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CONTENTS

SECTION 1

INTRODUCTION

Over the past several years, Acurex developed the HET catalytic combustor computer model as an aid in the solution of problems related to catalytic combustion applications for various systems such as boilers and gas turbines. The HET model differs from previous models in that it can handle the high temperature effects of catalytic combustion where bed radiative heat transfer and "flame type" phenomena are important by including gas phase reactions and wall radiation terms. For a balance between accuracy and economy of operation, the code utilizes a quasi-one-dimensional model. In the present project, the HET code is used as a basis for examining different concepts utilizing catalytic combustion for Stirling engine heater heads.

Current heater head designs for Stirling engines depend on convective heat transfer from the combustion mixture to heat the working fluid. This approach results in a nonuniform circumferential and axial heat transfer distribution on the heater tubes. Since the tube temperature distribution is somewhat dependent on the local heat transfer rate, a temperature difference will then also exist on the heater tubes. The maximum allowable material temperature then dictates the maximum allowable heat flux. Techniques which result in uniform tube temperatures or heat fluxes will maximize the net amount of energy that can be transferred to the working fluid.

Two advanced concepts that have the potential for more uniform heat fluxes are catalyzed heater head and radiative energy transfer from catalytic reactors to the working fluid heat exchanger. The catalytically coated heater head can react the fuel and transfer the heat of reaction directly into the engine working fluid in a single component. With this concept,

heating would be more spatially uniform allowing a higher average head temperature and thereby increased engine efficiency. Also, combustion temperature and extent of reaction could be tailored to achieve very low exhaust emission levels. Finally, construction would be simplified by incorporating the combustion surface into the head design. In the radiatively cooled concept, heat would be transferred radiatively as well as convectively from the catalytic reactor to the working fluid heat exchanger. The advantage of this concept is that catalyst surface temperatures could be maintained considerably above the working fluid temperature resulting in efficient combustion. With this concept, catalyst and heat exchanger temperatures could be more easily tailored for combustion and heat exchanger efficiency as well as emissions.

Section 2 will present the basic HET model and the modifications and additions introduced by various heater head concepts. Section 3 will describe the code input instructions.

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SECTION 2

THEORY

This section briefly summarizes the theoretical foundations upon which the calculation methods of the Stirling Engine HET Code program are based. An attempt has been made to present these fundamentals in a fashion most appropriate to a user unfamiliar with the code. To this end, and in the interest of brevity, explanations tend to be nonrigorous and perhaps somewhat heuristic. In discussing each type of problem treated by the program, the pertinent governing equations are developed and it is shown that these relations are sufficient to determine the unknown quantities for that particular problem. Since all problems related to the Stirling engine are essentially solved by a modification of the basic HET code developed earlier by Acurex (Reference 2-1), this section will begin with a description of the basic HET code. This is then followed by discussions on how the basic code is modified for each Stirling concept. Calculations and correlations for radiation view factors and transport properties are then discussed at the end of this section.

2.1 BASIC HET CODE

The basic model describes the reactions of a prevaporized and premixed fuel and air stream inside a catalytically coated channel. The following phenomena are treated:

- Homogeneous gas phase chemical reactions
- Heterogeneous surface chemical reactions
- Radial heat and mass transport
- Axial bed conduction
- Radiative heat exchange between walls

The following assumptions are made:

- Negligible gas phase axial heat and mass transport diffusion
- Wall fluxes can be treated by transfer coefficients which directly relate fluxes to the driving forces
- Radial conductive heat transfer is neglected

The resultant quasi one dimensional governing equations are:

Species

$$\dot{m} \frac{dY_i}{ds} = AW_i - C_w J_{w_i} \qquad (1)$$

where $\dot{m}$ = mass flowrate/channel

Y_i = mass fraction of species i in the bulk gas

s = axial distance

A = cross-sectional area of flow channel

C_w = perimeter of flow channel

W_i = chemical production rate (gas phase) of species i

J_{w_i} = flux of species i at the wall

Energy

$$\dot{m} \frac{dh}{ds} = - C_w q_w \tag{2}$$

where h = enthalpy in the bulk gas phase

q_w = heat flux at the wall

Species Flux at the Wall

The flux of species i at the wall is determined by the rate of transport of i to the wall and the rate of reaction of i at the wall. These are given by:

$$J_{w_i} = W_{w_i} \tag{3}$$

and

$$J_{w_i} = \frac{\dot{m}}{A} C_{m_i} (Y_i - Y_{w_i}) \tag{4}$$

where W_{w_i} = rate of destruction of species i at the wall

Y_{w_i} = mass fraction of species i at the wall

C_{m_i} = dimensionless mass transfer coefficient

($C_{m_i} = \frac{k_c}{v}$, k_c = mass transfer coefficient

v = free stream velocity)

Energy Flow at the Wall

The wall heat flux is governed by convective heat transfer, chemical reaction, radiation exchange between walls and conduction in the solid phase. These are given by:

$$q_w = q_r - \frac{A_s}{C_w} k_s \frac{d^2 T_w}{ds^2} \tag{5}$$

and

$$q_w = \frac{\dot{m}}{A} C_H \left[(h - \bar{h}_w) + \sum_i \frac{C_{m_i}}{C_H} h_{w_i} (Y_i - Y_{w_i}) \right] \tag{6}$$

where q_r = radiative heat loss

A_s = cross-sectional area of the solid bed

k_s = conductivity of the solid bed material

T_w = wall temperature

C_H = dimensionless heat transfer coefficient

($C_H = \frac{h_i}{v\rho C_p}$, h = heat transfer coefficient, ρ = density, C_p = heat capacity)

$\bar{h}_w$ = enthalpy of edge gas at wall temperature (defined as $\bar{h}_w = \sum_i Y_i h_{w_i}$).

h_{w_i} = enthalpy of species i at wall temperature

Chemical reaction rate constants are calculated by Arrhenius type rate expressions of the form:

$$k_R = aT^b \exp(-E/RT) \tag{7}$$

where k_R = reaction rate constant

E = activation energy

a,b = constants

Radiation heat exchange is calculated using a view factor approach where q_{r_j}, the wall radiative heat flux at station j is given by

$$q_{r_j} = \varepsilon\sigma\left[(1 - K_{jj})T_{w_j}^4 - \sum_{k\neq j} K_{jk}T_{w_k}^4 - K_{jr_1}T_{r_1}^4 - K_{jr_2}T_{r_2}^4\right] \qquad (8)$$

where K is the channel segment view factor

k denotes all other stations except j

r_1, r_2 denote upstream and downstream reservoirs

Derivation for the view factors for different geometries are given in Section 2.6. Transfer coefficient calculation/correlations used in the code are given in Section 2.7.

The boundary conditions required to solve the system of equations are:

$$s = 0\ ,\quad Y_i = Y_{o_i}\ ,\quad T = T_o\ ,\quad \left.\frac{dT_w}{ds}\right|_{s=0}^{*} = 0$$

$$\left.\frac{dT_w}{ds}\right|_{s=L}^{*} = 0$$

The above equations are solved simultaneously using a finite difference implicit numerical scheme. The results will provide both temperature and species distributions in the gas phase and at the catalyst surface. In the case when the catalyst wall temperature distributions are known, one can also over specify the problem by inputting this information into the program. The program will then automatically bypass the catalyst wall energy equation.

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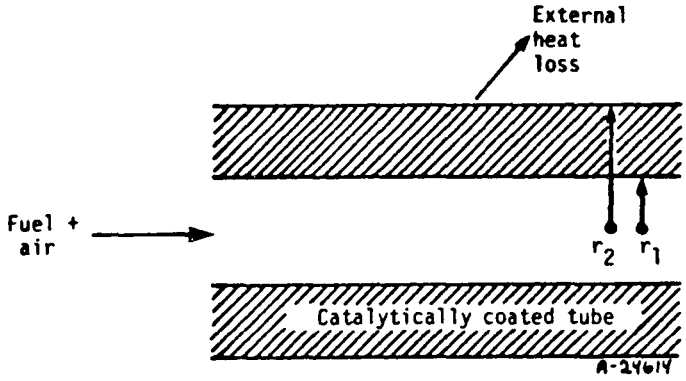
*These correspond to insulated edges. If heat transfer occurs from the ends of the channel to the surroundings, it can easily be taken into account by equating the conductive heat flux to heat loss from the ends, say by convection and/or radiation.

2.2 EXTERNALLY COOLED CATALYTIC CYLINDRICAL REACTOR/FLAT PLATE



This problem is essentially the same as the basic HET problem except that the heat is also removed externally from the tube. Heat conduction must therefore occur transversely as well as axially in the tube walls. To incorporate this effect, a two-dimensional heat conduction equation was implemented into the formulation. This is given by:

$$\frac{\partial^2 T}{\partial s^2} + \frac{\partial^2 T}{\partial r^2} = 0 \qquad (9)$$

where r = radial distance

r_1 = inside tube radius

r_2 = outside tube radius

The above equation is not exact since it does not account for area variations due to changes in radius. It is, however, a good approximation where $r_1 >> (r_2 - r_1)$ which is typical for cylindrical catalytic reactors.

Four boundary conditions are needed for this equation. For the radial direction, these are given by heat exchange between tube and coolant and tube and fuel.

$$h_\infty\left(T_w\Big|_{r=r_2} - \bar{T}_\infty\right) = -k_s \left.\frac{dT_w}{dr}\right|_{r=r_2} \tag{10}$$

$$q_w = q_r - C_{w_1} k_s \left.\frac{dT_w}{dr}\right|_{r=r_1} \tag{11}$$

where h_∞ = external heat transfer coefficient

C_{w_1} = inside tube perimeter

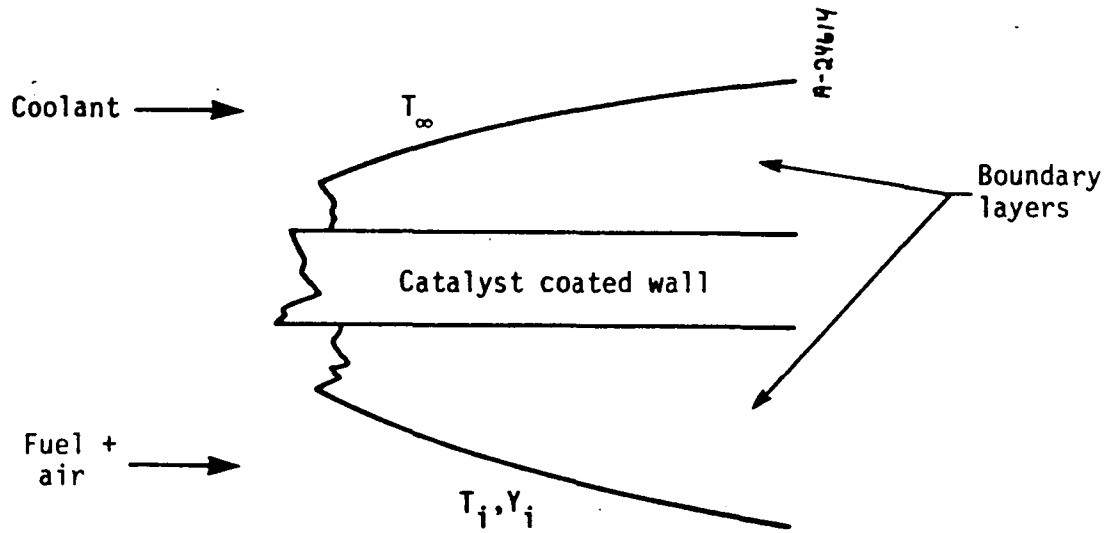
$\bar{T}_\infty$ = average external coolant temperature

The heat transfer occurring from the outside of the tube to the coolant is represented by an external heat transfer coefficient h_∞. Heat transfer may also occur by radiation. If heat transfer by radiation from the surface of the tube is important, then h_∞ can include this effect by linearizing the temperature term of radiation and assuming h_∞ is an effective heat transfer coefficient representing both convective and radiative heat transfer.

q_w, the wall heat flux, is the same as that defined in the basic model (Equation (5)), except the axial conduction term is replaced by a conduction term at the surface of the wall. The boundary conditions for the axial direction remain the same as in the basic model with either insulated ends (no heat transfer at the ends of the tube) or conductive heat transfer at the ends of the tube balanced by radiation and convection.

