	1.0*OH	+ 1.0*C2H2	=	1.0*C2H	+ 1.0*H2O	6.00000E 12	0.0000	7000.00
73	1.0*C2H	+ 1.0*O	=	1.0*CO	+ 1.0*CH	1.40000E 13	0.0000	3150.00
74	1.0*C2H	+ 1.0*O2	=	1.0*HCO	+ 1.0*CO	1.00000E 13	0.0000	7000.00
75	1.0*C2H2	+ 1.0*O2	=	2.0*HCO		4.00000E 12	0.0000	28000.00
76	M	+ 1.0*C2H2	=	1.0*C2H	+ 1.0*H	1.00000E 14	0.0000	114000.00
77	1.0*O	+ 1.0*C2H2	=	1.0*C2H	+ 1.0*OH	3.20000E 15	-0.6000	17000.00
78	M	+ 1.0*C2H5	=	1.0*C2H4	+ 1.0*H	6.80000E 17	0.0000	31800.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(O2	, 28) = 2.00000	M(O2	, 31) = 1.60000	M(N2	, 28) = 2.00000	M(N2	, 31) = 1.60000
M(H2O	, 28) = 32.50000	M(H2O	, 31) = 20.00000	M(CO2	, 28) = 7.50000	M(CO2	, 31) = 7.50000
M(CO	, 28) = 2.00000	M(CO	, 31) = 1.60000				

INTEGRATION CONTROLS

INITIAL STEP SIZE 0.10000E-06 CM

MAXIMUM RELATIVE ERROR 0.10000E-03

** ASSIGNED VARIABLE PROFILE **

WELL - STIRRED REACTOR CASE - AREA IS REACTOR VOLUME

HEAT TRANSFER CASE QDOT(CAL/SEC) = (0.00000)T**2 + (5.00000E-02)T + (-4.28800E 01)

** INITIAL CONDITIONS **

TIME 0.00000 SEC AREA 6.02600E 03 SQ CM AXIAL POSITION 2.00000E-01 CM

FLOW PROPERTIES

PRESSURE (ATM)	5.00000
VELOCITY (CM/SEC)	0.00
DENSITY (GM/CM**3)	2.96319E-03
TEMPERATURE (DEG K)	614.00
MASS FLOW RATE (GM/SEC)	8.50000E 01
ENTROPY CAL/GM/DEG K)	1.7275
MACH NUMBER	0.0000
GAMMA	1.2954
ENTHALPY (CAL/GM)	3.60538E 01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

HEAT LOSS(QDOT/TOTMAS) = -1.4329E-01 CAL/G

CHEMICAL PROPERTIES

SPECIES	MASS FRACTION	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE*CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
C3H8	8.73261E-02	5.91295E-02	-1.59235E-19	1	2.7136E-14	1.81351E-14	1.00000
C2H5	0.00000	0.00000	1.59235E-19	2	1.0298E-01	0.00000	0.00000
CH3	0.00000	0.00000	1.59235E-19	3	4.1516E 11	0.00000	0.00000
C2H4	0.00000	0.00000	0.00000	4	2.4721E 12	0.00000	0.00000
H	0.00000	0.00000	0.00000	5	4.3133E 09	0.00000	0.00000
O	0.00000	0.00000	1.34584E-35	6	6.6116E 01	0.00000	0.00000
CH2O	0.00000	0.00000	0.00000	7	7.3221E 09	0.00000	0.00000
CH2	0.00000	0.00000	0.00000	8	1.0625E 10	0.00000	0.00000
HCO	0.00000	0.00000	0.00000	9	2.1951E 11	0.00000	0.00000
CH4	0.00000	0.00000	0.00000	10	1.0000E 13	0.00000	0.00000
C3H7	0.00000	0.00000	0.00000	11	4.8195E 12	0.00000	0.00000
H2	0.00000	0.00000	0.00000	12	1.7670E 07	0.00000	0.00000
OH	0.00000	0.00000	0.00000	13	6.8000E 13	0.00000	0.00000
H2O	0.00000	0.00000	0.00000	14	1.3379E 12	0.00000	0.00000
CH	0.00000	0.00000	0.00000	15	1.1811E 12	0.00000	0.00000
O2	2.11232E-01	1.97115E-01	-6.72841E-36	16	1.1795E 11	0.00000	0.00000
CO	0.00000	0.00000	1.61026E-39	17	3.0000E 13	0.00000	0.00000
CO2	4.16200E-04	2.82370E-04	-1.61026E-39	18	2.0000E 13	0.00000	0.00000
HO2	0.00000	0.00000	0.00000	19	3.0000E 13	0.00000	0.00000
NO	0.00000	0.00000	0.00000	20	1.7569E 09	0.00000	0.00000
NO2	0.00000	0.00000	0.00000	21	5.6820E 09	0.00000	0.00000
N	0.00000	0.00000	0.00000	22	1.1565E 15	-1.83390E-34	1.00000
N2	6.89289E-01	7.34701E-01	0.00000	23	4.1796E-02	0.00000	0.00000
HCN	0.00000	0.00000	0.00000	24	2.3234E 08	0.00000	0.00000
CN	0.00000	0.00000	0.00000	25	7.5082E 09	0.00000	0.00000
HNCO	0.00000	0.00000	0.00000	26	2.5256E 11	0.00000	0.00000
NCO	0.00000	0.00000	0.00000	27	2.5721E 12	0.00000	0.00000
NH2	0.00000	0.00000	0.00000	28	3.4044E 15	0.00000	0.00000
NH	0.00000	0.00000	0.00000	29	2.4678E 14	-7.66288E-31	1.00000
C2H3	0.00000	0.00000	0.00000	30	1.3518E 15	0.00000	0.00000

C2H2	0.00000	0.00000	0.00000
C2H	0.00000	0.00000	0.00000
AR	1.17370E-02	8.77265E-03	0.00000

31	2.2231E 16	0.00000	0.00000
32	1.4180E 04	0.00000	0.00000
33	1.0640E 04	0.00000	0.00000
34	1.4180E 04	0.00000	0.00000
35	1.7062E 12	0.00000	0.00000
36	6.1356E 12	0.00000	0.00000
37	1.4542E 16	0.00000	0.00000
38	1.5115E 14	0.00000	0.00000
39	2.3426E 10	0.00000	0.00000
40	1.3017E-13	0.00000	0.00000
41	4.0000E 13	0.00000	0.00000
42	2.5391E 04	0.00000	0.00000
43	7.7920E 11	0.00000	0.00000
44	1.0632E 07	0.00000	0.00000
45	4.0310E 10	0.00000	0.00000
46	1.2000E 13	0.00000	0.00000
47	1.8293E 12	0.00000	0.00000
48	6.2589E 10	0.00000	0.00000
49	9.4292E 10	0.00000	0.00000
50	1.4100E 13	0.00000	0.00000
51	3.7000E 12	0.00000	0.00000
52	2.0000E 13	0.00000	0.00000
53	1.0000E 13	0.00000	0.00000
54	2.0000E 13	0.00000	0.00000
55	2.4053E 12	0.00000	0.00000
56	3.7000E 12	0.00000	0.00000
57	1.0372E 11	0.00000	0.00000
58	5.6780E 12	0.00000	0.00000
59	1.1518E 02	0.00000	0.00000
60	2.5062E 12	0.00000	0.00000
61	1.4440E 04	0.00000	0.00000
62	4.4125E 03	0.00000	0.00000
63	9.0654E 10	0.00000	0.00000
64	1.0000E 14	0.00000	0.00000
65	1.0000E 13	0.00000	0.00000
66	7.4000E 12	0.00000	0.00000
67	1.5392E 05	0.00000	0.00000
68	3.0000E 13	0.00000	0.00000
69	2.7938E 10	0.00000	0.00000
70	4.8000E 13	0.00000	0.00000
71	2.0000E 13	0.00000	0.00000
72	1.9344E 10	0.00000	0.00000
73	1.0590E 12	0.00000	0.00000
74	3.2240E 10	0.00000	0.00000
75	4.3214E 02	0.00000	0.00000
76	2.6445E-27	0.00000	0.00000
77	6.0422E 07	0.00000	0.00000
78	3.2620E 06	0.00000	0.00000

MIXTURE MOLECULAR WEIGHT 29.85855 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) 1.55311E-09 MASS FRACTION SUM 0.99999976

**EQUILIBRIUM CONDITIONS **

TIME 0.00000 SEC AREA 6.02600E 03 SQ CM AXIAL POSITION 2.00000E-01 CM

FLOW PROPERTIES

PRESSURE (ATM)	5.00000
VELOCITY (CM/SEC)	0.00
DENSITY (GM/CM**3)	7.12366E-04
TEMPERATURE (DEG K)	2205.19
MASS FLOW RATE (GM/SEC)	8.50000E 01
ENTROPY CAL/GM/DEG K)	2.3431
MACH NUMBER	0.0000
GAMMA	1.2663
ENTHALPY (CAL/GM)	3.60469E 01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

HEAT LOSS(QDOT/TOTMAS) = 7.9270E-01 CAL/G

CHEMICAL PROPERTIES

SPECIES	MASS FRACTION	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE*CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
C3H8	4.40970E-09	2.57804E-09	-1.23516E-05	1	1.7339E 08	2.43399E 01	1.00000
C2H5	2.90620E-09	2.57804E-09	-1.13991E-03	2	2.9243E 09	4.10432E 02	0.99980
CH3	1.50350E-09	2.57804E-09	1.50621E-03	3	7.9874E 12	4.55171E-05	0.99992
C2H6	2.80540E-09	2.57804E-09	2.64640E-03	4	1.2204E 13	6.95543E-05	1.00000
H	2.52253E-05	6.45174E-04	1.15914E-03	5	1.9065E 12	6.93072E-10	0.03635
O	9.11820E-07	1.46925E-06	1.02426E-07	6	2.0971E 10	2.94383E 03	1.00000
CH2O	2.42073E-08	2.07844E-08	3.19108E-09	7	8.3367E 12	-6.17024E-02	0.74731
CH2	1.40270E-09	2.57804E-09	7.69043E-08	8	2.4504E 12	-4.13041E-05	0.74732
HCO	8.92935E-08	7.93291E-08	3.61857E-07	9	7.6292E 12	-1.83030E-02	0.74732
CH4	1.60430E-09	2.57804E-09	4.06209E-08	10	1.0000E 13	5.42740E-05	1.00009
C3H7	4.30890E-09	2.57804E-09	-1.49389E-03	11	4.2984E 13	2.33265E-04	0.99989
H2	4.87684E-03	6.26233E-02	-1.13909E-06	12	6.9655E 10	3.75789E-07	0.99403
OH	1.37955E-04	2.09122E-04	2.78653E-06	13	6.8000E 13	3.85225E-04	0.99403
H2O	5.86391E-02	1.41165E-01	-2.91445E-06	14	9.4184E 12	-1.32565E-06	0.00001
CH	1.30130E-09	2.57804E-09	-4.31874E-07	15	1.7622E 13	-4.02171E-08	0.00005
O2	1.73561E-06	1.39921E-06	6.24289E-09	16	2.5738E 14	-4.98020E-05	0.00003
CO	1.16632E-01	1.07344E-01	1.47127E-07	17	3.0000E 13	-2.18871E-07	0.00034
CO2	7.86322E-02	4.60616E-02	-1.22491E-07	18	2.0000E 13	1.68094E-06	0.00000
HO2	3.30050E-09	2.57804E-09	-1.90870E-09	19	3.0000E 13	-1.61136E-05	0.00002
NO	3.63426E-05	3.12240E-05	3.59720E-07	20	1.0477E 13	-2.33873E-04	0.00000
NO2	4.60060E-09	2.57804E-09	-3.66425E-07	21	6.4447E 11	7.25409E-01	0.00003
N	2.54410E-09	4.68856E-09	8.63199E-09	22	7.8905E 13	-4.18470E-06	0.00001
N2	6.89277E-01	6.35342E-01	-2.45161E-09	23	4.0779E 07	7.08769E-07	0.00008
HCN	8.55613E-08	8.16173E-08	2.17332E-06	24	4.7689E 12	2.82328E-04	0.00004

CN	2.60180E-09	2.57804E-09	-2.34256E-06	25	5.2079E 12	-3.07811E-02	0.00004
HNCO	4.02312E-08	2.41063E-08	1.53472E-06	26	1.1795E 13	-5.25617E 00	0.00002
NCO	4.23170E-09	2.57804E-09	-1.39216E-06	27	4.9093E 12	6.48730E-03	0.00002
NH2	1.69[illegible]E-08	3.04965E-08	3.29301E-12	28	1.0845E 15	-1.27656E-02	0.02707
NH	1.5[illegible]95E-09	2.65607E-09	2.46584E-08	29	8.5713E 13	-6.53963E-10	0.00008
C2H3	2.[illegible]46E-09	2.57804E-09	-5.97269E-06	30	3.7638E 14	8.32724E-06	0.00000
C2H2	2.60[illegible]3E-09	2.57804E-09	5.75567E-06	31	1.7274E 15	-9.14938E-04	0.00002
C2H	2.60503E-09	2.57804E-09	-3.61833E-08	32	1.3317E 11	-1.81983E-02	0.98202
AR	1.17370E-02	7.57447E-03	0.00000	33	1.0121E 11	-3.14986E-05	0.98202
				34	1.3317E 11	-5.89881E-03	0.98202
				35	6.9712E 12	-9.20742E-03	0.91600
				36	8.7284E 12	4.56782E-05	0.91827
				37	7.3232E 15	-1.56952E-01	0.91828
				38	2.4138E 14	5.55864E-01	0.91828
				39	3.3901E 12	1.48937E-09	0.00004
				40	4.9930E 06	-3.35432E-07	0.00005
				41	4.0000E 13	5.77606E-08	0.00000
				42	1.9936E 09	4.85159E-03	1.00000
				43	1.7901E 13	4.28222E 00	0.98432
				44	5.5560E 11	-6.29184E-03	0.98432
				45	2.1113E 11	-1.97335E-08	0.00000
				46	1.2000E 13	6.73165E-05	0.98432
				47	6.3577E 13	2.38498E-02	0.46246
				48	1.2324E 13	3.02429E 00	0.97082
				49	1.4374E 13	6.49898E-06	0.00002
				50	2.5471E 13	6.39343E-05	0.46249
				51	3.7000E 12	3.05711E-01	0.46244
				52	2.0000E 13	1.10656E-04	0.97082
				53	1.0000E 13	1.76331E-07	0.97082
				54	2.0000E 13	4.85912E-02	0.97082
				55	1.4876E 13	-5.86712E-06	0.[illegible]0000
				56	3.7000E 12	6.61073E-01	1.00000
				57	1.5312E 13	-2.59470E-01	0.86[illegible]8
				58	4.4991E 13	-2.39312E-01	0.86[illegible]
				59	2.9059E 12	1.12709E 01	0.99991
				60	2.2352E 13	1.11546E-04	0.87567
				61	1.6828E 11	-1.37413E-02	0.9702[illegible]
				62	3.9219E 10	-7.40503E-06	0.970[illegible]7
				63	5.9710E 12	-1.58047E-01	0.97027
				64	1.0000E 14	1.21117E-02	1.00000
				65	1.0000E 13	1.21117E-03	1.00000
				66	7.4000E 12	5.96683E-03	0.99403
				67	1.0093E 10	6.63123E-05	0.02705
				68	3.0000E 13	-1.37384E-04	0.02707
				69	4.9400E 11	2.68475E-06	0.99980
				70	4.8000E 13	1.20100E-01	0.99980
				71	2.0000E 13	-1.41967E-05	0.98611
				72	1.2145E 12	-7.09864E-02	0.98631
				73	6.8225E 12	3.66564E-05	0.94277
				74	2.0242E 12	1.09861E-05	1.00000
				75	6.7152E 02	3.64460E-08	0.99999
				76	5.0326E 02	-1.40656E-07	0.98631
				77	6.52C2E 11	-2.67756E-04	0.98631
				78	4.7563E 14	1.86007E 03	0.99980

MIXTURE MOLECULAR WEIGHT 25.78036 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) 1.65254E 08 MASS FRACTION SUM 1.00001621

WELLSTIRRED REACTOR CALCULATION.... C3H8 - AIR WELL-STIRRED REACTOR + ROCKET EXPANSION PROB. GCKP84 CASE 9

	INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE ATM	5.00000	5.00000	1.00000
TEMP. DEG K	614.000	2198.85	3.58119
ENTROPY CAL/GM/K	1.72751	2.34214	1.35579
DENSITY GM/CM**3	2.96319E-03	7.14637E-04	0.24117
ENTHALPY CAL/GM	36.0938	35.2653	0.978130
MOL. WT. OF MIXT	29.0506	25.7282	
GAMMA	1.2954	1.2663	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
C3H8	5.91295E-02	8.73261E-02	2.57882E-09	4.40970E-09
C2H5	0.00000	0.00000	2.57882E-09	2.90620E-09
CH3	0.00000	0.00000	1.60404E-05	9.35652E-06
C2H4	0.00000	0.00000	1.17549E-06	1.27876E-06
H	0.00000	0.00000	1.17513E-03	4.59317E-05
O	0.00000	0.00000	5.11200E-06	3.17161E-06
CH2O	0.00000	0.00000	5.23931E-07	6.10029E-07
CH2	0.00000	0.00000	3.78767E-06	2.06023E-06
HCO	0.00000	0.00000	1.51413E-07	1.70380E-07
CH4	0.00000	0.00000	3.43997E-05	2.14003E-05
C3H7	0.00000	0.00000	2.57882E-09	4.30890E-09
H2	0.00000	0.00000	6.18211E-02	4.83264E-03
OH	0.00000	0.00000	3.82913E-04	2.52539E-04
H2O	0.00000	0.00000	1.41235E-01	9.86928E-02
CH	0.00000	0.00000	4.29721E-08	2.16942E-08
O2	1.97115E-01	2.11232E-01	2.33939E-05	2.90263E-05
CO	0.00000	0.00000	1.06415E-01	1.15588E-01
CO2	2.82370E-04	4.16200E-04	4.63922E-02	7.91727E-02
HO2	0.00000	0.00000	7.85497E-08	1.09532E-07
NO	0.00000	0.00000	5.43310E-05	6.32171E-05
NO2	0.00000	0.00000	2.57832E-09	4.60260E-09
N	0.00000	0.00000	2.87572E-08	1.56200E-08
N2	7.34701E-01	6.89289E-01	6.34516E-01	6.89256E-01
HCN	0.00000	0.00000	2.27749E-06	2.38660E-06
CN	0.00000	0.00000	2.57882E-09	2.60180E-09
HNCO	0.00000	0.00000	5.92172E-07	9.87979E-07
NCO	0.00000	0.00000	2.57882E-09	4.20170E-09
NH2	0.00000	0.00000	1.38724E-06	8.61933E-07
NH	0.00000	0.00000	2.27379E-08	1.32390E-08
C2H3	0.00000	0.00000	6.03991E-08	6.33451E-08
C2H2	0.00000	0.00000	2.84564E-04	2.87321E-04
C2H	0.00000	0.00000	7.14239E-06	6.93239E-06
AR	8.77265E-03	1.17370E-02	7.57678E-03	1.17370E-02

HEAT LOSS(QDOT/MDOT) = 7.8896E-01 CAL/G

VOLUME 6026.00 CM**3 MASS FLO 85.00 GM/SEC

MDOT/VOLUME = 0.01411 RESIDENCE TIME = 50.6636 MSEC ITERATIONS = 19

WELLSTIRRED REACTOR CALCULATION.... C3H8 - AIR WELL-STIRRED REACTOR + ROCKET EXPANSION PROB. GCKP84 CASE 9

	INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE ATM	5.00000	5.00000	1.00000
TEMP. DEG K	614.000	2182.60	3.55472
ENTROPY CAL/GM/K	1.72751	2.34167	1.35563
DENSITY GM/CM**3	2.96319E-03	7.19134E-04	0.24269
ENTHALPY CAL/GM	36.0538	35.9794	0.997938
MOL. WT. OF MIXT	29.8586	25.7587	
GAMMA	1.2954	1.2668	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
C3H8	5.91295E-02	8.73261E-02	7.05912E-08	1.20847E-07
C2H5	0.00000	0.00000	2.57587E-09	2.90620E-09
CH3	0.00000	0.00000	4.19402E-05	2.64799E-05
C2H4	0.00000	0.00000	4.20580E-06	4.58056E-06
H	0.00000	0.00000	3.2072xE-03	1.25502E-04
O	0.00000	0.00000	3.8411xE-05	2.38548E-05
CH2O	0.00000	0.00000	1.86505E-06	2.17402E-06
CH2	0.00000	0.00000	2.20528E-05	1.20089E-05
HCO	0.00000	0.00000	4.72258E-07	5.32024E-07
CH4	0.00000	0.00000	3.24704E-05	2.02231E-05
C3H7	0.00000	0.00000	2.57537E-09	4.30890E-09
H2	0.00000	0.00000	6.10244E-02	4.77582E-03
OH	0.00000	0.00000	1.02721E-03	6.78207E-04
H2O	0.00000	0.00000	1.40315E-01	9.81272E-02
CH	0.00000	0.00000	6.64732E-07	3.35969E-07
O2	1.97115E-01	2.11232E-01	1.06587E-04	1.32401E-04
CO	0.00000	0.00000	1.05722E-01	1.14966E-01
CO2	2.82370E-04	4.16200E-04	4.65879E-02	7.95975E-02
HO2	0.00000	0.00000	1.07095E-06	1.37228E-06
NO	0.00000	0.00000	8.85975E-05	1.03206E-04
NO2	0.00000	0.00000	2.57587E-09	4.60060E-09
N	0.00000	0.00000	1.92562E-07	1.04710E-07
N2	7.34701E-01	6.89289E-01	6.33768E-01	6.89231E-01
HCN	0.00000	0.00000	6.29488E-06	6.60456E-06
CN	0.00000	0.00000	1.45736E-05	1.47202E-08
HNCO	0.00000	0.00000	1.32950E-06	2.22068E-06
NCO	0.00000	0.00000	2.12527E-05	3.46668E-08
NH2	0.00000	0.00000	8.74725E-06	5.44115E-05
NH	0.00000	0.00000	1.02992E-07	6.00387E-08
C2H3	0.00000	0.00000	3.41653E-07	3.58726E-07
C2H2	0.00000	0.00000	3.97843E-06	4.02156E-06
C2H	0.00000	0.00000	2.68655E-05	2.61054E-05
AR	8.77265E-03	1.17370E-02	7.56812E-03	1.17370E-02

HEAT LOSS(QDOT/MDOT) = 7.4859E-02 CAL/G

VOLUME 6026.00 CM**3 MASS FLO 885.00 GM/SEC

MDOT/VOLUME = 0.14686 RESIDENCE TIME = 6.8966 MSEC ITERATIONS = 8

WELLSTIRRED REACTOR CALCULATION.... C3H8 - AIR WELL-STIRRED REACTOR + ROCKET EXPANSION PROB. GCKP84 CASE 9

	INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE ATM	5.00000	5.00000	1.00000
TEMP. DEG K	614.000	2172.26	3.53788
ENTROPY CAL/GM/K	1.72751	2.34155	1.35565
DENSITY GM/CM**3	2.96319E-03	7.22007E-04	0.24366
ENTHALPY CAL/GM	36.0538	36.0153	0.998932
MOL. WT. OF MIXT	29.8586	25.7391	
GAMMA	1.2954	1.2672	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
C3H8	5.91295E-02	8.73261E-02	1.46744E-07	2.51406E-07
C2H5	0.00000	0.00000	1.03167E-08	1.16486E-08
CH3	0.00000	0.00000	5.15940E-05	3.01377E-05
C2H4	0.00000	0.00000	5.89461E-06	6.42476E-06
H	0.00000	0.00000	4.34917E-03	1.70318E-04
O	0.00000	0.00000	7.01475E-05	4.36036E-05
CH2O	0.00000	0.00000	2.65920E-06	3.10210E-06
CH2	0.00000	0.00000	3.29857E-05	1.79762E-05
HCO	0.00000	0.00000	6.87362E-07	7.74941E-07
CH4	0.00000	0.00000	2.92865E-05	1.82541E-05
C3H7	0.00000	0.00000	2.57391E-09	4.30890E-09
H2	0.00000	0.00000	6.07133E-02	4.75510E-03
OH	0.00000	0.00000	1.37192E-03	9.06493E-04
H2O	0.00000	0.00000	1.39677E-01	9.77557E-02
CH	0.00000	0.00000	1.33003E-06	6.72738E-07
O2	1.97115E-01	2.11232E-01	1.63462E-04	2.03204E-04
CO	0.00000	0.00000	1.05464E-01	1.14773E-01
CO2	2.82370E-04	4.16200E-04	4.66539E-02	7.97713E-02
HO2	0.00000	0.00000	2.36449E-06	3.03197E-06
NO	0.00000	0.00000	9.80938E-05	1.14355E-04
NO2	0.00000	0.00000	2.57391E-09	4.60060E-09
N	0.00000	0.00000	3.07919E-07	1.67567E-07
N2	7.34701E-01	6.89289E-01	6.33276E-01	6.89223E-01
HCN	0.00000	0.00000	7.56242E-06	7.91953E-06
CN	0.00000	0.00000	2.27813E-08	2.30281E-08
HNCO	0.00000	0.00000	1.44177E-06	2.41004E-06
NCO	0.00000	0.00000	2.96390E-08	4.83834E-08
NH2	0.00000	0.00000	1.30674E-05	8.13469E-06
NH	0.00000	0.00000	1.48310E-07	8.65174E-08