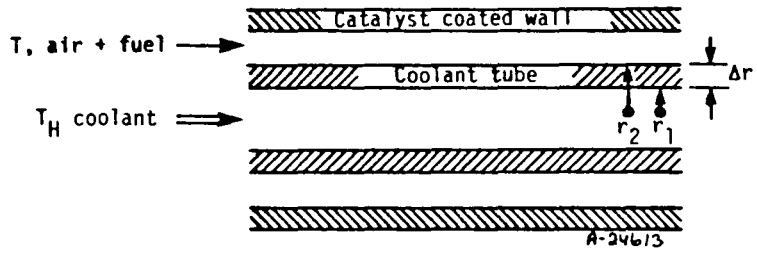
The input conditions for this problem are similar to the typical monolithic reactor problem except that the external heat transfer coefficient and coolant temperature must be inputted. The values of these input parameters, however, need not be constant.

2.3 FLOW ALONG FLAT PLATE



For the flat plate problem, the bulk gas temperature and composition remain constant and the boundary layer is growing as the gas streams travel down the tube. The basic HET model equations are easily adapted to this problem and much simplified. Equations (1) and (2) are not necessary since the bulk composition and temperatures remain constant Wall compositions and temperatures can be solved by equating Equations (3) and (4), and (5) and (6). Thus, the flat plate problem, in a way, is a subset problem of the HET code. Transfer coefficients, however, must be modified accordingly and also there is no radiation exchange between walls (only radiation heat loss to the ambient).

2.4 COANNULAR TUBE RADIATIVELY COOLED CONCEPT



In this problem, coolant and fuel flow in concentric tubes with coolant in the inner tube and fuel in the annular region. The inner walls of the outer tube are catalytically coated. Heat is transferred to the inner tube by convection and radiation. The following assumptions are made:

- The inner coolant tube has a thickness Δr which offers some resistance to heat transfer
- Axial conduction in the inner tube is neglected
- Radiation from the inner tube wall to the catalyst coated wall is neglected since the temperature of the inner tube wall is much lower than the catalyst wall

For this problem, the basic equations of the HET model can be adapted with a few minor modifications. Equation (2) has to be modified to include heat exchange with the inner tube in addition to the catalyst wall. This is given by:

$$\dot{m}\frac{dh}{ds} = -C_w q_w - C'_{w_2} h_t \left(T - T'_w\Big|_{r=r_2}\right) \qquad (12)$$

where C'_{w_2} = outer perimeter of inner coolant tube

h_t = heat transfer coefficient from bulk gas to wall surface of coolant tube

T'_w = wall temperature of coolant tube (function of both axial and radial directions)

To solve for the wall and coolant temperature distributions, the following heat balances on the coolant tube are needed:

$$h_t\left(T - T'_w\Big|_{r=r_2}\right) + k\left.\frac{dT'_w}{dr}\right|_{r=r_2} + q'_r = 0 \qquad (13)$$

$$h_H\left(T_H - T'_w\Big|_{r=r_1}\right) - k\left.\frac{dT_w}{dr}\right|_{r=r_1} = 0 \qquad (14)$$

$$\dot{m}_H C_{p_H}\frac{dT_H}{ds} - h_H C'_{w_1}\left(T'_w\Big|_{r=r_1} - T_H\right) = 0 \qquad (15)$$

where k = conductivity of the coolant tube

C'_{w_1} = inner perimeter of coolant tube

q'_r = heat transfer by radiation from catalyst wall to coolant tube wall

h_H = heat transfer coefficient of coolant

$\dot{m}_H, C_{p_H}$ = mass flowrate and heat capacity of coolant, respectively

If the axial condition is neglected, the radial conduction heat flow Q_c in the coolant tube is given by:

$$-kA\left.\frac{dT'_w}{dr}\right|_{r=r_1} = Q_c = k\,\frac{2\pi L}{\ell n\,\frac{r_2}{r_1}}\left(T'_w\Big|_{r=r_2} - T'_w\Big|_{r=r_1}\right) \qquad (16)$$

where A = tube surface area for heat transfer

L = tube length

Combining Equations (13), (14), and (16), and substituting into Equation (15) gives:

$$\dot{m}_H C_{p_H} \frac{dT_H}{ds} - U_1 C'_{w_1} \left[\frac{q'_r}{h_t} + (T - T_H) \right] = 0 \qquad (17)$$

boundary condition $T_H = T_{H_o}$ at $S = 0$

where U_1 = overall heat transfer coefficient

$$U_1 = \frac{1}{\frac{A_1}{A_2 h_t} + \frac{A_1 \ln (r_2/r_1)}{2\pi k L} + \frac{1}{h_H}}$$

A_2 = surface area at $r = r_2$

A_1 = surface area at $r = r_1$

If we assume that the tube wall is thin, U_1 can be simplified to

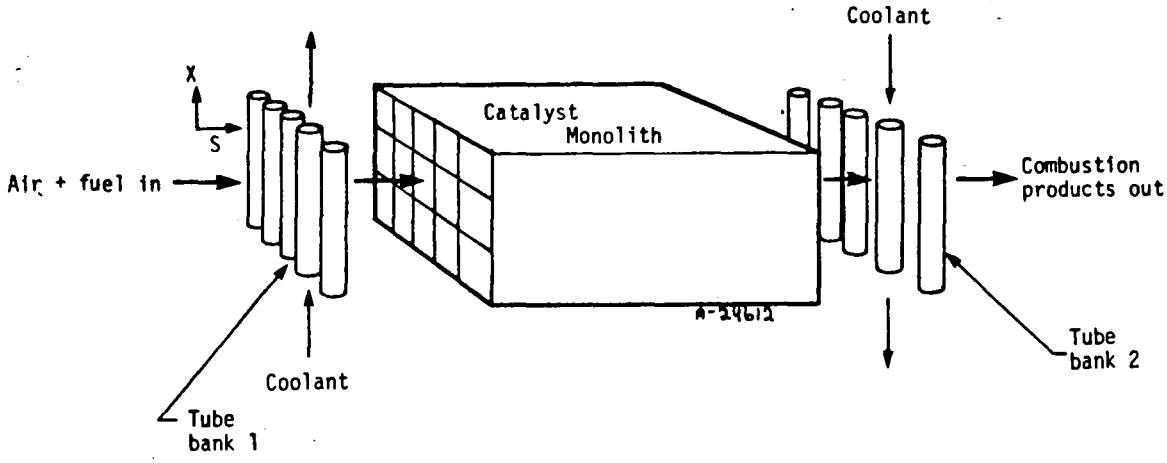
$$U_1 = \frac{1}{\frac{1}{h_t} + \frac{\Delta r}{k} + \frac{1}{h_H}} \qquad (19)$$

The second term on the right hand side of Equation (12) can also be expressed as functions of T and T_H only to give:

$$\dot{m} \frac{dh}{ds} = - C_w q_w - C'_{w_2} \left[U_1 \frac{A_1}{A_2} (T - T_H) + q'_r \frac{U_1}{h_t} \frac{A_1}{A_2} \right] \qquad (20)$$

Equations (17) and (20) can be incorporated into the basic HET equations and solved simultaneously. Once T_H and T are solved, the coolant wall temperature profile T'_w can readily be derived from Equations (13) and (14).

2.5 MONOLITHIC REACTOR RADIATING TO UPSTREAM AND DOWNSTREAM HEAT EXCHANGERS



The problem of a monolith placed between two banks of coolant tubes is rather straightforward in that no modification is necessary to the basic HET equations. The problem of heat transfer to the coolant is decoupled from the solution to the HET equations since heat transfer to the tube banks does not affect the HET equations. Heat transfer to the tube banks occurs by two mechanisms. The first is by convective flow of the fuel over the tube banks. The second is by radiation from the monolith walls to the tube banks. Back radiation from the tube banks to the monolith walls can be neglected since the tube walls are at significantly lower temperatures compared to the catalyst walls. The equation describing heat transfer to the tube banks is similar to Equations (13), (14), (15), and (17) except that convective heat transfer occurs by crossflow over the tubes and radiation heat transfer occurs from the whole monolith to the tube bank. The key equation to be solved is:

$$\dot{m}_H C_{p_H} \frac{dT_H}{dx} = U_1 C'_{w_1} \left[\frac{q_r}{h_t} + (\bar{T} - T_H) \right] \qquad (21)$$

boundary condition $\quad T_H = T_{H_o} \quad$ at $\quad x = 0$

where x = axial distance along coolant tube

$\bar{T} = \frac{T_i + T_o}{2}$ T_i = temperature of fuel air mixture approaching coolant tube

T_o = temperature of fuel air mixture after passing over coolant tube

q_r = radiation heat flux from the monolith to the tube bank, assumed uniformly distributed along the tube length

If the inlet fuel/air temperature (temperature after passing over the first tube bank) is known, the equations of the basic HET model can be solved without modification to give the wall and gas temperatures in the monolith. The monolith wall temperatures can be combined with suitable view factors to give the radiation heat transfer flow to the tube banks. The exit temperature of the gas stream from the monolith is the temperature of approach to the second tube bank. Equation (21) can be solved analytically by assuming the radiation heat flux term (q_r) is uniform over the length of the tube to give the hydrogen temperature as a function of distance x:

$$T_H = \frac{1}{A_1}\left[B_1(1 - e^{-A_1 x})\right] + T_{H_o} e^{-A_1 x} \qquad (22)$$

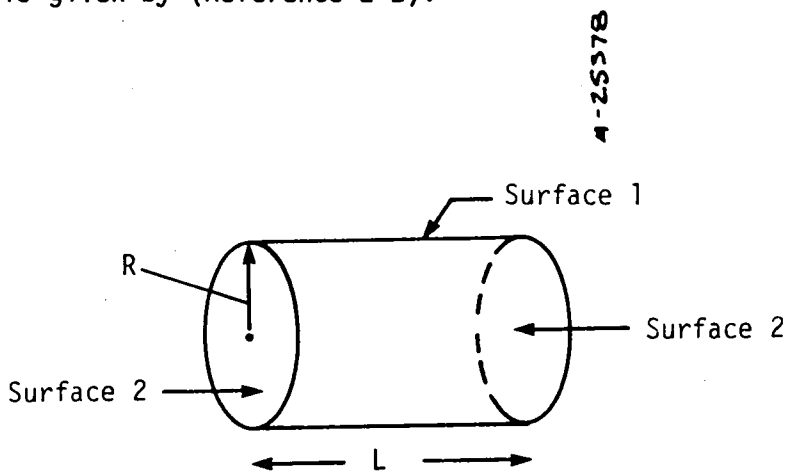
where $A_1 = \frac{U_1 C'_{w_1}}{\dot{m}_H C_{p_H}}$

$$B_1 = \left(\frac{U_1 q_r}{h_t} + U_1 \bar{T}\right)\left(\frac{C'_{w_1}}{\dot{m}_H C_{p_H}}\right)$$

The wall temperature distribution of the coolant tubes can easily be solved once T_H is known.

2.6 CALCULATION OF RADIATION VIEW FACTORS

Calculation of radiation view factors for different geometries is relatively straightforward. Radiation heat transfer between walls of a cylindrical tube is given by (Reference 2-2):



$$Y = \frac{R}{L} \qquad x = 2 + \frac{1}{Y^2}$$

$$F_{22} = 0.5\left\{x - \sqrt{x^2 - 4}\right\} \tag{23}$$

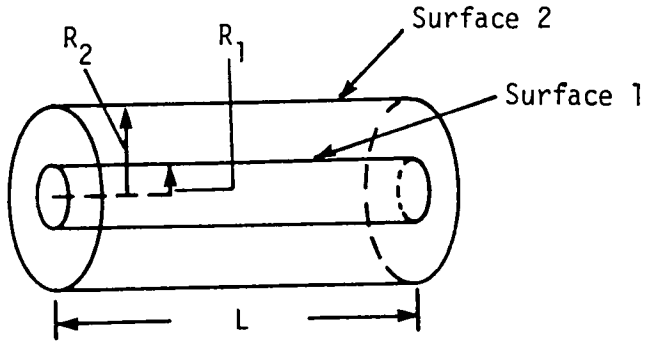
Radiation heat transfer between concentric tubes is given by (Reference 2-2):

$$R = \frac{R_2}{R_1}$$

$$G = \frac{L}{R_1}$$

$$A_o = R^2 + G^2 - 1$$

$$B = G^2 - R^2 + 1$$



$$F_{22} = 1 - \frac{1}{R} + \frac{2}{R}\tan^{-1}\left(\frac{2\sqrt{R^2 - 1}}{G}\right)$$

$$= \frac{1}{2\pi R}\left\{\frac{\sqrt{4R^2 + G^2}}{G}\sin^{-1}\left[\frac{4(R^2 - 1) + \frac{G^2}{R^2}(R^2 - 2)}{G^2 + 4(R^2 - 1)}\right]\right.$$

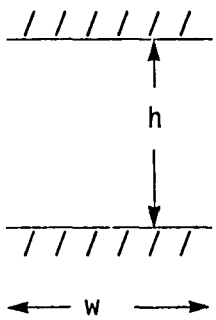
$$\left. - \sin^{-1}\left(\frac{R^2 - 2}{R^2}\right) + \frac{\pi}{2}\left(\frac{\sqrt{4R^2 + G^2}}{G} - 1\right)\right\} \qquad (24)$$

$$F_{21} = \frac{1}{R} - \frac{1}{\pi R}\left\{\cos^{-1}\left(\frac{B}{A_o}\right) - \frac{1}{2L}\left[\sqrt{(A_o + 2)^2 - (2R)^2}\ \cos^{-1}\left(\frac{B}{RA_o}\right)\right.\right.$$

$$\left.\left. + B\sin^{-1}\left(\frac{1}{R}\right) - \frac{\pi A_o}{2}\right]\right\} \qquad (25)$$

$$F_{23} = 0.5(1 - F_{21} - F_{22}) \qquad (26)$$

In the case of the monolith radiating to a bank of tubes, we can assume that the face of the monolith is very close to the tube bank for maximum heat transfer. The two faces can therefore be treated as semi-infinite plates with the view factor given as (Reference 2-2):



$$H = h/w$$

$$F_{12} = \sqrt{1 + H^2} - H \qquad (27)$$

To correct for the fact that one of the plates is really a bank of tubes of diameter D_t with center to center distance D_c, the actual view factor from monolith to tube bank F_{MT} is (Reference 2-3):

$$F_{MT} = yF_{12} \tag{28}$$

$$\begin{aligned} y &= -0.059Z^2 + 0.049Z + 1.01 \qquad 1 \leq Z \leq 2 \\ &= 0.0145Z^2 - 0.224Z + 1.26 \qquad 2 < Z \end{aligned} \tag{29}$$

where $Z = \dfrac{D_c}{D_t}$

2.7 TRANSFER COEFFICIENTS

Values for gas properties and transfer coefficients are based on correlations and theoretical equations. The fuel/air side consists of analytical equations and correlations already built into the HET code. They are more refined than the accuracy of the present problem requires but since they are already there, little effort is made to convert them to simpler correlations. Of the equations and correlations used for the fuel/air side, the following will be described in more detail.

The fuel/air side consists of a complex mixture of reactants and products that changes in concentration with distance down the channel. Transport properties such as diffusion, viscosity, and thermal conductivity must therefore make use of correlations based on mixtures. The development of expressions for these is discussed in detail elsewhere (Reference 2-8). A brief summary of this development, and the resulting expressions, is presented here.

Correlations for binary diffusion coefficients are given in terms of a bifurcation approximation discussed in detail in Reference 2-8. This is of the form:

$$D_{ij} = \frac{\bar{D}}{F_i F_j} \tag{30}$$

where $\bar{D}$ is a reference diffusion coefficient and F_i are diffusion factors. In the present code, oxygen is chosen as the reference species with $F_{O_2} = 1.0$. From the molecular theory of gases and liquids (Reference 2-9):

$$\bar{D} = 2.628 \times 10^{-3} \frac{T(T/M_{ref})^{1/2}}{P\sigma^2_{ref}\,\Omega^{(1,1)*}_{ij}} \ (cm^2/sec) \tag{31}$$

with T in °K, P in atmospheres, and collision cross section, σ in Å. For O_2 as the reference species, σ is equal to 3.467 Å. Using the data from Reference 2-9, the integral expression for transport properties is approximated by:

$$\Omega_{ij}^{(1,1)*} \simeq 1.07[T/(\varepsilon/k)]^{-0.159} \tag{32}$$

where the maximum energy of attraction function, ε/k, for O_2 is 106.7 and thus:

$$\bar{D} = 0.172 \times 10^{-4}\, T^{1.659} / P \ (cm^2/sec) \tag{33}$$

For system viscosity, use is made of the correlation suggested by Buddenberg and Wilke (Reference 2-10) and endorsed by Hirschfelder et al. (Reference 2-9), namely

$$\mu_{mix} = \sum_i \frac{X_i \mu_i}{X_i + 1.385 \frac{RT\mu_i}{PM_i} \sum_{\substack{j \\ j \neq i}} \frac{X_j}{D_{ij}}} \tag{34}$$

where X_i is the mole fraction for component i

M_i is the molecular weight of component i

μ_i is the viscosity of pure component i

By introducing the bifurcation relations, taking from Reference 2-9 the relation for pure component viscosity

$$\mu_i = \frac{5}{6A_{ii}^*} \rho_i D_{ii} \tag{35}$$

where A^*_{ij} is a ratio of collision integrals. Assuming $A^*_{ij} \simeq 1.12$ (actually varies from 1.10 to 1.14 in the temperature range of interest), and adjusting 1.385 to 1.344 for simplification, there is obtained

$$\mu_{mix} = \rho \bar{D} \frac{\beta_2}{1.344 \beta_1 M} \tag{36}$$

where $\beta_1 = X_i F_i$

$$\beta_2 = \frac{M_i X_i}{F_i}$$

The thermal conductivity of a mixture of polyatomic molecules can be written (Reference 2-10) as:

$$k_{mix} = k_{mono\text{-}mix} + k_{int} \tag{37}$$

where $k_{mono\text{-}mix}$ is the mixture thermal conductivity computed neglecting all internal energy modes and k_{int} is the contribution of the internal energy modes of the molecules to the mixture conductivity. An approximate relationship for $k_{mono\text{-}mix}$ developed by Mason and Saxena (Reference 2-11) is:

$$k_{mono\text{-}mix} = \sum_{i}^{I} \left[\frac{X_i k_{i_{mono}}}{X_i + 1.385 \frac{RT_i}{PM_i} \sum_{j \neq 1}^{I} \frac{X_i}{D_{ij}}} \right] \tag{38}$$

where $k_{i_{mono}}$ is the thermal conductivity of the pure species i, neglecting all internal degrees of freedom. Expressions for $k_{i_{mono}}$ can be written (Reference 2-9) as:

$$k_{i_{mono}} = \frac{15}{4}\frac{R}{M_i}\mu_i \tag{39}$$

The expression for $k_{mono\text{-}mix}$ then becomes:

$$k_{mono\text{-}mix} = \frac{\rho\bar{D}}{\beta_1}\left\{\sum\left[\frac{\frac{X_i}{F_i}\frac{15}{4}\frac{R}{M}}{1.344}\right]\right\} \tag{40}$$

To complete the definition of k, the expression for the internal energy mode contribution to thermal conductivity must be added to $k_{mono\text{-}mix}$.

From Equations (59) and (77) of Reference 2-12, the following relation can be obtained:

$$k_{int} = \sum_i \frac{\rho X_i \frac{M_i}{M}\left(C_{p_i} - \frac{5}{2}\frac{R}{M_i}\right)}{\sum_j X_j/D_{ij}} \tag{41}$$

$$k_{int} = \sum \frac{\rho\bar{D}X_i \frac{M_i}{M}\left(C_{p_i} - \frac{5}{2}\frac{R}{M_i}\right)}{\beta_1 F_i} \tag{42}$$

The value of k used is then:

$$k = \frac{\rho\bar{D}}{\beta_1}\left\{C_p + 0.29R\beta_3\right\} \tag{43}$$

where $$\beta_3 = \frac{1}{M}\sum_i \frac{X_i}{F_i} \quad \text{and} \quad C_p = \frac{1}{M}\sum \frac{M_i X_i C_{p_i}}{F_i} \tag{44}$$

The mass transfer coefficient is developed from the heat transfer coefficient by

$$C_{M_i} = C_H(Le_i)^{2/3} \tag{45}$$

where Le_i = Lewis number.

On the coolant side, the gases used are either hydrogen, helium or air. Since there are no reactions in the coolant, gas properties and transfer coefficients can be treated as a one component gas stream and simple expressions can be derived.

Gas viscosity can be represented by the Hirschfelder, Curtiss and Bird equation (Reference 2-9):

$$\mu = 26.69 \frac{\sqrt{MT}}{\sigma^2 \Omega_v} \tag{46}$$

where μ = viscosity (μp)

T = temperature (K)

M = molecular weight

σ = hard sphere diameter (Å)

Ω_v = collision integral

$$\Omega_v = \left(\frac{1.161}{0.150T_k}\right) + \frac{0.525}{\exp(0.773T_k)} + \frac{2.162}{\exp(2.438T_k)} \tag{47}$$

$$T_k = \frac{T}{\frac{\varepsilon}{k}} \tag{48}$$

$$\frac{\varepsilon}{k} = \frac{\text{characteristic energy of interaction between molecules}}{\text{Boltzmann constant}}$$

The values for σ and ε/k for the coolant used are given below:

Coolant	σ (Å)	ε/k (K)
Helium	2.551	10.22
Hydrogen	2.827	59.7
Air	3.711	78.6

Thermal conductivity can be calculated by the relation (Reference 2-4):

$$\frac{k_2}{k_1} = \left(\frac{T_2}{T_1}\right)^n \tag{49}$$

If we know the thermal conductivities of the gas at two temperatures, the value of n can be obtained from Equation (49).

Heat capacity of the coolant is correlated by the general expression:

$$C_p = a + bT + CT^{-2} \tag{50}$$

T = temperature (K)

C_p = heat capacity (cal/g mole °C)

Values for a, b, c for each gas can be readily obtained from any handbook.

REFERENCES FOR SECTION 2

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2-10 Buddenberg, J. W. and Wilke, C. R., "Calculation of Gas Mixture Viscosities," Ind. and Eng. Chem., 41: 1345, 1949.

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SECTION 3

CODE INPUT INSTRUCTIONS

This section describes the punched card input needed to activate the problem options described in Section 2. A number of comments are included to help guide the user in setting up input card decks.