C2H3	0.00000	0.00000	5.75936E-07	6.05179E-07
C2H2	0.00000	0.00000	4.12559E-04	4.17350E-04
C2H	0.00000	0.00000	3.71221E-05	3.60995E-05
AR	7.77265E-03	1.17370E-02	7.56234E-03	1.17370E-02

HEAT LOSS(QDOT/MDOT) = 3.9011E-02 CAL/G

VOLUME 6026.00 CM**3 MASS FLO 1685.00 GM/SEC

MDOT/VOLUME = 0.27962 RESIDENCE TIME = 2.5821 MSEC ITERATIONS = 7

** INITIAL CONDITIONS **

TIME 0.00000 SEC AREA 1.90000E 01 SQ CM AXIAL POSITION 2.00000E-01 CM

FLOW PROPERTIES

PRESSURE (ATM)	5.00000
VELOCITY (CM/SEC)	122830.23
DENSITY (GM/CM**3)	7.22007E-04
TEMPERATURE (DEG K)	2172.26
MASS FLOW RATE (GM/SEC)	1.68500E 03
ENTROPY (CAL/GM/DEG K)	2.3416
MACH NUMBER	1.3026
GAMMA	1.2672
ENTHALPY (CAL/GM)	3.60156E 01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHAMBER PRESS = 300.0 PSIA THROAT AREA = 2.20000E 00 SQ IN

ISP = 1228.3 METERS/SEC = 125.3 LB-SEC/LB IVAC = 1799.6 METERS/SEC = 183.5 LB-SEC/LB

CSTAR = 5716.3 FT/SEC THRUST COEFF = 0.7050 AREA RATIO = 1.339

HEAT LOSS(QDOT/MDOT) = 3.9011E-02 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	MASS FRACTION	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
C3H8	2.51406E-07	1.46744E-07	-5.32087E-04
C2H5	1.16486E-08	1.03167E-08	-2.18980E-05
CH3	3.01377E-05	5.15940E-05	1.37167E-03
C2H4	6.42476E-06	5.89461E-06	1.39478E-03
H	1.70318E-04	4.34917E-03	2.85693E-03
O	4.36036E-05	7.01474E-05	1.28576E-05
CH2O	3.10210E-06	2.65920E-06	2.49796E-06
CH2	1.79762E-05	3.29857E-05	-7.24463E-07
HCO	7.74941E-07	6.87362E-07	-8.31163E-05
CH4	1.82541E-05	2.92865E-05	-2.38145E-07
C3H7	4.30890E-09	2.57391E-09	-1.35026E-03
H2	4.75510E-03	6.07133E-02	-1.77066E-03
OH	9.06493E-04	1.37192E-03	-2.93721E-03
H2O	9.77557E-02	1.39677E-01	3.93281E-03
CH	6.72738E-07	1.33003E-06	-1.65300E-07
O2	2.03204E-04	1.63462E-04	-1.65603E-03
CO	1.14773E-01	1.05664E-01	8.25656E-04
CO2	7.97713E-02	4.66539E-02	7.70424E-04
HO2	3.03197E-06	2.36649E-06	1.19266E-07
NO	1.14355E-04	9.80937E-05	3.64220E-07
NO2	4.50060E-09	2.57391E-09	6.25406E-07
N	1.67567E-07	3.07919E-07	-6.75758E-10
N2	6.89223E-01	6.33276E-01	-5.93371E-07
HCN	7.91953E-06	7.56242E-06	1.45471E-07
CN	2.30281E-08	2.27813E-08	-6.25027E-08
HNCO	2.41004E-06	1.44177E-06	-2.64127E-08
NCO	4.83334E-08	2.96390E-08	-1.09782E-07
NH2	8.13469E-06	1.30674E-05	2.58515E-07
NH	8.65174E-08	1.48310E-07	1.50433E-09
C2H3	6.05179E-07	5.75936E-07	-4.69582E-05
C2H2	4.17350E-04	4.12559E-04	5.00481E-05
C2H	3.60995E-05	3.71221E-05	5.73308E-07
AR	1.17370E-02	7.56234E-03	0.00000

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE*CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.2926E 08	1.02068E 03	0.99399
2	2.5403E 09	1.84432E 02	0.13078
3	7.8504E 12	4.89387E 00	0.99880
4	1.2091E 13	7.56465E 00	1.00000
5	1.8397E 12	2.08273E-02	0.99063
6	1.8702E 10	2.59024E 03	0.99999
7	8.0005E 12	-7.89691E-01	0.00051
8	2.3737E 12	2.75660E-01	0.03745
9	7.4725E 12	9.91693E-01	0.00219
10	1.0000E 13	3.28165E 03	1.00000
11	4.2437E 13	3.65383E 02	1.00000
12	6.6362E 10	8.44704E-01	1.00000
13	6.8000E 13	3.71477E 02	1.00000
14	9.3115E 12	1.61052E 02	0.99078
15	1.7345E 13	4.84051E 00	0.99113
16	2.4606E 14	1.34254E 03	0.99380
17	3.0000E 13	2.15838E 00	0.98854
18	2.0000E 13	8.91729E 01	0.98809
19	3.0003E 13	4.21951E 01	0.98812
20	9.9578E 12	1.92977E 03	0.18679
21	6.2638E 11	1.81637E 03	0.01327
22	8.0154E 13	2.47586E 01	0.98610
23	3.6128E 07	5.50973E-01	0.58607
24	4.4908E 12	2.80306E 03	0.58050
25	4.9746E 12	1.21344E 03	0.03794
26	1.1536E 13	3.91633E 03	0.00270
27	4.8907E 12	-5.09020E 02	0.03534
28	1.8910E 15	3.63242E 00	0.03991
29	8.6251E 13	1.73666E-02	0.96642
30	3.8209E 16	3.01534E 03	0.93536
31	1.7801E 15	1.95013E 03	0.93540
32	1.2962E 11	-1.70815E 02	0.80699
33	9.1662E 10	-1.99514E 00	0.79937
34	1.2062E 11	-5.37025E 01	0.00646
35	6.9140E 12	2.35611E 00	0.97336
36	8.7194E 12	1.10603E-03	0.46594
37	7.3534E 15	2.00742E 00	0.93712
38	2.4122E 14	3.16277E 00	0.77596
39	3.2605E 12	2.43962E-01	0.93251
40	3.8353E 06	-1.18956E 00	0.82224
41	4.0000E 13	2.44437E 01	0.95836
42	1.6357E 09	2.33756E 00	0.99996
43	1.7576E 13	-2.80541E 00	0.07102
44	5.1871E 11	4.40238E-02	0.10627
45	2.0912E 11	1.17645E 00	0.36322
46	1.2000E 13	2.88926E-02	0.99816
47	6.2271E 13	9.57401E-01	0.32590
48	1.2431E 13	-7.31211E-01	0.02120
49	1.3958E 13	4.95910E-01	0.00375
50	2.5333E 13	1.02329E-01	0.71722
51	3.7000E 12	1.88071E 00	0.31684
52	2.0000E 13	6.27581E-02	0.99989
53	1.0000E 13	1.37754E-04	0.99998
54	2.0000E 13	3.81935E 00	0.98146

55	1.4662E 13	3.81646E 00	0.84750
56	3.7000E 12	3.46549E 02	1.00000
57	1.5356E 13	5.30974E 02	0.89372
58	4.4449E 13	4.85073E 02	0.85401
59	2.5260E 12	1.10615E 03	0.50372
60	2.2067E 13	9.63797E 02	0.99933
61	1.5219E 11	2.66041E 01	0.80726
62	3.6121E 10	1.02764E-01	0.81458
63	5.8065E 12	3.20282E 02	0.80778
64	1.0005E 14	1.96932E 01	1.00000
65	1.0069E 13	1.96931E 00	0.99929
66	7.6089E 12	7.90629E 02	1.00003
67	9.4607E 09	2.03787E 00	0.99405
68	3.0005E 13	9.91332E-01	0.19484
69	4.8555E 11	1.72640E-04	0.11939
70	4.8000E 13	3.20951E 00	0.92727
71	2.0000E 13	5.11954E 01	0.99547
72	1.1855E 12	4.36505E 01	0.04310
73	6.7485E 12	2.65248E 01	0.99997
74	1.9758E 12	1.80966E 01	1.00000
75	6.0953E 09	6.20455E-01	1.00000
76	3.3224E 02	-1.36303E-02	0.98474

TIME 3.39508E-06 SEC AREA 2.90000E 01 SQ CM AXIAL POSITION 7.0000CE-01 CM

FLOW PROPERTIES

PRESSURE (ATM)	2.04278
VELOCITY (CM/SEC)	162892.26
DENSITY (GM/CM**3)	3.56577E-04
TEMPERATURE (DEG K)	1797.05
MASS FLOW RATE (GM/SEC)	1.68442E 03
ENTROPY (CAL/GM/DEG K)	2.3417
MACH NUMBER	1.8928
GAMMA	1.2759
ENTHALPY (CAL/GM)	-1.00769E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	8
AVERAGE STEP SIZE	0.37500E-01
TOTAL NUMBER OF STEPS	97
FUNCT EVALUATIONS	192
JACOBIAN EVALUATIONS	22

CHAMBER PRESS = 300.0 PSIA THROAT AREA = 2.20000E 00 SQ IN

ISP = 1628.9 METERS/SEC = 166.1 LB-SEC/LB IVAC = 1985.3 METERS/SEC = 202.4 LB-SEC/LB

CSTAR = 5718.2 FT/SEC THRUST COEFF = 0.7346 AREA RATIO = 2.043

HEAT LOSS(QDOT/MDOT) = 2.7886E-02 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	MASS FRACTION	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
C3H8	9.23107E-12	5.38821E-12	7.17971E-11
C2H5	6.23046E-09	5.51818E-09	4.57334E-08
CH3	1.91284E-05	3.27474E-05	-2.93032E-05
C2H4	1.19536E-06	1.08757E-06	2.76660E-06
H	1.91497E-04	4.8[illegible]E-03	1.45251E-03
O	2.98617E-05	4.80410E-05	-6.93341E-05
CH2O	3.35971E-06	2.87238E-06	1.77221E-06
CH2	1.95739E-05	3.59181E-05	9.25916E-06
HCO	7.84030E-07	6.95437E-07	2.34940E-07
CH4	1.28263E-05	2.05754E-05	-2.14282E-05
C3H7	5.83500E-15	3.48558E-15	1.33798E-14
H2	4.74647E-03	6.06042E-02	1.72738E-04
OH	5.00395E-04	7.57332E-04	-1.63586E-03
H2O	9.79132E-02	1.39305E-01	4.66171E-05
CH	3.41595E-07	6.75360E-07	-1.86495E-06
O2	1.12835E-04	9.07684E-05	-1.09527E-04
CO	1.14366E-01	[illegible].05092E-01	-[illegible].51962E-03
CO2	8.05644E-02	4.71187E-02	1.69112E-03
HO2	5.34364E-06	4.16734E-06	7.31916E-06
NO	1.14402E-04	9.81356E-05	3.46674E-08
NO2	4.83739E-09	2.70643E-09	6.32073E-10
N	1.49185E-07	2.76137E-07	-1.58674E-07
N2	6.89223E-01	6.33208E-01	9.58549E-08
HCN	7.91861E-06	7.54171E-06	-5.97411E-08
CN	1.13641E-08	1.12425E-08	-2.93305E-08
HNCO	1.56286E-06	8.95631E-07	-1.61935E-06
NCO	2.12595E-08	1.30235E-08	-4.07176E-08
NH2	8.48466E-06	1.36299E-35	1.69099E-06
NH	8.60982E-08	1.47594E-07	-9.72346E-09
C2H3	1.04053E-06	9.90131E-07	3.95262E-06
C2H2	3.91106E-04	3.86624E-04	-6.34759E-05
C2H	3.45826E-05	3.55627E-05	-7.49669E-06
AR	1.17370E-02	7.56248[illegible]-03	0.00000

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE*CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	2.1282E 06	-5.64977E-04	0.31139
2	3.5474E 08	-5.02873E-01	0.00235
3	6.1649E 12	4.82735E-01	0.99307
4	1.0611E 13	8.36778E-01	1.00000
5	1.1179E 12	2.97636E-07	0.99973
6	3.7720E 09	1.92405E-07	0.00013
7	4.4992E 12	1.41025E 02	0.26639
8	1.5211E 12	5.38672E-01	0.23736
9	5.5902E 12	2.69676E 01	0.20511
10	1.0030E 13	9.25268E-01	1.00000
11	3.5483E 13	1.74609E 02	1.00000
12	3.3715E 10	1.51264E-01	1.00000
13	6.8300E 13	1.61472E 02	1.00000
14	7.9377E 12	1.67675E 02	0.99636
15	1.3905E 13	2.88611E 00	0.99650
16	1.3121E 14	4.29240E 02	0.99435
17	3.0000E 13	1.51264E 00	0.99987
18	2.0000E 13	1.02647E 02	0.99987
19	3.0000E 13	2.38455E 01	0.99987
20	4.8905E 12	6.64838E 02	0.12950
21	4.2573E 11	1.34636E 04	0.26335
22	9.7838E 13	1.05386E 01	0.99989
23	6.6469E 06	5.76456E-02	0.66234
24	1.9975E 12	6.15338E 02	0.46018
25	2.6753E 12	4.58845E 02	0.03922
26	8.4226E 12	-9.43521E 02	0.00161
27	4.6309E 12	-1.69627E 02	0.04057
28	1.9348E 15	6.11505E 01	0.51454
29	9.4043E 13	4.53714E-03	0.99973
30	4.6187E 14	2.30906E 02	0.99985
31	2.6011E 15	8.87654E 02	0.99985
32	3.0647E 10	-6.39275E 01	0.89616
33	2.3245E 10	-4.55601E-01	0.89194
34	3.0647E 10	-9.91838E 00	0.89633
35	6.1622E 12	3.77690E 00	0.99293
36	8.4629E 12	1.59132E-03	0.95515
37	7.7770E 15	7.61777E-01	0.99364
38	2.3212E 14	4.53212E 00	0.97741
39	1.9982E 12	7.46629E-02	0.99487
40	9.5951E 04	-1.22753E 00	0.99642
41	4.0000E 13	1.24155E 01	0.99049
42	7.3548E 08	4.73460E-01	0.99991
43	1.3601E 13	-1.09295E 00	0.07247
44	2.0133E 11	1.19645E-02	0.10867
45	1.8261E 11	8.38775E-01	0.53279
46	1.2000E 13	9.78145E-03	0.99988
47	4.6585E 13	3.05653E-01	0.51055

48	8.0437E 12	-2.79288E-01	0.02832
49	9.2526E 12	1.32995E 01	0.21660
50	2.4184E 13	2.74081E-02	0.73579
51	3.7000E 12	9.92750E-01	0.33557
52	2.0000E 13	1.88872E-02	1.00000
53	1.0000E 13	5.38853E-05	1.00000
54	2.0000E 13	1.90640E 00	0.99161
55	1.2106E 13	1.98287E 00	0.97079
56	3.7000E 12	1.77716E 02	1.00000
57	1.0178E 13	7.72407E 00	0.09454
58	3.7527E 13	4.34235E 00	0.09308
59	3.5618E 11	-1.90427E 01	0.03454
60	1.8451E 13	5.17264E 02	0.99998
61	3.7894E 10	9.36328E 00	0.93203
62	9.3414E 09	2.27404E-02	0.93668
63	3.9496E 12	1.51122E 02	0.93192
64	1.0000E 14	1.00037E 01	1.00000
65	1.0000E 13	1.00037E 00	1.00000
66	7.4000E 12	2.77009E 02	1.00000
67	5.8292E 09	1.45949E 00	0.99984
68	3.0000E 13	1.65041E 00	0.57740
69	3.8462E 11	1.49284E-04	0.51339
70	4.8000E 13	1.95473E 00	0.99985
71	2.0000E 13	3.55052E 01	0.99994
72	8.4497E 11	-3.66907E 01	0.02946
73	5.7943E 12	1.49631E 01	1.00000
74	1.4083E 12	6.86144E 00	1.00000
75	1.5733E 09	8.33359E-02	1.00000
76	1.3670E 00	-5.84953E-03	0.99986
77	3.0545E 11	-4.59793E-01	0.05096
78	9.2282E 13	-1.81223E 00	0.00235

TIME 1.05294E-05 SEC AREA 5.50000E 01 SQ CM AXIAL POSITION 2.00000E 00 CM

FLOW PROPERTIES

PRESSURE (ATM)	0.72397
VELOCITY (CM/SEC)	193173.55
DENSITY (GM/CM**3)	1.58621E-04
TEMPERATURE (DEG K)	1431.73
MASS FLOW RATE (GM/SEC)	1.68528E 03
ENTROPY CAL/GM/DEG K)	2.3418
MACH NUMBER	2.5019
GAMMA	1.2891
ENTHALPY (CAL/GM)	-2.29670E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	41
AVERAGE STEP SIZE	0.31707E-01
TOTAL NUMBER OF STEPS	138
FUNCT EVALUATIONS	272
JACOBIAN EVALUATIONS	33

CHAMBER PRESS = 380.0 PSIA THROAT AREA = 2.20000E 00 SQ IN

ISP = 1931.7 METERS/SEC = 197.0 LB-SEC/LB IVAC = 2171.1 METERS/SEC = 221.4 LB-SEC/LB

CSTAR = 5715.3 FT/SEC THRUST COEFF = 1.1089 AREA RATIO = 3.875

HEAT LOSS(QDOT/MDOT) = 1.7034E-02 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	MASS FRACTION	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
C3H8	4.76334E-10	2.78044E-10	5.29215E-10
C2H5	1.22009E-07	1.08063E-07	2.19289E-07
CH3	1.51057E-05	2.58612E-05	-2.61791E-06
C2H4	3.25916E-06	2.99035E-06	1.59259E-06
H	2.08429E-04	5.32257E-03	1.96431E-04
O	1.59317E-05	2.56312E-05	-1.12542E-05
CH2O	3.99085E-06	3.42120E-06	1.29634E-07
CH2	2.06991E-05	3.79838E-05	4.13792E-07
HCO	9.83427E-07	8.72322E-07	1.93690E-07
CH4	9.85904E-06	1.58183E-05	-1.55657E-06
C3H7	2.58313E-14	1.54309E-14	2.12115E-14
H2	4.74563E-03	6.05948E-02	-5.55342E-05
OH	1.90850E-04	2.88852E-04	-2.07508E-04
H2O	9.79513E-02	1.39962E-01	6.79214E-05
CH	9.33037E-08	1.84473E-07	-1.81819E-07
O2	8.26380E-05	6.64785E-05	-8.45129E-06
CO	1.13928E-01	1.04691E-01	-1.39525E-04
CO2	8.13196E-02	4.75614E-02	1.52567E-04
HO2	8.25691E-06	6.43945E-06	1.00055E-06
NO	1.14403E-04	9.81385E-05	-3.23465E-09
NO2	5.22704E-09	2.92450E-09	5.61064E-12
N	1.17306E-07	2.15569E-07	-3.32409E-08
N2	6.89223E-01	6.33302E-01	2.18582E-08
HCN	7.89936E-06	7.52352E-06	-6.57941E-09
CN	3.49414E-09	3.45683E-09	-3.08808E-09
HNCO	7.76264E-07	4.64407E-07	-1.83123E-07
NCO	5.71315E-09	3.49995E-09	-3.28465E-09
NH2	8.76700E-06	1.40837E-05	1.89576E-07
NH	8.46345E-08	1.45038E-07	-7.67635E-10
C2H3	3.95191E-06	3.76110E-06	2.33321E-06
C2H2	3.74235E-04	3.69953E-04	-7.61684E-06
C2H	3.22256E-05	3.31399E-05	-1.14222E-06
AR	1.17370E-02	7.56265E-03	0.00000

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE*CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	4.9365E 03	-2.10392E-02	0.98427
2	1.9361E 07	-1.25150E 01	0.02384
3	4.3122E 12	4.97305E-01	0.99690
4	8.7690E 12	1.01211E 00	1.00000
5	5.3550E 11	5.81158E-06	0.99999
6	3.5434E 08	4.96853E-06	0.00371
7	1.9225E 12	5.56459E 01	0.22778
8	7.8826E 11	1.62554E-01	0.33699
9	3.6411E 12	6.05665E 00	0.24120
10	1.0000E 13	1.85094E-01	1.00000
11	2.7240E 13	1.03815E 02	1.00000
12	1.2392E 10	3.21729E-02	1.00000
13	6.8000E 13	6.80309E 01	1.00000
14	6.2794E 12	1.72122E 02	0.99877
15	1.0032E 13	1.32629E 00	0.99894
16	5.1326E 13	7.72071E 01	0.99879
17	3.0000E 13	1.01239E 00	1.00000
18	2.0000E 13	1.40154E 02	1 00000
19	3.0000E 13	1.14091E 01	1.00000
20	1.7108E 12	1.43672E 02	0.06378
21	2.4037E 11	6.10956E 03	0.55689
22	1.3811E 14	3.44658E 00	1.00000
23	5.4514E 05	4.63900E-03	0.81011
24	6.0182E 11	1.83670E 02	0.57146
25	1.1287E 12	3.74189E 02	0.14143
26	5.2941E 12	2.43174E 03	0.01739
27	4.2904E 12	-7.80579E 01	0.12624
28	2.1318E 15	4.28167E 01	0.94532
29	1.0686E 14	6.52945E-04	1.00000
30	5.7972E 14	1.52753E 02	1.00000
31	4.0979E 15	2.58492E 02	1.00000
32	4.1951E 09	-1.34835E 01	0.93929
33	3.1746E 09	-4.17375E-02	0.92929
34	4.1951E 09	-7.18194E-01	0.93821
35	5.1985E 12	4.95163E 00	0.99362
36	8.1100E 12	9.15836E-04	0.99815
37	8.4490E 15	1.97638E-01	0.99982

38	2.1930E 14	5.14814E 00	0.99921
39	1.0186E 12	2.20206E-02	0.99952
40	4.1294E 02	-9.02591E-01	0.99999
41	4.0000E 13	3.75500E 00	0.99887
42	1.8871E 08	3.32626E-02	0.99965
43	9.3136E 12	-2.18865E-01	0.06919
44	5.1566E 10	3.01417E-03	0.20083
45	1.4950E 11	3.46124E-01	0.70565
46	1.2000E 13	1.60474E-03	1.00000
47	3.0343E 13	3.21748E-02	0.70361
48	4.2283E 12	-8.96285E-02	0.06211
49	5.0407E 12	7.53663E 00	0.40065
50	2.2517E 13	6.81784E-03	0.87299
51	3.7000E 12	3.04016E-01	0.33112
52	2.0000E 13	2.70794E-03	1.00000
53	1.0000E 13	1.13874E-05	1.00000
54	2.0000E 13	5.60464E-01	0.99668
55	9.3671E 12	5.90974E-01	0.99742
56	3.7000E 12	4.89967E 01	1.00000
57	5.5448E 12	-3.47786E 01	0.20704
58	2.9224E 13	-9.11205E 00	0.19301
59	1.9719E 10	-1.36623E 02	0.54965
60	1.4165E 13	2.02722E 02	1.00000
61	5.0426E 09	1.51883E 00	0.98708
62	1.3009E 09	1.89034E-03	0.98891
63	2.2962E 12	3.75419E 01	0.98730
64	1.0000E 14	2.73244E 00	1.00000
65	1.000JE 13	2.73244E-01	1.00000
66	7.4000E 12	8.34323E 01	1.00000
67	1.0065E 09	5.92765E-01	1.00000
68	3.0000E 13	2.49135E 00	0.94880
69	2.7178E 11	2.78178E-03	0.94398
70	4.8000E 13	4.16694E 01	1.00000
71	2.0000E 13	2.96520E 01	1.00000
72	5.1241E 11	-3.62414E 01	0.30484
73	4.6269E 12	5.93181E 00	1.00000
74	8.5402E 11	2.83973E 00	1.00000
75	2.1278E 08	7.89824E-03	1.00000
76	3.9642E-04	-1.99755E-03	1.00000
77	1.0390E 11	-3.82052E-01	0.20441
78	9.5128E 12	-3.78938E 01	0.02384