3.1 CARD INPUT DECK

Card 1		(Format 20A4)
1 - 80		Title of run
Card 2		(Format 7I3)
1 - 3	IS	Number of species
4 - 6	NL	Number of grid points
7 - 9	NIT	Number of iterations allowed
10 - 12	ILOSS	Heat loss option,
		0 - adiabatic reactor option
		1 - traverse heat loss option
		2 - assigned catalyst temperature option
13 - 15	IGEOM	Reactor geometry option,
		0 - monolith or cylindrical reactor option
		1 - flat plat option
		2 - coannular tube radiatively cooled reactor option
		3 - monolith reactor radiating to up- and downstream heat exchangers problem option

16 - 18	ICOEF	Input external heat transfer coefficient option
		>0 - invoke this option and bypass the built-in correlation
19 - 21	KR7	Diagnostic output option,
		>3 - invoke diagnostic output option
Card 3		(Format 5F10.0)
1 - 10	DTUB	Effective cell diameter (cm)
11 - 20	VF	Void fraction of monolith
21 - 30	DIAMS	Diameter/height of reactor (cm)
31 - 40	AK	Thermal conductivity of reactor (cal/s/cm-K)
41 - 50	EMIV	Emissivity of reactor
Card 4		(Format 3F10.0)
1 - 10	AM	Mass flowrate (gm/s) for IGEOM $\neq$ 1. Mass flux (gm/cm^2-s) for IGEOM = 1.
11 - 20	TI	Inlet temperature (K)
21 - 30	P	Pressure (atm)
Card 5		(Format 2F10.0)
1 - 10	TRES(1)	Upstream reservoir temperature (K)
11 - 20	TRES(2)	Downstream reservoir temperature (K)
Card Set 6		Spatial grid parameters
Card(s) 1		(Format 8E10.5)
1 - 10	S(N),N=1,NL	Selected grid locations (cm)
11 - 20		
...		

Card Set 7		First guessed/assigned wall temperature profile
Card(s) 1		(Format 8E10.5)
1 - 10	TL(N),N=1,NL-1	Wall temperature at node point N (K)
11 - 20		
...		
Card Set 8		(Format 40I2)
Card(s) 1		
1 - 2 3 - 4 ...	IKIN(N),N=1,NL-1	If the node is a noncatalytic surface, enter zero. If it is a catalytic surface, enter 1
Card Set 9		Parameters for ILOSS >0 and IGEOM >0 options
Card 1		(Format 5F10.5)
1 - 10	VL	Coolant initial velocity (cm/s)
11 - 20	AMH	Coolant flowrate (gm/s)
21 - 30	TTI	Coolant inlet temperature (K)
31 - 40	PT	Coolant pressure (atm)
41 - 50	WT	Coolant molecular weight (gm/gmole)
Card 2		
1 - 10	AKT	Thermal conductivity (for coolant tube) (cal/s-cm-K)
11 - 20	DR	Coolant tube thickness (cm)
21 - 30	DT	Coolant tube diameter (cm). Leave blank if IGEOM >2.
41 - 50	CC	Distance between monolith and tube bank (cm). Leave blank unless IGEOM = 3.

Card 3		(Format 4F10.5). (See Equation 49.)
1 - 10	TK1	Lower reference temperature for thermal conductivity of the coolant (K)
11 - 20	TK2	Upper reference temperature for thermal conductivity of the coolant (K)
21 - 30	GKT1	Coolant thermal conductivity corresponding to TK1
31 - 40	GKT2	Coolant thermal conductivity corresponding to TK2
Card 4		(Format 5F10.5)
1 - 10	SG	Parameters for calculation of coolant viscosity (see Equations 46 to 48)
11 - 20	EK	
21 - 30	C1	Coefficients for coolant specific heat correlation (see Equation 50) $C_1 = a$, $C_2 = b$, $C_3 = c$
31 - 40	C2	
41 - 50	C3	
Card Set 10		Initial species concentrations, wall species concentration guesses, and species diffusion factors
Card(s) 1 to IS		(Format 2A4, 2X, 2E10.3, F10.4)
1 - 8	NAMA	Species name utilized in kinetic reaction input. (These names must also be compatible with the names on the thermochemical input data file.) See Section 3.2 for a description of thermochemical data.
11 - 20	ALPHF	Initial species concentration in relative mole concentrations

21 - 30	ALPHE	Estimate of final wall species concentrations in relative mole concentrations
31 - 40	BPA	Bifurcation diffusion factors, $1/F_i$, for each species. (See Appendix A for the definition of these factors)

Card Set 11 — Kinetic data

Reactions and their associated rates are given in the form:

$$\sum_i \mu^R_{i_m} B_i \rightleftharpoons \sum_i \mu^P_{i_m} B_i$$

and

$$R_m = k_{f_m} \left[e^{\Sigma \mu^R_{i_m} \ln P_i} - e^{\Sigma \mu^P_{i_m} \ln p_i - \ln K_{p_m}} \right]$$

where μ are the stoichiometric coefficients on species B_i, P_i is the partial pressure of species i, and K_{p_m} is the corresponding equilibrium constant. The forward reaction rate coefficient, k_{f_m}, has the Arrhenius form

$$k_{f_m} = aT^b e^{-(E/RT)}$$

The backward reaction rate coefficient is taken to be equal to the forward reaction rate coefficient divided by the equilibrium constant.

Card 1 — (Format 2I3)

1 - 3	MT	Total number of reactions input (including both gas phase and surface reactions)
4 - 6	MGAS	Number of gas phase reactions

Card(s) 2, 4,...,2MT			(Format 10(A4,1X), 3E10.4)
1 - 4	NA(1)	}	Name of reactants (must be compatible with Card Set 10
...	...		
21 - 24	NA(5)		
26 - 29	NB(1)	}	Name of products (must be compatible with Card Set 10
...	...		
46 - 49	NB(2)		
51 - 60	FKF(M)		Pre-exponential factor of the mth reaction (in mole, cm, sec units)
61 - 70	EXK(M)		Temperature exponent
71 - 80	EAK(M)		Activation energy (kcal/gmole-K)
Card(s) 3, 5,...,2MT+1			(Format 5F5.0, T41, 5F5.0)
1 - 5	AMU(1)	}	μ_i^R associated with NA(i)
...	...		
21 - 25	AMU(5)		
41 - 45	BMU(1)	}	μ_i^P associated with NB(i)
...	...		
61 - 65	BMU(5)		

3.2 THERMOCHEMICAL INPUT DATA FORMAT

For the program operation, thermochemical data (i.e., specific heat, enthalpy and entropy) for all species included in Card Set 10 must be present on mass storage devices designated by unit 11. The order of this data on the storage device is not important. However, it is important that the species names input on Card Set 10 match identically with the species names on the thermochemical data files and the kinetic reaction input data, Card Set 11. The thermochemical data files can be full libraries of data, from which only a limited number of species will be selected for each problem of interest.

Curve fits of data are in the form $Cp = F_3 + F_4T + F_5/T^2$ and cover a lower and upper temperature range. Cp units are cal/mole/K.

Card 1		(Format 10X, 2A4, 2X, 2F10.0)
11 - 18	NAMA	Species name utilized in initial concentration and reaction input
21 - 20	MW	Molecular weight of species
Card 2		(Format 6E9.6, 6X, F6.0, 6X, A4) Low temperature curve fit.
1 - 9	F_1	Heat of formation at 298K (cal/mole)
10 - 18	F_2	Change in enthalpy from 298K to 3000K (cal/mole)
19 - 27	F_3	Coefficient in above Cp expression
28 - 36	F_4	Coefficient in above Cp expression
36 - 45	F_5	Coefficient in above Cp expression
46 - 54	F_6	Entropy constant at 3000K (cal/mole)
61 - 66	TU	Upper temperature limit of low temperature range curve fit (K)
73 - 76	NAMA	Name of species used in reaction set
Card 3		(Format 6E9.6, 6X, F6.0, 6X, A4) High temperature curve fit
1 - 9	F_1	Heat of formation at 298K (cal/mole)
10 - 18	F_2	Change in enthalpy from 298K to 3000K (cal/mole)
19 - 27	F_3	Coefficient in above Cp expression
28 - 36	F_4	Coefficient in above Cp expression
36 - 45	F_5	Coefficient in above Cp expression
46 - 54	F_6	Coefficient in above Cp expression
61 - 66	TU	Upper temperature limit of low temperature range curve fit (K)
73 - 76	NAMA	Name of species used in reaction set

SECTION 4

SAMPLE PROBLEMS

Several sample problems were run with the Stirling Engine Combustor Code to show the variety of problems that can be solved. In this section, each problem is briefly described, input card data is shown and select output results are presented.

SAMPLE PROBLEM NO. 1
ADIABATIC CYLINDRICAL REACTOR (CERAMIC)

Description: This problem represents a fuel/air mixture flow in a catalytic ceramic tube with no heat loss to the environment. This problem is also the same as catalytic combustion in an adiabatic honeycomb reactor.

Fuel: Propane/air

Equivalence ratio	$\Phi = 0.2$
Mixture flowrate	$\dot{m} = 0.0394$ g/s
Preheat temperature	$T_{in} = 800$K
Pressure	$P^{in} = 3 \times 10^5$ Pa

Geometry:

Cell diameter	$D_{Tub} = 0.32$ cm
Reactor length	$\ell = 20$ cm
Void fraction	$V_F = 0.87$

```
SAMPLE PROBLEM A - UNCOOLED CATALYST MONOLITH F/A EQUIV RATIO=0.2
  5 32  1  0  0  0  0
0.15875   0.87      0.17      0.0005    0.8
0.0394    800.0     3.0
800.0     -1.0
0.0       0.05      0.10       0.15      0.2       0.25      0.3       0.35
0.4       0.45       0.5       0.75      1.0        1.5       1.75       2.0
2.5       3.        3.5       4.        4.5       5.        5.5        6.
6.5       7.        7.5       8.        8.5         9.      9.5        10.
1200.     1200.     1200.     1200.     1200.     1200.     1200.     1200.
1200.     1200.     1200.     1200.     1200.     1200.     1200.     1200.
1200.     1200.     1200.     1200.     1200.     1200.     1200.     1200.
1200.     1200.     1200.     1200.     1200.     1200.     1200.     1200.
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
N2        .78334    .77686    1.03475
O2        .20833    .16529    1.10045
C3H8      .00833    2.0   E-031.2758
H2O       1.0   E-10 .03306   .844069
CO2       1.0   E-10 .02479   1.27446
  2  1
C3H8 O2                  C3H8 O2   H2O  CO2       4.1    E+9          40.61
.25  1.04                                -.75 -3.964.0  3.0
C3H8                     O2   H2O  CO2            1.1   E+09 0.       17.6
1.0                                 -5.0 4.0  3.0
```

SAMPLE PROBLEM A - UNCOOLED CATALYST MONOLITH F/A EQUIV RATIO=0.2

* INTEGRAL PARAMETERS *

IS (NUMBER OF SPECIES)	=	5
NL (GRID POINTS)	=	32
NIT (NUMBER OF OVERALL ITERATIONS)	=	1
ILOSS (HEAT LOSS OPTION)	=	0
IGEOM (PROBLEM GEOMETRY OPTION)	=	0
ICOEFF (HEAT TRANSFER INPUT OPTION)	=	0
KR7 (PRINT OPTION)	=	0

* NONINTEGRAL PARAMETERS *

*** REACTOR DATA ***

MONOLITH HONEYCOMB CATALYTIC COMBUSTOR

NUMBER OF TUBES	=	1.00
VOID FRACTION	=	.870
DIAMETER OF COMBUSTOR	=	.17 (CM)
EFFECTIVE CELL DIAMETER	=	.16 (CM)

INLET TEMPERATURE	=	800.00 (K)
PRESSURE	=	3.00 (ATM)
MASS FLOW RATE	=	.394-001 (G/S)
CONDUCTIVITY	=	.500-003 (CAL/S-CM-K)
EMISSIVITY	=	.80

*** RESERVOIR TEMPERATURES ***

UPSTREAM	=	800.00
DOWNSTREAM	=	1.0000

GRID POINTS CHOSEN (S)

.0000	.5000-001	.1000+000	.1500	.2000	.2500	.3000	.3500	.4000	.4500
.5000	.7500	1.000	1.500	1.750	2.000	2.500	3.000	3.500	4.000
4.500	5.000	5.500	6.000	6.500	7.000	7.500	8.000	8.500	9.000
9.500	10.00								

INITIAL GUESSED WALL TEMPERATURES (TL)

1200.	1200.	1200.	1200.	1200.	1200.	1200.	1200.	1200.	1200.
1200.	1200.	1200.	1200.	1200.	1200.	1200.	1200.	1200.	1200.
1200.	1200.	1200.	1200.	1200.	1200.	1200.	1200.	1200.	1200.
1200.									