TIME 2.04557E-05 SEC AREA 9.50000E 01 SQ CM AXIAL POSITION 4.00000E 00 CM

FLOW PROPERTIES

PRESSURE (ATM)	0.31984
VELOCITY (CM/SEC)	210275.23
DENSITY (GM/CM**3)	8.43822E-05
TEMPERATURE (DEG K)	1189.82
MASS FLOW RATE (GM/SEC)	1.68563E 03
ENTROPY (CAL/GM/DEG K)	2.3418
MACH NUMBER	2.9737
GAMMA	1.3019
ENTHALPY (CAL/GM)	-3.12154E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	9
AVERAGE STEP SIZE	0.11111E 00
TOTAL NUMBER OF STEPS	152
FUNCT EVALUATIONS	294
JACOBIAN EVALUATIONS	37

CHAMBER PRESS = 300.0 PSIA THROAT AREA = 2.20000E 00 SQ IN

ISP = 2102.8 METERS/SEC = 214.4 LB-SEC/LB IVAC = 2285.4 METERS/SEC = 233.0 LB-SEC/LB

CSTAR = 5714.1 FT/SEC THRUST COEFF = 1.2073 AREA RATIO = 6.693

HEAT LOSS(QDOT/MDOT) = 9.8306E-03 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	MASS FRACTION	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE*CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
C3H8	4.041112E-09	2.35891E-09	1.19028E-09	1	1.1168E 01	-1.67187E-01	0.99993
C2H5	1.27746E-06	1.13144E-06	5.96604E-07	2	1.0441E 06	-1.31721E 02	0.19197
CH3	1.37130E-05	2.34773E-05	-4.62625E-07	3	3.0123E 12	3.00389E-01	0.99812
C2H4	4.78581E-06	4.39117E-06	6.12563E-08	4	7.2032E 12	7.20155E-01	1.00000
H	2.14753E-04	5.48417E-03	2.13772E-05	5	2.5575E 11	2.13765E-05	1.00000
O	9.36999E-06	1.50749E-05	-1.93177E-06	6	3.2964E 07	1.90768E-05	0.02229
CH2O	3.86753E-06	3.31555E-06	-7.96975E-08	7	8.1359E 11	2.15416E 01	0.21720
CH2	2.06488E-05	3.78921E-05	-1.38327E-07	8	4.0738E 11	6.70930E-02	0.49652
HCO	1.36835E-06	1.21378E-06	1.27527E-07	9	2.3674E 12	1.60342E 00	0.28356
CH4	9.12308E-06	1.46378E-05	-1.65278E-07	10	1.0000E 13	4.38445E-02	1.00000
C3H7	9.43936E-14	5.63891E-14	1.63745E-14	11	2.0389E 13	7.11130E 01	1.00000
H2	4.73994E-03	6.05236E-02	-1.52684E-05	12	4.5410E 09	9.57818E-03	1.00000
OH	7.14320E-05	1.08115E-04	-3.04452E-05	13	6.8000E 13	3.63223E 01	1.00000
H2O	9.80119E-02	1.40051E-01	2.01492E-05	14	4.9484E 12	1.35715E 02	0.99939
CH	2.46936E-08	4.88232E-08	-1.80301E-08	15	7.2272E 12	5.44968E-01	0.99960
O2	7.39971E-05	5.95284E-05	-1.13747E-06	16	2.0393E 13	1.10264E 01	0.99944
CO	1.13824E-01	1.04598E-01	-1.07034E-05	17	3.0000E 13	8.28470E-01	1.00000
CO2	8.15011E-02	4.76085E-02	1.24370E-05	18	2.0000E 13	2.00929E 02	1.00000
HO2	9.38542E-06	7.31969E-06	1.57889E-07	19	3.0000E 13	5.94165E 00	1.00000
NO	1.14396E-04	9.81342E-05	-2.12823E-09	20	5.9588E 11	-6.56051E 01	0.05669
NO2	5.02843E-09	2.81344E-09	-5.15331E-11	21	1.3539E 11	1.75825E 03	0.76087
N	9.87368E-08	1.81448E-07	-7.09934E-09	22	1.9127E 14	1.49216E 00	1.00000
N2	6.89223E-01	6.33314E-01	4.99755E-09	23	4.4251E 04	3.83499E-04	0.92221
HCN	7.89481E-06	7.51933E-06	-4.35210E-10	24	1.8043E 11	5.99789E 01	0.67468
CN	1.01242E-09	1.00162E-09	-3.61216E-10	25	4.9497E 11	2.41458E 02	0.35426
HNCO	5.06231E-07	3.01667E-07	-2.87627E-08	26	3.3209E 12	2.78021E 03	0.08477
NCO	1.61755E-09	9.90948E-10	-3.57729E-10	27	3.9663E 12	-2.92052E 01	0.29445

NH2	8.87106E-06	1.42512E-05	2.92762E-08
NH	8.43212E-08	1.44554E-07	-7.53198E-11
C2H3	6.42110E-06	6.11119E-06	3.80357E-07
C2H2	3.66989E-04	3.62718E-04	-1.36027E-06
C2H	3.12598E-05	3.21473E-05	-1.63350E-07
AR	1.17370E-02	7.56279E-03	0.00000

28	2.2983E 15	2.38200E 01	0.99682
29	1.2148E 14	1.36592E-04	1.00000
30	6.9806E 14	1.03874E 02	1.00000
31	5.9416E 15	7.69285E 01	1.00000
32	5.8599E 08	-2.74290E 00	0.96014
33	4.4262E 08	-3.59372E-03	0.93827
34	5.8599E 08	-4.92992E-02	0.95645
35	4.3825E 12	4.74961E 00	0.99968
36	7.7705E 12	4.97348E-04	0.99990
37	9.1823E 15	6.72080E-02	1.00000
38	2.0714E 14	4.82356E 00	0.99997
39	5.4022E 11	8.80634E-03	0.99996
40	1.7377E 08	-7.06114E-01	1.00000
41	4.0000E 13	1.18416E 00	0.99988
42	4.8279E 07	2.24963E-03	0.99850
43	6.3676E 12	-1.72378E-02	0.02874
44	1.3518E 10	8.62203E-04	0.37282
45	1.2229E 11	1.17583E-01	0.78365
46	1.2000E 13	2.73465E-04	1.00000
47	1.9729E 13	2.63882E-03	0.81840
48	2.2168E 12	-4.54489E-02	0.18473
49	2.7393E 12	4.11162E 00	0.60114
50	2.0958E 13	1.77454E-03	0.94092
51	3.7000E 12	6.41431E-02	0.24058
52	2.0000E 13	4.50918E-04	1.00000
53	1.0000E 13	2.71373E-06	1.00000
54	2.0000E 13	1.63812E-01	0.99860
55	7.3952E 12	1.74390E-01	0.99976
56	3.7000E 12	1.29964E 01	1.00000
57	3.0132E 12	-5.99468E 01	0.35574
58	2.2734E 13	-6.77952E 00	0.29388
59	1.0788E 09	-1.20145E 02	0.92352
60	1.0862E 13	8.96403E 01	1.00000
61	6.8555E 08	2.14431E-01	0.99730
62	1.8355E 08	1.57966E-04	0.99826
63	1.3606E 12	8.39153E 00	0.99753
64	1.0000E 14	7.23118E-01	1.00000
65	1.0000E 13	7.23118E-02	1.00000
66	7.4000E 12	2.83483E 01	1.00000
67	2.6311E 08	1.75920E-01	1.00000
68	3.0000E 13	3.26048E 00	0.99663
69	1.9177E 11	1.94177E-02	0.99605
70	4.8000E 13	4.49527E 02	1.00000
71	2.0000E 13	2.68528E 01	1.00000
72	3.1010E 11	-1.86259E 01	0.50368
73	3.6989E 12	2.69958E 00	1.00000
74	5.1683E 11	1.49273E 00	1.00000
75	2.8540E 07	9.30067E-04	1.00000
76	1.1117E-07	-8.37423E-04	1.00000
77	3.4302E 10	-1.19336E-01	0.29655
78	9.7149E 11	-4.01781E 02	0.19497

DISTANCE-AREA VERSION GENERAL CHEMICAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

GCKP84 HIGH TEMPERATURE AIR IONIZATION CASE 10

REACTION NUMBER	REACTION					REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1.0*N	+ 1.0*O2	= 1.0*NO	+ 1.0*O		6.40000E 09	1.0000	6250.00
2	1.0*O	+ 1.0*N2	= 1.0*NO	+ 1.0*N		1.80000E 14	0.0000	76250.00
3	1.0*N	+ 1.0*O	= 1.0*NO	+ M		6.40000E 16	-0.5000	0.00
4	1.0*O	+ 1.0*O	= 1.0*O2	+ M		5.70000E 13	0.0000	-1788.00
5		2.0*N	= 1.0*N2	+ M		2.80000E 17	-0.7500	0.00
6	1.0*NO	+ 1.0*O	= 1.0*NO2	+ M		5.62000E 15	0.0000	-1160.00
7	M	+ 1.0*N2O	= 1.0*N2	+ 1.0*O		1.42000E 14	0.0000	51280.00
8	1.0*O	+ 1.0*N2O	= 1.0*N2	+ 1.0*O2		6.23000E 13	0.0000	24520.00
9	1.0*NO+	+ 1.0*E	= 1.0*N	+ 1.0*O		1.45000E 21	-1.5000	0.00
10	1.0*O+	+ 1.0*E	= 1.0*O	+ M		2.00000E 26	-2.5000	0.00
11	1.0*O2	+ 1.0*E	= 1.0*O2-	+ M		1.52000E 21	-1.0000	1198.00
12	1.0*O2	+ 1.0*O-	= 1.0*O2-	+ 1.0*O		6.00000E 12	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(N2O , 3) = 2.25000 M(N2 , 6) = 1.55000 M(N2 , 11) = 0.00002 M(N , 10) = 0.03000
M(O2 , 10) = 4.50000 M(NO , 10) = 50.00000 M(O , 10) = 0.03000

INTEGRATION CONTROLS

INITIAL STEP SIZE 0.50000E-08 CM MAXIMUM RELATIVE ERROR 0.10000E-04

** ASSIGNED VARIABLE PROFILE **

THE AREA IS CALCULATED FROM THE FOLLOWING POLYNOMIAL

AREA (CM**2) = (0.00000)X**3 + (0.00000)X**2 + (0.00000)X + (1.00000E 03)

** INITIAL CONDITIONS **

TIME 0.00000 SEC AREA 1.00000E 03 SQ CM AXIAL POSITION 0.00000 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.68030
VELOCITY (CM/SEC)	47002.00
DENSITY (GM/CM**3)	1.22557E-04
TEMPERATURE (DEG K)	4820.00
MASS FLOW RATE (GM/SEC)	5.76044E 03
ENTROPY CAL/GM/DEG K)	2.3906
MACH NUMBER	0.3535
GAMMA	1.2726
ENTHALPY (CAL/GM)	1.35461E 03

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
N	0.00000	0.00000	1.57091E-05	1	1.6063E 13	0.00000	0.00000
O2	8.90048E-07	2.09500E-01	-2.25142E-02	2	6.2795E 10	0.00000	0.00000
NO	0.00000	0.00000	0.00000	3	9.2184E 14	0.00000	0.00000
O	0.00000	0.00000	4.26393E-02	4	6.8698E 13	-1.33983E 06	1.00000
N2	3.35839E-06	7.90500E-01	-2.39786E-03	5	4.8403E 14	-5.22929E 02	1.00000
NO2	0.00000	0.00000	0.00000	6	6.3436E 15	0.00000	0.00000
N2O	0.00000	0.00000	2.39000E-03	7	6.7164E 11	0.00000	0.00000
NO+	0.00000	0.00000	0.00000	8	4.8161E 12	-1.59118E 05	1.00000
E	0.00000	0.00000	4.38514E-07	9	4.3331E 15	0.00000	0.00000
O+	0.00000	0.00000	0.00000	10	1.2400E 17	0.00000	0.00000
O2-	4.24844E-15	9.99999E-10	-4.38514E-07	11	2.7851E 17	-2.91947E 01	1.00000
O-	0.00000	0.00000	0.00000	12	6.0000E 12	0.00000	0.00000

MIXTURE MOLECULAR WEIGHT 28.84763 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) 1.72299E 11 MASS FRACTION SUM 0.99999994

TIME 2.14084E-06 SEC AREA 1.00000E 03 SQ CM AXIAL POSITION 1.00000E-01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.68655
VELOCITY (CM/SEC)	45902.88
DENSITY (GM/CM**3)	1.25492E-04
TEMPERATURE (DEG K)	4681.24
MASS FLOW RATE (GM/SEC)	5.76044E 03
ENTROPY CAL/GM/DEG K)	2.3998
MACH NUMBER	0.3482
GAMMA	1.2763
ENTHALPY (CAL/GM)	1.35583E 03

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	3
AVERAGE STEP SIZE	0.13333E-01
TOTAL NUMBER OF STEPS	116
FUNCT EVALUATIONS	172
JACOBIAN EVALUATIONS	37

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
N	9.68342E-10	2.20547E-06	2.90961E-06	1	1.5302E 13	7.86471E 05	0.97754
O2	8.55070E-07	1.94748E-01	-2.79544E-02	2	6.9595E 10	8.01154E 05	0.92244
NO	3.13757E-08	7.14603E-03	2.49509E-02	3	9.3560E 14	-3.25854E 03	0.99379
O	8.05914E-08	1.83553E-02	3.10500E-02	4	6.9080E 13	-8.96860E 05	0.99986
N2	3.42202E-06	7.79390E-01	-1.25286E-02	5	4.9475E 14	-2.58482E 02	0.99952
NO2	1.04184E-13	2.37286E-08	5.27478E-08	6	6.3664E 15	3.34944E 00	0.00052
N2O	6.11579E-10	1.39292E-04	-9.23674E-05	7	5.7308E 11	9.76119E 04	0.99894
NO+	3.68811E-14	8.39993E-09	4.35476E-08	8	4.4642E 12	-9.17466E 04	0.86784
E	4.11175E-14	9.36481E-09	4.34129E-08	9	4.5272E 15	-2.76523E 00	0.99984
O+	3.51861E-19	8.01387E-14	2.41358E-13	10	1.3339E 17	-1.53260E-05	1.00000
O2-	8.98571E-17	2.04656E-11	9.58971E-11	11	2.8571E 17	8.56994E-03	0.01387
O-	2.42233E-17	5.51704E-12	3.98644E-11	12	6.0000E 12	-2.48056E-03	0.23916

MIXTURE MOLECULAR WEIGHT 28.58171 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) 1.53580E 11 MASS FRACTION SUM 1.00000000

AA	BB	D(AREA)/D(IVAR)	D2(AREA)/D(IVAR)2	(1/AREA)*D(AREA)/D(IVAR)-AA
-0.20684E 00	0.28482E 00	0.00000	0.00000	0.20684E 00

VARIABLE DERIVATIVES

V	-0.10894E 05	RHO	0.29538E-04	T	-0.12964E 04
N	0.50510E-04	N2O	-0.16035E-04		
O2	-0.48528E-02	NO+	0.75598E-08		
NO	0.43314E-02	E	0.75364E-08		
O	0.51902E-02	O+	0.41899E-13		
N2	-0.21749E-02	O2-	0.16648E-10		
NO2	0.91569E-08	O-	0.67815E-11		

OMEGA(I,J) RATE OF PRODUCTION OF SPECIES I BY REACTION J

SPECIES	REACTION 1	2	3	4	5	6	7	8
	9	10	11	12				
N	-0.12386E-01	0.12617E-01	0.51316E-04	0.00000	0.84563E-05	0.00000	0.00000	0.00000
	-0.43548E-07	0.00000	0.00000	0.00000				
O2	-0.12386E-01	0.00000	0.00000	-0.14124E-01	0.00000	0.00000	0.00000	-0.14448E-02
	0.00000	0.00000	-0.13496E-09	0.39064E-10				
NO	0.12386E-01	0.12617E-01	-0.51316E-04	0.00000	0.00000	-0.52748E-07	0.00000	0.00000
	0.00000	0.00000	0.00000	0.00000				
O	0.12386E-01	-0.12617E-01	0.51316E-04	0.28248E-01	0.00000	-0.52748E-07	0.15372E-02	0.14448E-02
	-0.43543E-07	-0.24136E-12	0.00000	-0.39064E-10				
N2	0.00000	-0.12617E-01	0.00000	0.00000	-0.42281E-05	0.00000	0.15372E-02	-0.14448E-02
	0.00000	0.00000	0.00000	0.00000				
NO2	0.00000	0.00000	0.00000	0.00000	0.00000	0.52748E-07	0.00000	0.00000
	0.00000	0.00000	0.00000	0.00000				
N2O	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.15372E-02	0.14448E-02
	0.00000	0.00000	0.00000	0.00000				
NO+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	0.43548E-07	0.00000	0.00000	0.00000				
E	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	0.43548E-07	0.24136E-12	-0.13496E-09	0.00000				
O+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	0.00000	0.24136E-12	0.00000	0.00000				
O2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	0.00000	0.00000	0.13496E-09	-0.39064E-10				
O-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	0.00000	0.00000	0.00000	0.39064E-10				

TIME 1.58663E-05 SEC AREA 1.00000E 03 SQ CM AXIAL POSITION 7.00000E-01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.70890
VELOCITY (CM/SEC)	41969.32
DENSITY (GM/CM**3)	1.37253E-04
TEMPERATURE (DEG K)	4241.22
MASS FLOW RATE (GM/SEC)	5.76040E 03
ENTROPY CAL/GM/DEG K)	2.4165
MACH NUMBER	0.3293
GAMMA	1.2874
ENTHALPY (CAL/GM)	1.35996E 03

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	8
AVERAGE STEP SIZE	0.25000E-01
TOTAL NUMBER OF STEPS	143
FUNCT EVALUATIONS	210
JACOBIAN EVALUATIONS	44

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
N	1.45253E-09	2.95807E-04	-1.33947E-05	1	1.2930E 13	3.03689E 05	0.45382
O2	6.71204E-07	1.36691E-01	-9.46123E-03	2	2.1189E 10	2.96219E 05	0.24173
NO	3.47193E-07	7.07059E-02	1.11739E-02	3	9.8273E 14	-6.71895E 03	0.98346
O	3.03760E-07	6.18609E-02	7.75595E-03	4	7.0471E 13	-1.85881E 05	0.99096
N2	3.58659E-06	7.30411E-01	-5.57165E-03	5	5.3277E 14	-2.30633E 01	0.98746
NO2	9.13358E-12	1.86006E-06	7.72697E-07	6	6.4493E 15	4.10173E 01	0.00017
N2O	1.59421E-10	3.24662E-05	-9.04746E-06	7	3.2347E 11	1.31439E 04	0.97786
NO+	1.54077E-12	3.13779E-07	1.07089E-07	8	3.3960E 12	-1.26636E 04	0.59194
E	1.53462E-12	3.12527E-07	1.05941E-07	9	5.2497E 15	-5.63464E 00	0.89613
O+	2.77319E-18	5.64761E-13	8.23092E-14	10	1.7073E 17	-4.36925E-06	0.99979
O2-	3.46291E-15	7.05223E-10	2.44765E-10	11	3.1119E 17	6.09472E-02	0.00271
O-	7.44300E-15	1.51577E-09	9.03378E-10	12	6.0000E 12	-4.79543E-02	0.02926

MIXTURE MOLECULAR WEIGHT 27.95158 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) 3.72301E 10 MASS FRACTION SUM 1.00000381

AA	BB	D(AREA)/D(IVAR)	D2(AREA)/D(IVAR)2	(1/AREA)*D(AREA)/D(IVAR)-AA
-0.72639E-01	0.91444E-01	0.00000	0.00000	0.72639E-01

VARIABLE DERIVATIVES

V	-0.36194E 04	RHO	0.11183E-04	T	-0.37706E 03
N	-0.23253E-05	N2O	-0.15706E-05		
O2	-0.16425E-02	NO+	0.18591E-07		
NO	0.19398E-02	E	0.18391E-07		
O	0.13464E-02	O+	0.14289E-13		
N2	-0.96723E-03	O2-	0.42491E-10		
NO2	0.13414E-06	O-	0.15683E-09		

OMEGA(I,J) RATE OF PRODUCTION OF SPECIES I BY REACTION J

SPECIES	REACTION 1	2	3	4	5	6	7	8
	9	10	11	12				
N	-0.57210E-02	0.55803E-02	0.12657E-03	0.00000	0.86895E-06	0.00000	0.00000	0.00000
	-0.10709E-06	0.00000	0.00000	0.00000				

O2	-0.57210E-02 0.00000	0.00000 0.00000	0.00000 -0.11481E-08	-0.35017E-02 0.90338E-09	0.00000	0.00000	0.00000	-0.23856E-03
NO	0.57210E-02 0.00000	0.55803E-02 0.00000	-0.12657E-03 0.00000	0.00000 0.00000	0.00000	-0.77270E-06	0.00000	0.00000
O	0.57210E-02 -0.10709E-06	-0.55803E-02 -0.82309E-13	0.12657E-03 0.00000	0.70034E-02 -0.90338E-09	0.00000	-0.77270E-06	0.24761E-03	0.23856E-03
N2	0.00000 0.00000	-0.55803E-02 0.00000	0.00000 0.00000	0.00000 0.00000	-0.43447E-06	0.00000	0.24761E-03	-0.23856E-03
NO2	0.00000 0.00000	0.00000 0.00000	0.00000 0.00000	0.00000 0.00000	0.00000	0.77270E-06	0.00000	0.00000
H2O	0.00000 0.00000	0.00000 0.00000	0.00000 0.00000	0.00000 0.00000	0.00000	0.00000	-0.24761E-03	0.23856E-03
NO+	0.00000 0.10709E-06	0.00000 0.00000	0.00000 0.00000	0.00000 0.00000	0.00000	0.00000	0.00000	0.00000
E	0.00000 0.10709E-06	0.00000 0.82309E-13	0.00000 -0.11481E-08	0.00000 0.00000	0.00000	0.00000	0.00000	0.00000
O+	0.00000 0.00000	0.00000 0.82309E-13	0.00000 0.00000	0.00000 0.00000	0.00000	0.00000	0.00000	0.00000
O2-	0.00000 0.00000	0.00000 0.00000	0.00000 0.11481E-08	0.00000 -0.90338E-09	0.00000	0.00000	0.00000	0.00000
O-	0.00000 0.00000	0.00000 0.00000	0.00000 0.00000	0.00000 0.90338E-09	0.00000	0.00000	0.00000	0.00000

(GCKP) END OF THIS CASE - READ DATA FOR NEXT CASE

TIME-AREA VERSION GENERAL CHEMICAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

GCKP84 HIGH PRESSURE H2 - CO REACTION CASE 11

REACTION NUMBER	REACTION					REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1.0*CH3	+ 1.0*OH	= 1.0*CH2O	+ 1.0*H2		7.40000E 12	0.0000	0.00
2		1.0*CH4	= 1.0*CH3	+ 1.0*H		2.00000E 15	0.0000	104000.00
3	1.0*H	+ 1.0*CH4	= 1.0*CH3	+ 1.0*H2		1.26000E 14	0.0000	11900.00
4	1.0*O	+ 1.0*CH4	= 1.0*CH3	+ 1.0*OH		2.00000E 13	0.0000	9200.00
5	1.0*OH	+ 1.0*CH4	= 1.0*CH3	+ 1.0*H2O		3.00000E 13	0.0000	6000.00
6	1.0*CH2O	+ 1.0*H	= 1.0*HCO	+ 1.0*H2		2.00000E 13	0.0000	3300.00
7	1.0*CH2O	+ 1.0*O	= 1.0*HCO	+ 1.0*OH		2.00000E 13	0.0000	0.00
8	1.0*CH2O	+ 1.0*OH	= 1.0*HCO	+ 1.0*H2O		2.30000E 13	0.0000	0.00
9	M	+ 1.0*CH2O	= 1.0*H	+ 1.0*HCO		5.00000E 16	0.0000	72000.00
10	1.0*O	+ 1.0*HCO	= 1.0*H	+ 1.0*CO2		5.30000E 13	0.0000	0.00
11	1.0*HCO	+ 1.0*O	= 1.0*CO	+ 1.0*OH		1.26000E 14	0.0000	0.00
12	1.0*HCO	+ 1.0*H	= 1.0*CO	+ 1.0*H2		1.00000E 14	0.0000	0.00
13	1.0*HCO	+ 1.0*OH	= 1.0*CO	+ 1.0*H2O		1.00000E 14	0.0000	0.00
14	M	+ 1.0*HCO	= 1.0*H	+ 1.0*CO		5.00000E 14	0.0000	19000.00
15	1.0*CO	+ 1.0*OH	= 1.0*CO2	+ 1.0*H		4.00000E 12	0.0000	800.00
16	1.0*CO	+ 1.0*O	= 1.0*CO2	+ M		2.80000E 13	0.0000	-4540.00
17	1.0*O	+ 1.0*H2	= 1.0*OH	+ 1.0*H		1.80000E 10	1.0000	8900.00
18	1.0*H2	+ 1.0*OH	= 1.0*H2O	+ 1.0*H		5.20000E 13	0.0000	6500.00
19	1.0*OH	+ 1.0*OH	= 1.0*O	+ 1.0*H2O		6.30000E 12	0.0000	1093.00
20	1.0*H	+ 1.0*H	= 1.0*H2	+ M		3.30000E 17	-1.0000	0.00
21	1.0*H	+ 1.0*OH	= 1.0*H2O	+ M		8.40000E 21	-2.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2 , 14) = 5.00000 M(H2 , 20) = 1.70000 M(H2 , 21) = 4.00000 M(CO , 14) = 2.00000
M(CO , 20) = 2.00000 M(H2O , 20) = 9.60000 M(CO2 , 20) = 3.50000