* SPECIES INITIAL MOLE FRACTIONS,FIRST GUESSES,AND DIFFUSION FACTORS *

SPECIE	ALPF	ALPL	DIFFUSION FACTOR
N2	.783+000	.777+000	1.0347
O2	.208+000	.163+000	1.1004
C3H8	.833-002	.200-002	1.2758
H2O	.100-009	.331-001	.8441
CO2	.100-009	.248-001	1.2745

* THERMOCHEMISTRY DATA *

CURVE FIT OF DATA IN FORM CP=RB+RC*T+RD/(T*T) (CAL/(MOLE*K)

HF(CAL/MOL)	H(CAL/MOL)	RB	RC	RD	S(CAL/MOL/K)	TU(K)		NAME
N2	28.000							
.79000+000	.23993+005	.61391+001	.16415-002	.29727+005	.64548+002	300.	1000.	N2
.79000+000	.22188+005	.83049+001	.23357-003	-.74806+006	.63774+002	1000.	2500.	N2
O2	32.000							
.00000	.25541+005	.67044+001	.16795-002	-.19419+005	.68908+002	300.	1000.	O2
.00000	.23450+005	.80725+001	.50513-003	-.21319+006	.67976+002	1000.	2500.	O2
H2O	18.000							
-.57798+005	.31716+005	.68290+001	.29575-002	.27843+005	.69022+002	300.	1000.	H2O
-.57798+005	.30303+005	.99698+001	.12774-002	-.14328+007	.68463+002	1000.	2500.	H2O
CO2	44.000							
-.94054+005	.41438+005	.95778+001	.36020-002	-.16589+006	.81997+002	300.	1000.	CO2
-.94054+005	.36573+005	.13972+002	.38449-003	-.13412+007	.79867+002	1000.	2500.	CO2
C3H8	44.000							
-.24820+005	.10888+006	.32090+002	.11928-001	-.20372+007	.15940+003	300.	2500.	C3H8
-.24820+005	.10888+006	.32090+002	.11928-001	-.20372+007	.15940+003	2500.	6000.	C3H8

* KINETIC REACTION DATA *

TOTAL NUMBER OF REACTIONS 2
NUMBER OF GAS PHASE REACTIONS 1

M	TYPE	REACTION	PRE EXP FACTOR (MOLE-CM-S)	TEMP EXP	ACTIVATION (KCAL/MOLE)
1	GAS	5.0 O2 + 1.0 C3H8--=4.0 H2O + 3.0 CO2	.4100+010	.000	40.6100
2	SURF	5.0 O2 + 1.0 C3H8--=4.0 H2O + 3.0 CO2	.1100+010	.000	17.6000

	AXIAL DISTANCE ALONG MONOLITH, CYLINDER OR PLATE S (CM)									
	.050	.100	.150	.200	.250	.300	.350	.400	.450	.500
BULK TEMP (K)	813.5	823.8	832.5	840.2	847.2	853.8	859.9	865.6	871.1	876.5
WALL TEMP (K)	1197.8	1216.8	1226.0	1231.7	1235.3	1237.5	1239.1	1240.2	1241.5	1243.8
MOLE FRACTION										
BULK SPECIES										
N2	.78314	.78299	.78286	.78276	.78266	.78257	.78248	.78240	.78233	.78226
O2	.20697	.20599	.20517	.20445	.20380	.20320	.20264	.20211	.20161	.20114
C3H8	.00807	.00784	.00772	.00758	.00745	.00734	.00723	.00713	.00703	.00694
H2O	.00104	.00180	.00243	.00298	.00348	.00394	.00437	.00478	.00516	.00553
CO2	.00078	.00135	.00182	.00224	.00261	.00296	.00328	.00358	.00387	.00414
WALL SPECIES										
N2	.77687	.77687	.77687	.77687	.77687	.77687	.77687	.77687	.77687	.77687
O2	.16531	.16531	.16530	.16530	.16530	.16530	.16530	.16530	.16530	.16530
C3H8	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
H2O	.03304	.03304	.03304	.03304	.03304	.03304	.03304	.03304	.03304	.03304
CO2	.02478	.02478	.02478	.02478	.02478	.02478	.02478	.02478	.02478	.02478

	AXIAL DISTANCE ALONG MONOLITH , CYLINDER OR PLATE S (CM)									
	.750	1.000	1.500	1.750	2.000	2.500	3.000	3.500	4.000	4.500
BULK TEMP (K)	898.4	918.0	950.6	965.6	979.7	1004.9	1027.5	1048.0	1066.8	1084.0
WALL TEMP (K)	1247.3	1249.4	1251.1	1250.7	1251.5	1253.2	1254.0	1254.7	1255.3	1255.8
MOLE FRACTION										
BULK SPECIES										
N2	.78196	.78169	.78125	.78104	.78085	.78050	.78019	.77990	.77964	.77940
O2	.19913	.19737	.19441	.19304	.19175	.18945	.18737	.18547	.18374	.18215
C3H8	.00655	.00621	.00564	.00537	.00512	.00467	.00427	.00391	.00357	.00326
H2O	.00706	.00842	.01069	.01175	.01274	.01450	.01610	.01755	.01888	.02011
CO2	.00530	.00631	.00802	.00881	.00955	.01088	.01207	.01317	.01416	.01508
WALL SPECIES										
N2	.77687	.77687	.77687	.77687	.77687	.77687	.77687	.77687	.77687	.77687
O2	.16530	.16530	.16530	.16530	.16530	.16530	.16530	.16530	.16530	.16530
C3H8	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
H2O	.03304	.03304	.03304	.03304	.03304	.03304	.03304	.03304	.03304	.03304
CO2	.02478	.02478	.02478	.02478	.02478	.02478	.02478	.02478	.02478	.02478

	AXIAL DISTANCE ALONG MONOLITH , CYLINDER OR PLATE S (CM)									
	5.000	5.500	6.000	6.500	7.000	7.500	8.000	8.500	9.000	9.500
BULK TEMP (K)	1099.8	1114.4	1127.9	1140.4	1152.1	1162.9	1173.0	1182.5	1191.3	1199.7
WALL TEMP (K)	1256.2	1256.6	1257.0	1257.3	1257.6	1257.8	1258.0	1258.2	1258.4	1259.2
MOLE FRACTION										
BULK SPECIES										
N2	.77918	.77898	.77879	.77861	.77844	.77829	.77815	.77801	.77788	.77777
O2	.18067	.17931	.17805	.17687	.17578	.17475	.17379	.17290	.17206	.17127
C3H8	.00298	.00271	.00247	.00224	.00203	.00183	.00164	.00147	.00131	.00116
H2O	.02124	.02229	.02326	.02416	.02500	.02579	.02652	.02721	.02786	.02846
CO2	.01593	.01671	.01744	.01812	.01875	.01934	.01989	.02041	.02089	.02135
WALL SPECIES										
N2	.77687	.77687	.77687	.77687	.77687	.77687	.77687	.77687	.77687	.77687
O2	.16530	.16530	.16530	.16530	.16530	.16530	.16530	.16530	.16530	.16530
C3H8	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
H2O	.03304	.03304	.03304	.03304	.03304	.03304	.03304	.03304	.03304	.03304
CO2	.02478	.02478	.02478	.02478	.02478	.02478	.02478	.02478	.02478	.02478

AXIAL DISTANCE ALONG MONOLITH , CYLINDER OR PLATE S (CM)

10.000

BULK TEMP (K) 1207.6

WALL TEMP (K) 1260.8

MOLE FRACTION

BULK SPECIES

N2	.77766
O2	.17053
C3H8	.00101
H2O	.02903
CO2	.02177

WALL SPECIES

N2	.77687
O2	.16530
C3H8	.00000
H2O	.03304
CO2	.02478

****

ITERATIONS = 1 TEMP ERROR = .11931-001

****

SAMPLE PROBLEM NO. 2
NONADIABATIC CYLINDRICAL REACTOR (CERAMIC)

Description: This problem is the same as sample problem No. 1 except for a change in the fuel/air conditions and the inclusion of a convective flow of air over the outer surface of the cylindrical reactors

Fuel: Propane/air

Equivalence ratio	$\phi = 0.8$
Mixture flowrate	$\dot{m} = 0.0278$ g/s
Preheat temperature	$T_{in} = 1000$K
Pressure	$P = 1 \times 10^5$ Pa

Coolant: Air

Bulk temperature	$T_c = 1000$K
Heat transfer coefficient	$h_c = 1.51 \times 10^{-4}$ cal/cm^2-s-K

Geometry:

Cell diameter	$D_{Tub} = 0.32$ cm
Reactor length	$\ell = 20$ cm
Void fraction	$V_F = 0.87$

```
SAMPLE PROBLEM B2: COOLED MONOLITH TUBE, EQUIVALENCE RATIO = 0.8
  5 30  2  1  0  1  0
0.3175      0.87      0.3404      0.0005      0.8
2.78       1000.       1.
1000.      1500.
0.0        .05        .10        .20        .40        .60        .80        1.0
1.5        2.0        2.5        3.0        3.5        4.0        4.5        5.0
6.0        6.5        7.0        8.0        9.0        10.0       11.0       12.0
13.0       14.0       15.0       16.0       18.0       20.0
1700.      1700.      1700.      1700.      1700.      1700.      1700.      1700.
1700.      1700.      1700.      1700.      1700.      1700.      1700.      1700.
1700.      1700.      1700.      1700.      1700.      1700.      1700.      1700.
1700.      1700.      1700.      1700.      1700.      1700.      1700.      1700.
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
0.000151  0.000151  0.000151  0.000151  0.000151  0.000151  0.000151  0.000151
0.000151  0.000151  0.000151  0.000151  0.000151  0.000151  0.000151  0.000151
0.000151  0.000151  0.000151  0.000151  0.000151  0.000151  0.000151  0.000151
0.000151  0.000151  0.000151  0.000151  0.000151  0.000151  0.000151  0.000151
1000.      0.0005     .01145
N2         .764       .7401      1.03475
O2         .203       .0394      1.10045
C3H8       .0325      5.    E-051.2758
H2O        1.0   E-10 .126       .844069
CO2        1.0   E-10 .0945      1.27446
  2  1
C3H8 O2                    C3H8 O2   H2O  CO2        4.1    E+9            40.61
.25  1.04                                 -.75 -3.964.0  3.0
C3H8                       O2   H2O  CO2             1.1    E+09 0.        17.6
1.0                                      -5.0 4.0  3.0
```

SAMPLE PROBLEM B2: COOLED MONOLITH TUBE, EQUIVALENCE RATIO = 0.8

* INTEGRAL PARAMETERS *

IS (NUMBER OF SPECIES)	=	5
ML (GRID POINTS)	=	30
NIT (NUMBER OF OVERALL ITERATIONS)	=	2
ILOSS (HEAT LOSS OPTION)	=	1
IGEOM (PROBLEM GEOMETRY OPTION)	=	0
ICOEFF (HEAT TRANSFER INPUT OPTION)	=	1
KPZ (PRINT OPTION)	=	0

* NONINTEGRAL PARAMETERS *

*** REACTOR DATA ***

MONOLITH HONEYCOMB CATALYTIC COMBUSTOR

NUMBER OF TUBES	=	1.00
VOID FRACTION	=	.870
DIAMETER OF COMBUSTOR	=	.34 (CM)
EFFECTIVE CELL DIAMETER	=	.32 (CM)

INLET TEMPERATURE	=	1000.00 (K)
PRESSURE	=	1.00 (ATM)
MASS FLOW RATE	=	.278+001 (G/S)
CONDUCTIVITY	=	.500-003 (CAL/S-CM-K)
EMISSIVITY	=	.80

*** RESERVOIR TEMPERATURES ***

UPSTREAM = 1000.0
DOWNSTREAM =. 1500.0

GRID POINTS CHOSEN (S)

.0000	.5000-001	.1000+000	.2000	.4000	.6000	.8000	1.000	1.500	2.000
2.500	3.000	3.500	4.000	4.500	5.000	6.000	6.500	7.000	8.000
9.000	10.00	11.00	12.00	13.00	14.00	15.00	16.00	18.00	20.00

INITIAL GUESSED WALL TEMPERATURES (TL)

1700.	1700.	1700.	1700.	1700.	1700.	1700.	1700.	1700.	1700.
1700.	1700.	1700.	1700.	1700.	1700.	1700.	1700.	1700.	1700.
1700.	1700.	1700.	1700.	1700.	1700.	1700.	1700.	1700.	