INTEGRATION CONTROLS

INITIAL STEP SIZE 0.10000E-14 SEC MAXIMUM RELATIVE ERROR 0.50000E-05

** ASSIGNED VARIABLE PROFILE **

THIS IS A V=0 PROBLEM - AN ASSIGNED VARIABLE IS NOT REQUIRED

THE VOLUME (DENSITY) WILL BE HELD CONSTANT FOR THIS CASE

THE TEMPERATURE WILL BE HELD CONSTANT FOR THIS CASE

** INITIAL CONDITIONS **

TIME 0.00000 SEC AREA 1.00000E 00 SQ CM AXIAL POSITION 0.00000 CM

FLOW PROPERTIES

PRESSURE (ATM)	100.00003
VELOCITY (CM/SEC)	0.00
DENSITY (GM/CM**3)	2.77354E-03
TEMPERATURE (DEG K)	1000.00
MASS FLOW RATE (GM/SEC)	0.00000
ENTROPY CAL/GM/DEG K)	13.5436
MACH NUMBER	0.0000
GAMMA	1.3793
ENTHALPY (CAL/GM)	2.05691E 03

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
CH3	0.00000	0.00000	7.52445E-16	1	7.4000E 12	-9.78155E-11	1.00000
OH	1.21868E-12	9.99999E-10	2.70900E-02	2	3.7312E-08	0.00000	0.00000
CH2O	1.21868E-11	9.99999E-09	-3.00453E-08	3	3.1595E 11	0.00000	0.00000
H2	1.20649E-03	9.89999E-01	-3.29357E-02	4	1.9515E 11	0.00000	0.00000
CH4	0.00000	0.00000	0.00000	5	1.4649E 12	0.00000	0.00000
H	0.00000	0.00000	3.29754E-02	6	3.8003E 12	0.00000	0.00000
O	1.21868E-10	9.99999E-08	-3.05305E-02	7	2.0000E 13	3.86137E-03	1.00000
H2O	0.00000	0.00000	2.90298E-03	8	2.3000E 13	4.44058E-05	1.00000
HCO	0.00000	0.00000	3.00455E-08	9	9.1914E 00	1.77458E-08	1.00000
CO2	0.00000	0.00000	5.37505E-04	10	5.3000E 13	0.00000	0.00000
CO	1.21868E-05	9.99999E-03	-5.37505E-04	11	1.2600E 14	-3.92327E-17	1.00000
				12	1.0000E 14	-2.67088E-08	1.00000
				13	1.0000E 14	0.00000	0.00000
				14	3.5199E 10	0.00000	0.00000
				15	2.6744E 12	5.16335E 00	1.00000
				16	2.7503E 14	6.47106E 01	1.00000
				17	2.0426E 11	3.90415E 03	1.00000
				18	1.9744E 12	3.77378E 02	1.00000
				19	3.6347E 12	7.01742E-07	1.00000
				20	8.3000E 14	-1.67382E-08	1.00000
				21	8.4000E 15	0.00000	0.00000

MIXTURE MOLECULAR WEIGHT 2.27585 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) -6.73595E 06 MASS FRACTION SUM 0.99999988

PREDICTOR TROUBLE FOR Y 2, VALUE = -0.1908725831251670D-13, T= 0.4216519575485210-07, H= 0.2712403213476019D-08

TIME 1.00000E 06 SEC AREA 1.00000E 00 SQ CM AXIAL POSITION 0.00000 CM

FLOW PROPERTIES

PRESSURE (ATM)	99.98323
VELOCITY (CM/SEC)	0.00
DENSITY (GM/CM**3)	2.77354E-03
TEMPERATURE (DEG K)	1000.00
MASS FLOW RATE (GM/SEC)	0.00000
ENTROPY CAL/GM/DEG K)	13.5434
MACH NUMBER	0.0000
GAMMA	1.3792
ENTHALPY (CAL/GM)	2.05493E 03

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	6
AVERAGE STEP SIZE	0.16500E 06
TOTAL NUMBER OF STEPS	397
FUNCT EVALUATIONS	661
JACOBIAN EVALUATIONS	98

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
CH3	4.75154E-16	3.89958E-13	1.38562E-14	1	7.4000E 12	-1.31195E-08	1.00000
OH	5.24783E-20	4.30688E-17	3.77788E-16	2	3.7312E-08	-2.66540E-12	0.00539
CH2O	1.63497E-09	1.34181E-06	8.99420E-18	3	3.1596E 11	-1.13164E-08	0.00001
H2	1.20619E-03	9.89916E-01	-2.87297E-13	4	1.9515E 11	-3.96370E-24	0.00011
CH4	1.01365E-07	8.31896E-05	8.70655E-14	5	1.4649E 12	7.96817E-13	0.00078
H	2.74103E-13	2.24956E-10	-3.65253E-14	6	3.8003E 12	-2.37840E-10	0.00000
O	1.37524E-29	1.12947E-26	1.13502E-26	7	2.0000E 13	-6.03478E-24	0.00010
H2O	1.00043E-07	8.21054E-05	9.93012E-14	8	2.3000E 13	2.03544E-13	0.00079
HCO	7.46970E-15	6.13036E-12	2.22911E-14	9	9.1914E 00	-1.28830E-08	0.00538
CO2	1.44417E-09	1.18522E-06	1.24262E-15	10	5.3000E 13	4.25631E-27	0.00601
CO	1.20824E-05	9.91597E-03	-1.24464E-13	11	1.2600E 14	8.89137E-27	0.00528
				12	1.0000E 14	1.43249E-10	0.00538
				13	1.0000E 14	3.14525E-17	0.00617
				14	3.5199E 10	-1.61617E-08	0.00000
				15	2.6744E 12	1.61537E-10	0.00073

16	2.7503E 14	4.353146-20	0.00601
17	2.0426E 11	-4.49958E-20	0.00010
18	1.9744E 12	1.29078E-08	0.00079
19	3.6347E 12	1.16655E-24	0.00090
20	8.3000E 14	9.05653E-11	0.00538
21	8.4000E 15	4.68954E-16	0.00617

MIXTURE MOLECULAR WEIGHT 2.27623 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) -6.90521E-04 MASS FRACTION SUM 0.99999976

TIME 1.00000E 09 SEC AREA 1.00000E 00 SQ CM AXIAL POSITION 0.00000 CM

FLOW PROPERTIES

PRESSURE (ATM)	98.0089
VELOCITY (CM/SEC)	0.00
DENSITY (GM/CM**3)	2.77354E-03
TEMPERATURE (DEG K)	1000.00
MASS FLOW RATE (GM/SEC)	0.00000
ENTROPY (CAL/GM/DEG K)	13.4245
MACH NUMBER	0.0000
GAMMA	1.3707
ENTHALPY (CAL/GM)	1.91998E 03

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	46
AVERAGE STEP SIZE	0.19565E 08
TOTAL NUMBER OF STEPS	458
FUNCT EVALUATIONS	738
JACOBIAN EVALUATIONS	112

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
CH3	5.75250E-14	4.84168E-11	-2.52164E-13	1	7.4000E 12	-4.94387E-12	0.93218
OH	6.46574E-18	5.41375E-15	-3.68809E-15	2	3.7312E-08	-4.58436E-12	0.00008
CH2O	6.81406E-13	5.70540E-10	-3.77030E-16	3	3.1596E 11	-3.27810E-08	0.00000
H2	1.16995E-03	9.79596E-01	-2.55534E-13	4	1.9515E 11	5.81914E-22	0.00000
CH4	1.21515E-05	1.01996E-02	2.52202E-13	5	1.4649E 12	9.02382E-14	0.00000
H	2.69237E-13	2.25432E-10	-1.00199E-13	6	3.8003E 12	4.36691E-11	0.00048
O	1.71730E-27	1.43789E-24	-5.54770E-25	7	2.0000E 13	1.46996E-24	0.00048
H2O	1.21816E-05	1.01996E-02	3.72504E-15	8	2.3000E 13	6.35030E-15	0.00048
HCO	3.15108E-18	2.6384CE-15	3.56043E-13	9	9.1914E 00	3.93365E-13	0.00040
CO2	7.78972E-11	6.52252E-08	1.07361E-18	10	5.3000E 13	-1.69742E-29	0.00046
CO	5.19188E-09	4.34716E-06	-3.55705E-13	11	1.2600E 14	-4.14142E-29	0.00047
				12	1.0000E 14	-5.16787E-15	0.00047
				13	1.0000E 14	-1.24041E-19	0.00047
				14	3.5195E 10	-4.62403E-08	0.00055
				15	2.6744E 12	1.39565E-13	0.00001
				16	2.7503E 14	3.45060E-23	0.00009
				17	2.0426E 11	7.14788E-20	0.00000
				18	1.9744E 12	4.84147E-10	0.00000
				19	3.6347E 12	-2.15403E-23	0.00000
				20	8.3000E 14	1.28117E-12	0.00008
				21	8.4000E 15	6.93805E-16	0.00068

MIXTURE MOLECULAR WEIGHT 2.32228 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) -7.35104E-04 MASS FRACTION SUM 0.99999243

(GCKP) END OF THIS CASE - READ DATA FOR NEXT CASE

TIME-AREA VERSION GENERAL CHEMICAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

GCKP84 HYDROGEN - OXYGEN LOW TEMP PHOTOLYTIC IGNITION CASE 12

REACTION NUMBER	REACTION						REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1.0*H	+ 1.0*O2	=	1.0*OH	+ 1.0*O		2.20000E 14	0.0000	16790.00
2	1.0*O	+ 1.0*H2	=	1.0*OH	+ 1.0*H		1.80000E 10	1.0000	8900.00
3	1.0*H2	+ 1.0*OH	=	1.0*H2O	+ 1.0*H		5.20000E 13	0.0000	6500.00
4	1.0*OH	+ 1.0*OH	=	1.0*O	+ 1.0*H2O		6.30000E 12	0.0000	1093.00
5	1.0*H	+ 1.0*O2	=	1.0*HO2	+ M		1.50000E 15	0.0000	-1000.00
6	1.0*O	+ 1.0*O	=	1.0*O2	+ M		5.70000E 13	0.0000	-1788.00
7	1.0*H	+ 1.0*H	=	1.0*H2	+ M		8.30000E 17	-1.0000	0.00
8	1.0*H	+ 1.0*OH	=	1.0*H2O	+ M		8.40000E 21	-2.0000	0.00
9	1.0*H2	+ 1.0*HO2	=	1.0*H2O	+ 1.0*OH		7.20000E 11	0.0000	18700.00
10	M	+ 1.0*H2O2	=	2.0*OH			1.30000E 17	0.0000	45500.00
11	1.0*H2	+ 1.0*O2	=	2.0*OH			1.00000E 13	0.0000	43000.00
12	1.0*H	+ 1.0*HO2	=	1.0*OH	+ 1.0*OH		2.50000E 14	0.0000	1900.00
13	1.0*O	+ 1.0*HO2	=	1.0*OH	+ 1.0*O2		5.00000E 13	0.0000	1000.00
14	1.0*OH	+ 1.0*HO2	=	1.0*H2O	+ 1.0*O2		5.00000E 13	0.0000	1000.00
15		2.0*HO2	=	1.0*H2O2	+ 1.0*O2		1.80000E 12	0.0000	0.00
16	1.0*OH	+ 1.0*H2O2	=	1.0*H2O	+ 1.0*HO2		1.00000E 13	0.0000	1800.00
17	1.0*O	+ 1.0*H2O2	=	1.0*OH	+ 1.0*HO2		8.00000E 13	0.0000	1000.00
18	1.0*H	+ 1.0*H2O2	=	1.0*H2O	+ 1.0*OH		3.20000E 14	0.0000	9000.00
19	HNU	+ 1.0*H2	>	2.0*H			3.00000E-03	0.0000	0.00
20	HNU	+ 1.0*O2	>	2.0*O			5.00000E-03	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	, 5) = 5.00000	M(H2	, 7) = 5.00000	M(H2	, 8) = 4.00000	M(H2	, 10) = 2.30000
M(O2	, 5) = 2.00000	M(O2	, 7) = 2.00000	M(O2	, 8) = 1.60000	M(O2	, 10) = 0.78000
M(H2O	, 5) = 32.50000	M(H2O	, 7) = 15.00000	M(H2O	, 8) = 20.00000	M(H2O	, 10) = 6.00000
M(H2O2	, 10) = 6.60000						