*** COOLANT PROPERTIES ***

COOLANT
INLET TEMPERATURE =1000.00 (K)
PRESSURE = .00 (ATM)
MASS FLOW RATE = .000 (G/S)
APPROACH VELOCITY = .00 (CM/S)
MOLECULAR WEIGHT = .00

FOR COOLANT TUBE:
TUBE DIAMETER = .00 (CM)
TUBE THICKNESS = .011 (CM)
CONDUCTIVITY = .500-003 (CAL/S-CM-K)

* THERMOCHEMICAL DATA FOR COOLANT

TEMPERATURE	THERMAL CONDUCTIVITY
.00	.000
.00	.000

HEAT CAPACITY CPH = C1 + C2 * T + C3 / T**2 (CAL/G-MOLE - K)

C1 = .000 (CAL/G-MOLE - K)
C2 = .000 (CAL/G-MOLE - K**2)
C3 = .000 (CAL-K/G-MOLE)

VISCOSITY PARAMETERS
SIGMA = .000 (A)
E/K = .000 (K)

* SPECIES INITIAL MOLE FRACTIONS, FIRST GUESSES, AND DIFFUSION FACTORS *

SPECIE	ALPF	ALPL	DIFFUSION FACTOR
N2	.764+000	.740+000	1.0347
O2	.203+000	.394-001	1.1004
C3H8	.325-001	.500-004	1.2759
H2O	.100-009	.126+000	.8441
CO2	.100-009	.945-001	1.2745

* THERMOCHEMISTRY DATA *

CURVE FIT OF DATA IN FORM CP=RB+RC*T+RD/(T*T) (CAL/(MOLE*K)

HF(CAL/MOL)	H(CAL/MOL)	RB	RC	RD	S(CAL/MOL/K)	TU(K)		NAME
N2	28.000							
.79000+000	.23993+005	.61591+001	.16415-002	.29727+005	.64548+002	300.	1000.	N2
.79000+000	.22188+005	.83049+001	.23357-003	-.72806+006	.63774+002	1000.	2500.	N2
O2	32.000							
.00000	.25541+005	.67044+001	.16795-002	-.19419+005	.68908+002	300.	1000.	O2
.00000	.23458+005	.80725+001	.50513-003	-.21319+006	.67976+002	1000.	2500.	O2
H2O	18.000							
-.57798+005	.31716+005	.68290+001	.29575-002	.27843+005	.69022+002	300.	1000.	H2O
-.57798+005	.30303+005	.99698+001	.12774-002	-.14328+007	.68463+002	1000.	2500.	H2O
CO2	44.000							
-.94054+005	.41438+005	.95778+001	.36020-002	-.16389+006	.81997+002	300.	1000.	CO2
-.94054+005	.36573+005	.13972+002	.38449-003	-.13412+007	.79867+002	1000.	2500.	CO2
C3H8	44.000							
-.24820+005	.10888+006	.32090+002	.11928-001	-.20372+007	.15940+003	300.	2500.	C3H8
-.24820+005	.10888+006	.32090+002	.11928-001	-.20372+007	.15940+003	2500.	6000.	C3H8

* KINETIC REACTION DATA *

TOTAL NUMBER OF REACTIONS 2
NUMBER OF GAS PHASE REACTIONS 1

M	TYPE	REACTION	PRE EXP FACTOR (MOLE-CM-S)	TEMP EXP	ACTIVATION (KCAL/MOLE)
1	GAS	5.0 O2 + 1.0 C3H8--=4.0 H2O + 3.0 CO2	.4100+010	.000	40.6100
2	SURF	5.0 O2 + 1.0 C3H8--=4.0 H2O + 3.0 CO2	.1100+010	.000	17.6000

```
**  OVERALL HEAT TRANSFER RESULTS **
     COOLANT TEMPERATURE  IN  =1000.00 (K)
     COOLANT TEMPERATURE OUT  =1000.00 (K)
     TOTAL HEAT TRANSFERED TO
     COOLANT                  =  .451+001(CAL/S)
```

	AXIAL DISTANCE ALONG MONOLITH , CYLINDER OR PLATE S (CM)									
	.050	.100	.200	.400	.600	.800	1.000	1.500	2.000	2.500
BULK TEMP (K)	1003.1	1006.3	1013.0	1026.7	1040.6	1054.6	1068.6	1102.8	1136.4	1169.2
WALL TEMP (K)	2260.1	2312.6	2364.2	2421.6	2456.3	2473.1	2482.6	2490.4	2493.4	2494.5
MOLE FRACTION										
BULK SPECIES										
N2	.76453	.76427	.76416	.76394	.76373	.76351	.76330	.76278	.76226	.76176
O2	.20273	.20235	.20160	.20012	.19864	.19718	.19573	.19217	.18868	.18525
C3H8	.03244	.03237	.03222	.03192	.03163	.03134	.03105	.03035	.02965	.02897
H2O	.00029	.00058	.00115	.00230	.00343	.00455	.00567	.00841	.01109	.01372
CO2	.00022	.00043	.00086	.00172	.00257	.00341	.00425	.00630	.00832	.01029
WALL SPECIES										
N2	.74031	.74031	.74031	.74031	.74031	.74031	.74031	.74031	.74031	.74031
O2	.03925	.03925	.03925	.03925	.03925	.03925	.03925	.03925	.03925	.03925
C3H8	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
H2O	.12596	.12596	.12597	.12597	.12597	.12597	.12597	.12597	.12597	.12597
CO2	.09447	.09447	.09447	.09447	.09447	.09447	.09447	.09447	.09447	.09447
COOLANT TEMP (K)	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00
COOLANT TUBE TEMP (K)	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
HEAT LOSS TO COOLANT (CAL/S)	.9514-002	.9910-002	.2060-001	.4293-001	.4398-001	.4449-001	.4477-001	.1125	.1128	.1128

AXIAL DISTANCE ALONG MONOLITH , CYLINDER OR PLATE S (CM)										
	3.000	3.500	4.000	4.500	5.000	6.000	6.500	7.000	8.000	9.000
BULK TEMP (K)	1201.2	1232.5	1263.1	1293.0	1322.4	1378.6	1406.3	1433.4	1485.6	1536.3
WALL TEMP (K)	2495.0	2495.3	2495.6	2496.4	2497.1	2498.2	2497.5	2498.3	2499.8	2500.3
MOLE FRACTION										
BULK SPECIES										
N2	.76127	.76078	.76031	.75984	.75939	.75851	.75808	.75765	.75683	.75604
O2	.18190	.17861	.17538	.17221	.16911	.16314	.16019	.15730	.15172	.14630
C3H8	.02831	.02766	.02701	.02639	.02577	.02459	.02400	.02343	.02232	.02124
H2O	.01630	.01883	.02131	.02375	.02613	.03072	.03299	.03521	.03950	.04367
CO2	.01223	.01412	.01598	.01781	.01960	.02304	.02474	.02641	.02962	.03275
WALL SPECIES										
N2	.74031	.74031	.74031	.74031	.74031	.74031	.74031	.74031	.74031	.74031
O2	.03925	.03925	.03925	.03925	.03925	.03925	.03925	.03925	.03925	.03925
C3H8	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
H2O	.12597	.12597	.12597	.12597	.12597	.12597	.12597	.12597	.12597	.12597
CO2	.09447	.09447	.09447	.09447	.09447	.09447	.09447	.09447	.09447	.09447
COOLANT TEMP (K)	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00
COOLANT TUBE TEMP (K)	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
HEAT LOSS TO COOLANT (CAL/S)	.1129	.1129	.1129	.1130	.1130	.2262	.1131	.1131	.2265	.2266

	AXIAL DISTANCE ALONG MONOLITH , CYLINDER OR PLATE S (CM)								
	10.000	11.000	12.000	13.000	14.000	15.000	16.000	18.000	20.000
BULK TEMP (K)	1585.6	1634.0	1681.7	1729.0	1776.3	1823.9	1872.0	1963.5	2055.1
WALL TEMP (K)	2500.7	2501.2	2501.6	2502.0	2502.6	2503.3	2504.2	2505.0	2479.3
MOLL FRACTION									
BULK SPECIES									
N2	.75526	.75450	.75374	.75299	.75225	.75149	.75073	.74928	.74779
O2	.14101	.13581	.13068	.12559	.12049	.11536	.11017	.10031	.09015
C3H8	.02019	.01916	.01815	.01713	.01612	.01510	.01408	.01212	.01010
H2O	.04773	.05173	.05567	.05959	.06351	.06745	.07144	.07903	.08684
CO2	.03580	.03880	.04175	.04469	.04763	.05059	.05358	.05927	.06513
WALL SPECIES									
N2	.74031	.74031	.74031	.74031	.74031	.74031	.74031	.74031	.74031
O2	.03925	.03925	.03925	.03925	.03925	.03925	.03925	.03925	.03925
C3H8	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
H2O	.12597	.12597	.12597	.12597	.12597	.12597	.12597	.12597	.12597
CO2	.09448	.09448	.09448	.09448	.09448	.09448	.09448	.09448	.09448
COOLANT TEMP (K)	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00
COOLANT TUBE TEMP (K)	.00	.00	.00	.00	.00	.00	.00	.00	.00
HEAT LOSS TO COOLANT (CAL/S)	.2266	.2267	.2267	.2268	.2269	.2270	.2271	.4545	.4467

SAMPLE PROBLEM NO. 3
NONADIABATIC FLAT PLATE REACTOR (STAINLESS STEEL)

Description: This problem represents a semi-infinite stream of a fuel/air mixture passing over one side of a catalytic flat plate. A flow of coolant (air) flows over the other side. The mass flowrate is given in terms of the unit cross-sectional flow area.