INTEGRATION CONTROLS

INITIAL STEP SIZE 0.50000E-06 SEC MAXIMUM RELATIVE ERROR 0.50000E-06

** ASSIGNED VARIABLE PROFILE **

THIS IS A V=0 PROBLEM - AN ASSIGNED VARIABLE IS NOT REQUIRED

THE VOLUME (DENSITY) WILL BE HELD CONSTANT FOR THIS CASE

** INITIAL CONDITIONS **

TIME 0.00000 SEC AREA 1.00000E 00 SQ CM AXIAL POSITION 0.00000 CM

FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	2.00000	STEPS FROM LAST PRINT	0
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.00000
DENSITY (GM/CM**3)	4.17819E-04	TOTAL NUMBER OF STEPS	0
TEMPERATURE (DEG K)	700.00		
MASS FLOW RATE (GM/SEC)	0.00000		
ENTROPY (CAL/GM/DEG K)	3.5908	FUNCT EVALUATIONS	0
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	0
GAMMA	1.3728		
ENTHALPY (CAL/GM)	2.38997E 02		

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
H	0.00000	0.00000	1.39367E-07	1	1.2599E 09	0.00000	0.00000
O2	1.15949E-05	3.33000E-01	-5.80755E-08	2	2.0973E 10	0.00000	0.00000
OH	0.00000	0.00000	2.02323E-10	3	4.8597E 11	0.00000	0.00000
O	0.00000	0.00000	1.15949E-07	4	2.8714E 12	0.00000	0.00000
H2	2.32246E-05	6.67000E-01	-6.97748E-08	5	3.0783E 15	0.00000	0.00000
H2O	0.00000	0.00000	0.00000	6	2.0612E 14	-1.05084E-24	1.00000
HO2	0.00000	0.00000	0.00000	7	1.1857E 15	-2.41134E-19	1.00000
H2O2	0.00000	0.00000	0.00000	8	1.7143E 16	0.00000	0.00000
				9	1.0446E 06	0.00000	0.00000
				10	8.0948E 02	0.00000	0.00000
				11	3.7567E-01	5.79481E-04	1.00000
				12	6.3787E 13	0.00000	0.00000
				13	2.4364E 13	0.00000	0.00000
				14	2.4364E 13	0.00000	0.00000
				15	1.8600E 12	0.00000	0.00000
				16	2.7417E 12	0.00000	0.00000
				17	3.8983E 13	0.00000	0.00000
				18	4.9570E 11	0.00000	0.00000
				19	3.0000E-03	3.99109E-01	1.00000
				20	5.0000E-03	3.32092E-01	1.00000

MIXTURE MOLECULAR WEIGHT 11.99961 TOTAL ENERGY EXCHANGE RATE 8.11349E 04 (CAL-CM**3/GM**2/SEC) MASS FRACTION SUM 0.99999994

NEGATIVE CONCENTRATIONS-HALVE STEP SIZE -SAVE1(8) = -0.71672910D-12

TIME 1.14598E 00 SEC AREA 1.00000E 00 SQ CM AXIAL POSITION 0.00000 CM

FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	2.66052	STEPS FROM LAST PRINT	90
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.25088E-02
DENSITY (GM/CM**3)	4.17819E-04	TOTAL NUMBER OF STEPS	180
TEMPERATURE (DEG K)	943.84		
MASS FLOW RATE (GM/SEC)	0.00000		
ENTROPY (CAL/GM/DEG K)	3.7174	FUNCT EVALUATIONS	208
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	33
GAMMA	1.3538		
ENTHALPY (CAL/GM)	2.77280E 02		

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
H	1.32974E-11	3.87085E-07	8.66740E-09	1	2.8485E 10	2.41408E 01	1.00000
O2	1.11262E-05	3.23880E-01	-3.71813E-05	2	1.4762E 11	1.04634E 01	1.00000
OH	1.92902E-12	5.61534E-08	1.07888E-09	3	1.6252E 12	4.01887E 02	0.99967
O	5.52493E-13	1.60830E-08	4.71222E-10	4	3.5176E 12	-9.81015E-03	0.99241
H2	2.23868E-05	6.51676E-01	-7.52605E-05	5	2.5565E 15	3.43171E 02	0.99996
H2O	7.41959E-07	2.15983E-02	7.72944E-05	6	1.4787E 14	8.88241E-09	1.00000

HO2	3.89123E-09	1.13273E-04	1.14348E-06	7	8.7939E 14	1.29522E-04	1.00000
H2O2	9.38444E-08	2.73179E-03	-2.61056E-06	8	9.4794E 15	1.69429E-04	1.00000
				9	3.3671E 07	1.68020E 01	1.00000
				10	3.7862E 06	1.32790E 02	1.00000
				11	1.1045E 03	1.57583E 00	1.00000
				12	9.0779E 13	2.69068E 01	1.00000
				13	2.9337E 13	3.61287E-01	1.00000
				14	2.9337E 13	1.26142E 00	1.00000
				15	1.8000E 12	1.56599E 02	0.99023
				16	3.8330E 12	3.97054E 00	0.99972
				17	6.4939E 13	1.39409E 01	1.00000
				18	2.6373E 12	1.88519E 01	1.00000
				19	3.0000E-03	3.84713E-01	1.00000
				20	5.0000E-03	3.18668E-01	1.00000

MIXTURE MOLECULAR WEIGHT 12.16265 TOTAL ENERGY EXCHANGE RATE (CAL/CM**3/GM**2/SEC) -2.50960E 07 MASS FRACTION SUM 0.99999940

KFLAG = -1 FROM INTEGRATOR AT T = 0.11474745E 01
ERROR TEST FAILED WITH DABS(H) = HMIN

H HAS BEEN REDUCED TO 0.50000000E-0[illegible] AND STEP WILL BE RETRIED

TIME 1.14748E 00 SEC AREA 1.00000E 00 SQ CM AXIAL POSITION -0.03000 CM

FLOW PROPERTIES

PRESSURE (ATM)	3.15072
VELOCITY (CM/SEC)	0.00
DENSITY (GM/CM**3)	4.17819E-04
TEMPERATURE (DEG K)	1127.80
MASS FLOW RATE (GM/SEC)	0.00000
ENTROPY # CAL/GM/DEG K)	3.7932
MACH NUMBER	0.0000
GAMMA	1.3396
ENTHALPY (CAL/GM)	3.05692E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	90
AVERAGE STEP SIZE	0.16615E-04
TOTAL NUMBER OF STEPS	270
FUNCT EVALUATIONS	348
JACOBIAN EVALUATIONS	50

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
H	1.00543E-08	2.95314E-04	1.01354E-02	1	1.2268E 11	7.61912E 04	0.99566
O2	1.07978E-05	3.17152E-01	-5.30604E-02	2	3.8265E 11	4.51135E 04	0.99918
OH	1.42617E-09	4.77636E-05	1.74164E-03	3	2.8602E 12	5.78175E 05	0.99783
O	9.47137E-10	2.78192E-05	1.01943E-03	4	3.8624E 12	-5.54618E 01	0.61964
H2	2.17475E-05	6.38766E-01	-1.03936E-01	5	2.3436E 15	2.25709E 05	0.99995
H2O	1.38492E-06	4.06777E-02	1.07350E-01	6	1.2658E 14	2.21452E-02	1.00000
HO2	3.40681E-08	1.00064E-03	4.71587E-03	7	7.3395E 14	6.44460E 01	1.00000
H2O2	6.92178E-08	2.03306E-03	-6.71012E-03	8	6.6042E 15	8.16960E 01	1.00000
				9	1.7122E 08	7.76669E 02	1.00000
				10	1.9303E 08	5.27176E 03	0.99829
				11	4.6479E 04	6.25205E 01	1.00000
				12	1.0709E 14	2.10123E 05	1.00000
				13	3.2003E 13	5.91519E 03	1.00000
				14	3.2803E 13	1.01560E 04	1.00000
				15	1.8000E 12	1.19474E 04	0.99835
				16	4.4791E 12	2.88755E 03	0.99985
				17	5.1294E 13	1.92280E 04	0.99994
				18	5.7688E 12	2.29975E 04	1.00000
				19	3.0000E-03	3.73727E-01	1.00000
				20	5.0000E-03	3.09264E-01	1.00000

MIXTURE MOLECULAR WEIGHT 12.27213 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) -3.08082E 10 MASS FRACTION SUM 0.99999869

KFLAG = -1 FROM INTEGRATOR AT T = 0.11474790E 01
ERROR TEST FAILED WITH DABS(H) = HMIN

H HAS BEEN REDUCED TO 0.50000000E-08 AND STEP WILL [illegible]

TIME 1.14748E 00 SEC AREA 1.00000E 00 SQ CM AXIAL POSITION 0.00000 CM

FLOW PROPERTIES

PRESSURE (ATM)	5.36731
VELOCITY (CM/SEC)	0.00
DENSITY (GM/CM**3)	4.17819E-04
TEMPERATURE (DEG K)	2009.07
MASS FLOW RATE (GM/SEC)	0.00000
ENTROPY CAL/GM/DEG K)	4.1157
MACH NUMBER	0.0000
GAMMA	1.2825
ENTHALPY (CAL/GM)	4.34163E 02

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	90
AVERAGE STEP SIZE	0.21193E-07
TOTAL NUMBER OF STEPS	360
FUNCT EVALUATIONS	511
JACOBIAN EVALUATIONS	64

C-2

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
H	2.92008E-06	8.96900E-02	4.52829E 01
O2	6.59361E-06	2.02534E-01	-6.46656E 01
OH	8.72374E-07	2.67949E-02	2.14097E 01
O	8.28353E-07	2.54428E-02	1.62954E 01
H2	1.30697E-05	4.01434E-01	-1.25208E 02
H2O	8.24495E-06	2.53243E-01	9.19?A[illegible] 01
HO2	2.53931E-08	7.79948E-04	-1.68427E-01
H2O2	1.00734E-09	3.09405E-05	1.72424E-02

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/CM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	3.2806E 12	3.05621E 08	0.84436
2	3.8915E 12	2.00857E 08	0.83228
3	1.0208E 13	5.20426E 08	0.78063
4	4.7912E 12	-6.4[illegible]249E 06	0.23546
5	1.9270E 15	7.43341E 07	0.99575
6	8.9202E 13	1.14148E 04	0.99997
7	4.1313E 14	4.17403E 06	0.99997
8	2.0811E 15	7.05668E 06	0.99999
9	6.6544E 09	1.26505E 04	0.99996
10	1.4601E 12	-9.66662E 05	0.56225
11	2.1009E 08	1.01031E 05	0.97390
12	1.5533E 14	6.59653E 07	0.99983
13	3.8921E 13	4.68459E 06	0.99891
14	3.8921E 13	4.93189E 05	0.99858
15	1.8000E 12	6.53276E 03	0.98258
16	[illegible].3708E 12	2.94558E 04	0.91849
17	6.2274E 13	2.79113E 05	0.93768
18	3.3583E 13	5.65857E 05	0.99999
19	3.0000E-03	2.24600E-01	1.00000
20	5.0000E-03	1.68907E-01	1.00000

MIXTURE MOLECULAR WEIGHT 12.83329 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) -1.02211E 13 MASS FRACTION SUM 0.99999487

(GCKP) END OF THIS CASE - READ DATA FOR NEXT CASE

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