Fuel:	Propane/air	
	Equivalence ratio	$\phi = 0.8$
	Mixture flowrate	$\dot{m} = 0.3574$ g/cm^2-s
	Preheat temperature	$T_{in} = 1000$K
	Pressure	$P = 1 \times 10^5$ Pa
Coolant:	Air	
	Bulk temperature	$T_c = 1000$K
	Heat transfer coefficient	$h_c = 1.51 \times 10^{-4}$ cal/cm^2-s-K
Geometry:	Plate thickness	$t = 0.3175$ cm
	Initial noncatalytic length	$\ell_o = 30.5$ cm

SAMPLE PROBLEM B2-FLAT PLATE EQUIVALENCE RATIO = 0.8

```
  5 16 15  1  1  1  0
1.0       0.87      1.0       0.055     0.8
0.3574     1000.     1.
1000.     1000.
0.0       10.       20.       30.5       30.51      30.52     30.53     30.54
30.55     30.75     31.       31.5      32.        32.5       33.        34.
1800.     1800.     1800.     1800.     1800.     1800.     1800.     1800.
1800.     1800.     1800.     1800.     1800.     1800.     1800.     1800.
 0 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
0.000151  0.000151  0.000151  0.000151  0.000151  0.000151  0.000151  0.000151
0.000151  0.000151  0.000151  0.000151  0.000151  0.000151  0.000151  0.000151
.3175
N2        .764      .7401     1.03475
O2        .203      .0394     1.10045
C3H8      .0325     5.    E-051.2758
H2O       1.0   E-10 .126     .844069
CO2       1.0   E-10 .0945    1.27446
  2  1
C3H8 O2                  O2   H2O  CO2            1.7   E+13          21.0
1.0  1.0                                  -4.0 4.0  3.0
C3H8                     O2   H2O  CO2            1.1   E+09 0.       17.0
1.0                                    -5.0 4.0  3.0
```

SAMPLE PROBLEM B2-FLAT PLATE EQUIVALENCE RATIO = 0.8

* INTEGRAL PARAMETERS *

IS (NUMBER OF SPECIES)	= 5
NL (GRID POINTS)	= 16
NIT (NUMBER OF OVERALL ITERATIONS)	= 15
ILOSS (HEAT LOSS OPTION)	= 1
IGEOM (PROBLEM GEOMETRY OPTION)	= 1
ICOEFF (HEAT TRANSFER INPUT OPTION)	= 1
KR7 (PRINT OPTION)	= 0

* NONINTEGRAL PARAMETERS *

*** REACTOR DATA ***

FOR CYLINDER COOLED EXTERNALLY OR FLAT PLATE PROBLEM

THICKNESS OF CYLINDER OR THICKNESS OF PLATE	= .317 (CM)
INLET TEMPERATURE	=1000.00 (K)
PRESSURE	= 1.00 (ATM)
MASS FLOW RATE	= .357+00 (G/S)
CONDUCTIVITY	= .550-01 (CAL/S-CM-K)
EMISSIVITY	= .80

*** RESERVOIR TEMPERATURES ***

UPSTREAM	= 1000.0
DOWNSTREAM	= 1000.0

GRID POINTS CHOSEN (S)

.0000	10.00	20.00	30.50	30.51	30.52	30.53	30.54	30.55	30.75
31.00	31.50	32.00	32.50	33.00	34.00				

INITIAL GUESSED WALL TEMPERATURES (TL)

1800.	1800.	1800.	1800.	1800.	1800.	1800.	1800.	1800.	1800.
1800.	1800.	1800.	1800.	1800.					

*** COOLANT PROPERTIES ***

COOLANT
INLET TEMPERATURE = .00 (K)
PRESSURE = .00 (ATM)
MASS FLOW RATE = .000 (G/S)
APPROACH VELOCITY = .00 (CM/S)
MOLECULAR WEIGHT = .00

FOR COOLANT TUBE:
TUBE DIAMETER = .00 (CM)
TUBE THICKNESS = .317 (CM)
CONDUCTIVITY = .550-01 (CAL/S-CM-K)

CENTER TO CENTER DISTANCE (TUBE BANK) = .00 (CM)
DISTANCE BETWEEN MONOLITH AND TUBE BANK = .000 (CM)

* THERMOCHEMICAL DATA FOR COOLANT

TEMPERATURE	THERMAL CONDUCTIVITY
.00	.000
.00	.000

HEAT CAPACITY CPH = C1 + C2 * T + C3 / T**2 (CAL/G-MOLE - K)

C1 = .000 (CAL/G-MOLE - K)
C2 = .000 (CAL/G-MOLE - K**2)
C3 = .000 (CAL-K/G-MOLE)

VISCOSITY PARAMETERS
SIGMA = .000 (A)
E/K = .000 (K)

* SPECIES INITIAL MOLE FRACTIONS,FIRST GUESSES,AND DIFFUSION FACTORS *

SPECIE	ALPF	ALPL	DIFFUSION FACTOR
N2	.764+00	.740+00	1.0347
O2	.203+00	.394-01	1.1004
C3H8	.325-01	.500-04	1.2758
H2O	.100-09	.126+00	.8441
CO2	.100-09	.945-01	1.2745

* THERMOCHEMISTRY DATA *

CURVE FIT OF DATA IN FORM CP=RB+RC*T+RD/(T*T) (CAL/(MOLE*K)

HF(CAL/MOL)	H(CAL/MOL)	RB	RC	RD	S(CAL/MOL/K)	TU(K)		NAME
N2	28.000							
.79000+00	.23993+05	.61391+01	.16415-02	.29727+05	.64548+02	300.	1000.	N2
.79000+00	.22188+05	.83049+01	.23357-03	-.72806+06	.63774+02	1000.	2500.	N2
O2	32.000							
.00000	.25541+05	.67044+01	.16795-02	-.19419+05	.68908+02	300.	1000.	O2
.00000	.23450+05	.80725+01	.50513-03	-.21319+06	.67976+02	1000.	2500.	O2
H2O	18.000							
-.57798+05	.31716+05	.68290+01	.29575-02	.27843+05	.69022+02	300.	1000.	H2O
-.57798+05	.30303+05	.99698+01	.12774-02	-.14328+07	.68463+02	1000.	2500.	H2O
CO2	44.000							
-.94054+05	.41438+05	.95778+01	.36020-02	-.16389+06	.81997+02	300.	1000.	CO2
-.94054+05	.36573+05	.13972+02	.38449-03	-.13412+07	.79867+02	1000.	2500.	CO2
C3H8	44.000							
-.24820+05	.12785+06	.32090+02	.11928-01	-.20372+07	.15567+03	300.	2500.	C3H8
-.24820+05	.12785+06	.32090+02	.11928-01	-.20372+07	.15567+03	2500.	6000.	C3H8

* KINETIC REACTION DATA *

TOTAL NUMBER OF REACTIONS 2
NUMBER OF GAS PHASE REACTIONS 1

M		REACTION	PRE EXP FACTOR (MOLE-CM-S)	TEMP EXP	ACTIVATION (KCAL/MOLE)
1	GAS	5.0 O2 + 1.0 C3H8--=4.0 H2O + 3.0 CO2	.1700+14	.000	21.0000
2	SURF	5.0 O2 + 1.0 C3H8--=4.0 H2O + 3.0 CO2	.1100+10	.000	17.0000

```
**  OVERALL HEAT TRANSFER RESULTS **
     COOLANT TEMPERATURE  IN  =     .00 (K)
     COOLANT TEMPERATURE OUT  =     .00 (K)
     TOTAL HEAT TRANSFERED TO
     COOLANT                  =    .525+01(CAL/S)
```

	AXIAL DISTANCE ALONG MONOLITH , CYLINDER OR PLATE S (CM)									
	10.000	20.000	30.500	30.510	30.520	30.530	30.540	30.550	30.750	31.000
BULK TEMP (K)	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0
WALL TEMP (K)	988.7	988.7	1006.8	1763.5	1762.2	1758.2	1751.6	1742.3	1646.5	1516.4
MOLE FRACTION										
BULK SPECIES										
N2	.76400	.76400	.76400	.76400	.76400	.76400	.76400	.76400	.76400	.76400
O2	.20300	.20300	.20300	.20300	.20300	.20300	.20300	.20300	.20300	.20300
C3H8	.03250	.03250	.03250	.03250	.03250	.03250	.03250	.03250	.03250	.03250
H2O	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
CO2	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
WALL SPECIES										
N2	.76438	.76438	.76438	.74031	.74031	.74031	.74031	.74031	.74031	.74031
O2	.20310	.20310	.20310	.03924	.03924	.03924	.03924	.03924	.03924	.03924
C3H8	.03252	.03252	.03252	.00000	.00000	.00000	.00000	.00000	.00000	.00000
H2O	.00000	.00000	.00000	.12597	.12597	.12597	.12597	.12597	.12597	.12597
CO2	.00000	.00000	.00000	.09448	.09448	.09448	.09448	.09448	.09448	.09448
COOLANT TEMP (K)	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
HEAT LOSS TO COOLANT (CAL/S)	1.493	1.493	1.596	.2663-02	.2661-02	.2655-02	.2645-02	.2631-02	.4972-01	.5724-01

	AXIAL DISTANCE ALONG MONOLITH , CYLINDER OR PLATE S (CM)				
	31.500	32.000	32.500	33.000	34.000
BULK TEMP (K)	1000.0	1000.0	1000.0	1000.0	1000.0
WALL TEMP (K)	1366.3	1254.1	1188.6	1150.6	1120.0
MOLE FRACTION					
BULK SPECIES					
N2	.76400	.76400	.76400	.76400	.76400
O2	.20300	.20300	.20300	.20300	.20300
C3H8	.03250	.03250	.03250	.03250	.03250
H2O	.00000	.00000	.00000	.00000	.00000
CO2	.00000	.00000	.00000	.00000	.00000
WALL SPECIES					
N2	.74031	.74031	.74031	.74031	.74031
O2	.03924	.03924	.03924	.03924	.03925
C3H8	.00000	.00000	.00000	.00000	.00000
H2O	.12597	.12597	.12597	.12597	.12597
CO2	.09448	.09448	.09448	.09448	.09448
COOLANT TEMP (K)	.00	.00	.00	.00	.00
HEAT LOSS TO COOLANT (CAL/S)	.1032	.9468-01	.8974-01	.8687-01	.1691

****

ITERATIONS = 15 TEMP ERROR = .18058-02

SAMPLE PROBLEM NO. 4
COANNULAR TUBES

Description: In this problem, a coolant passes axially through the ID of the inner tube and a fuel/air mixture passes axially and in the same direction in the annulus formed by the coannular tubes. The outer surface of the larger tube is adiabatic and the inner surface is catalytic. Heat is transferred from the larger tube to the smaller tube by radiation and convection.

Fuel: Propane/air

Equivalence ratio	$\phi = 0.8$
Mixture flowrate	$\dot{m} = 1.045$ gm/cm^2-s
Preheat temperature	$T_{in} = 866$K
Pressure	$P = 1 \times 10^5$ Pa

Coolant: Air

Velocity	$V_\ell = 3000$ cm/s
Flowrate	$\dot{m}_c = 2.046$ g/s
Initial temperature	$T_i = 294$K
Pressure	$P_i = 1 \times 10^5$ Pa
Molecular weight	$M = 28.84$ g/mole

Geometry:

Coolant tube conductivity	$k_T = 0.055$ cal/s-cm-K
Coolant tube thickness	$D_r = 0.05$ cm
Coolant tube outside dia.	$D_T = 0.925$ cm
Reactor tube inside dia.	$D_{Tub} = 1.70$ cm
Length	$\ell = 61$ cm
Catalyst begins	$\ell_1 = 5$ cm
Catalyst ends	$\ell_2 = 50$ cm

```
SAMPLE PROBLEM D-COANNULAR TUBE EQUIVALENCE RATIO = 0.8
  5 28  5  0  2  0  0
1.5875     0.87       1.702      0.055       0.8
1.045      866.       1.0
866.0      -1.0
0.0        2.5        5.0        5.1         5.2         5.3         5.4         5.5
5.75       6.         6.5        7.          8.          10.         12.         15.
20.        25.        30.        35.         40.         45.         50.         50.8
51.        55.        60.        61.
1700.      1700.      1700.      1700.       1700.       1700.       1700.       1700.
1700.      1700.      1700.      1700.       1700.       1700.       1700.       1700.
1700.      1700.      1700.      1700.       1700.       1700.       1700.       1700.
1700.      1700.      1700.      1700.       1700.       1700.       1700.       1700.
 0 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 0 0 0
3000.      2.046       294.      1.0         28.84
0.055      0.05       0.925      1.          1.
373.       973.       0.000073   0.000155
3.711      78.6        6.9       0.00092      -18504.
N2         .764       .7401      1.03475
O2         .203       .0394      1.10045
C3H8       .0325      5.     E-051.2758
H2O        1.0    E-10 .126      .844069
CO2        1.0    E-10 .0945     1.27446
  2  1
C3H8 O2                    C3H8 O2   H2O  CO2        4.1    E+9          40.61
.25  1.04                                 -.75 -3.96 4.   3.0
C3H8                       O2   H2O  CO2             1.1    E+09 0.      17.6
1.0                                     -5.0 4.0  3.0
```

SAMPLE PROBLEM D-COANNUALR TUBE EQUIVALENCE RATIO = 0.8

* INTEGRAL PARAMETERS *

IS (NUMBER OF SPECIES)	= 5
NL (GRID POINTS)	= 28
NIT (NUMBER OF OVERALL ITERATIONS)	= 5
ILOSS (HEAT LOSS OPTION)	= 0
IGEOM (PROBLEM GEOMETRY OPTION)	= 2
ICOEFF (HEAT TRANSFER INPUT OPTION)	= 0
KR7 (PRINT OPTION)	= 0

* NONINTEGRAL PARAMETERS *

*** REACTOR DATA ***

MONOLITH HONEYCOMB CATALYTIC COMBUSTOR

NUMBER OF TUBES	= 1.00
VOID FRACTION	= .870
DIAMETER OF COMBUSTOR	= 1.70 (CM)
EFFECTIVE CELL DIAMETER	= 1.59 (CM)

INLET TEMPERATURE	= 866.00 (K)
PRESSURE	= 1.00 (ATM)
MASS FLOW RATE	= .105+01 (G/S)
CONDUCTIVITY	= .550-01 (CAL/S-CM-K)
EMISSIVITY	= .80

*** RESERVOIR TEMPERATURES ***

UPSTREAM	= 866.00
DOWNSTREAM	= 1.0000

GRID POINTS CHOSEN (S)

.0000	2.500	5.000	5.100	5.200	5.300	5.400	5.500	5.750	6.000
6.500	7.000	8.000	10.00	12.00	15.00	20.00	25.00	30.00	35.00
40.00	45.00	50.00	50.80	51.00	55.00	60.00	61.00		

INITIAL GUESSED WALL TEMPERATURES (TL)

1700.	1700.	1700.	1700.	1700.	1700.	1700.	1700.	1700.	1700.
1700.	1700.	1700.	1700.	1700.	1700.	1700.	1700.	1700.	1700.
1700.	1700.	1700.	1700.	1700.	1700.	1700.			

*** COOLANT PROPERTIES ***

COOLANT
INLET TEMPERATURE = 294.00 (K)
PRESSURE = 1.00 (ATM)
MASS FLOW RATE = .205+01 (G/S)
APPROACH VELOCITY =3000.00 (CM/S)
MOLECULAR WEIGHT = 28.84

FOR COOLANT TUBE:
TUBE DIAMETER = .92 (CM)
TUBE THICKNESS = .050 (CM)
CONDUCTIVITY = .550-01 (CAL/S-CM-K)

* THERMOCHEMICAL DATA FOR COOLANT

TEMPERATURE	THERMAL CONDUCTIVITY
373.00	.730-04
973.00	.155-03

HEAT CAPACITY CPH = C1 + C2 * T + C3 / T**2 (CAL/G-MOLE - K)

C1 = .690+01 (CAL/G-MOLE - K)
C2 = .920-03 (CAL/G-MOLE - K**2)
C3 = -.185+05 (CAL-K/G-MOLE)

VISCOSITY PARAMETERS
SIGMA = 3.711 (A)
E/K = 78.600 (K)

* SPECIES INITIAL MOLE FRACTIONS,FIRST GUESSES,AND DIFFUSION FACTORS *

SPECIE	ALPF	ALPE	DIFFUSION FACTOR
N2	.764+00	.740+00	1.0347
O2	.203+00	.394-01	1.1004
C3H8	.325-01	.500-04	1.2758
H2O	.100-09	.126+00	.8441
CO2	.100-09	.945-01	1.2745

* THERMOCHEMISTRY DATA *

CURVE FIT OF DATA IN FORM CP=RB+RC*T+RD/(T*T) (CAL/(MOLE*K)

HF(CAL/MOL)	H(CAL/MOL)	RB	RC	RD	S(CAL/MOL/K)	TU(K)		NAME
N2	28.000							
.79000+00	.23993+05	.61391+01	.16415-02	.29727+05	.64548+02	300.	1000.	N2
.79000+00	.22188+05	.83049+01	.23357-03	-.72806+06	.63774+02	1000.	2500.	N2
O2	32.000							
.00000	.25541+05	.67044+01	.16795-02	-.19419+05	.68908+02	300.	1000.	O2
.00000	.23450+05	.80725+01	.50513-03	-.21319+06	.67976+02	1000.	2500.	O2
H2O	18.000							
-.57798+05	.31716+05	.68290+01	.29575-02	.27843+05	.69022+02	300.	1000.	H2O
-.57798+05	.30303+05	.99698+01	.12774-02	-.14328+07	.68463+02	1000.	2500.	H2O
CO2	44.000							
-.94054+05	.41438+05	.95778+01	.36020-02	-.16389+06	.81997+02	300.	1000.	CO2
-.94054+05	.36573+05	.13972+02	.38449-03	-.13412+07	.79867+02	1000.	2500.	CO2
C3H8	44.000							
-.24820+05	.10888+06	.32090+02	.11928-01	-.20372+07	.15940+03	300.	2500.	C3H8
-.24820+05	.10888+06	.32090+02	.11928-01	-.20372+07	.15940+03	2500.	6000.	C3H8

* KINETIC REACTION DATA *

TOTAL NUMBER OF REACTIONS 2
NUMBER OF GAS PHASE REACTIONS 1

M		REACTION	PRE EXP FACTOR (MOLE-CM-S)	TEMP EXP	ACTIVATION (KCAL/MOLE)
1	GAS	5.0 O2 + 1.0 C3H8--=4.0 H2O + 3.0 CO2	.4100+010	.000	40.6100
2	SURF	5.0 O2 + 1.0 C3H8--=4.0 H2O + 3.0 CO2	.1100+010	.000	17.6000

```
**  OVERALL HEAT TRANSFER RESULTS **
    COOLANT TEMPERATURE  IN  = 294.00 (K)
    COOLANT TEMPERATURE OUT  = 500.58 (K)
    TOTAL HEAT TRANSFERED TO
    COOLANT                  =   .104+03(CAL/S)
```

	AXIAL DISTANCE ALONG MONOLITH , CYLINDER OR PLATE S (CM)									
	2.500	5.000	5.100	5.200	5.300	5.400	5.500	5.750	6.000	6.500
BULK TEMP (K)	843.3	844.4	848.3	852.6	857.0	861.5	866.0	877.1	887.5	906.4
WALL TEMP (K)	810.8	936.9	1511.2	1555.3	1583.8	1596.9	1594.9	1579.1	1557.5	1523.4
MOLE FRACTION										
BULK SPECIES										
N2	.76434	.76434	.76434	.76421	.76409	.76397	.76385	.76356	.76327	.76273
O2	.20279	.20279	.20279	.20195	.20111	.20029	.19947	.19749	.19555	.19187
C3H8	.03246	.03245	.03245	.03229	.03212	.03196	.03180	.03140	.03102	.03029
H2O	.00024	.00024	.00024	.00089	.00153	.00216	.00279	.00432	.00580	.00863
CO2	.00018	.00018	.00018	.00067	.00115	.00162	.00209	.00324	.00435	.00648
WALL SPECIES										
N2	.76434	.76434	.76434	.74031	.74031	.74031	.74031	.74031	.74031	.74031
O2	.20279	.20279	.20279	.03925	.03925	.03925	.03925	.03925	.03925	.03925
C3H8	.03246	.03245	.03245	.00000	.00000	.00000	.00000	.00000	.00000	.00000
H2O	.00024	.00024	.00024	.12597	.12597	.12597	.12597	.12597	.12597	.12597
CO2	.00018	.00018	.00018	.09448	.09448	.09448	.09448	.09448	.09448	.09448
COOLANT TEMP (K)	311.07	328.73	329.86	331.06	332.33	333.64	334.97	338.54	342.07	349.23
COOLANT TUBE TEMP (K)	653.51	696.86	936.91	985.20	1021.43	1046.89	1063.20	1119.01	1120.88	1144.12
HEAT LOSS TO COOLANT (CAL/S)	8.424	8.765	.5600	.6023	.6331	.6539	.6661	1.781	1.766	3.583

AXIAL DISTANCE ALONG MONOLITH , CYLINDER OR PLATE S (CM)

	7.000	8.000	10.000	12.000	15.000	20.000	25.000	30.000	35.000	40.000
BULK TEMP (K)	923.4	951.9	994.0	1026.1	1059.2	1102.4	1128.5	1143.1	1149.3	1148.9
WALL TEMP (K)	1498.4	1459.9	1411.4	1375.5	1331.1	1276.3	1230.6	1190.5	1154.4	1121.2
MOLE FRACTION										
BULK SPECIES										
N2	.76222	.76127	.75966	.75825	.75648	.75416	.75225	.75066	.74932	.74818
O2	.18836	.18194	.17095	.16136	.14930	.13349	.12054	.10970	.10056	.09281
C3H8	.02959	.02832	.02614	.02423	.02184	.01870	.01613	.01398	.01217	.01063
H2O	.01133	.01627	.02472	.03209	.04136	.05351	.06347	.07180	.07883	.08479
CO2	.00850	.01220	.01854	.02407	.03102	.04014	.04760	.05385	.05912	.06359
WALL SPECIES										
N2	.74031	.74031	.74031	.74031	.74031	.74031	.74031	.74031	.74031	.74031
O2	.03925	.03925	.03925	.03925	.03925	.03925	.03925	.03925	.03925	.03925
C3H8	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
H2O	.12597	.12597	.12597	.12597	.12597	.12597	.12597	.12597	.12597	.12597
CO2	.09448	.09448	.09448	.09448	.09448	.09448	.09448	.09448	.09448	.09448
COOLANT TEMP (K)	356.10	369.43	394.18	416.66	446.92	454.09	460.96	467.55	473.88	479.95
COOLANT TUBE TEMP (K)	1129.44	1129.84	1117.06	1101.89	1084.62	1212.99	1180.56	1150.90	1123.13	1096.77
HEAT LOSS TO COOLANT (CAL/S)	3.445	6.700	12.47	11.39	15.41	3.670	3.524	3.386	3.253	3.123

	AXIAL DISTANCE ALONG MONOLITH • CYLINDER OR PLATE S (CM)						
	45.000	50.000	50.800	51.000	55.000	60.000	61.000
BULK TEMP (K)	1143.3	1133.6	1130.9	1130.0	1103.0	1069.4	1062.6
WALL TEMP (K)	1090.5	1061.4	1032.4	998.1	886.1	852.4	858.4
MOLE FRACTION							
BULK SPECIES							
N2	.74721	.74640	.74627	.74627	.74622	.74617	.74617
O2	.08624	.08067	.07981	.07979	.07945	.07916	.07913
C3H8	.00933	.00822	.00805	.00805	.00798	.00792	.00791
H2O	.08984	.09412	.09478	.09480	.09506	.09528	.09531
CO2	.06738	.07059	.07109	.07110	.07130	.07146	.07148
WALL SPECIES							
N2	.74031	.74031	.74031	.74627	.74622	.74617	.74617
O2	.03925	.03925	.03925	.07979	.07945	.07916	.07913
C3H8	.00000	.00000	.00000	.00805	.00798	.00792	.00791
H2O	.12597	.12597	.12597	.09480	.09506	.09528	.09531
CO2	.09448	.09448	.09448	.07110	.07130	.07146	.07148
COOLANT TEMP (K)	485.77	491.33	492.16	492.35	495.82	499.81	500.58
COOLANT TUBE TEMP (K)	1071.62	1046.91	1009.07	959.61	924.58	892.92	876.93
HEAT LOSS TO COOLANT (CAL/S)	2.996	2.868	.4308	.9748-01	1.790	2.062	.3974

SAMPLE PROBLEM NO. 5
CYLINDRICAL REACTOR (CERAMIC), ASSIGNED BED TEMPERATURE

Description: This problem represents a fuel air mixture flow in a catalytic ceramic tube with no heat loss to the environment, and the catalyst bed temperature is assigned at 1200K. This problem is also the same as the catalytic combustion in a honeycomb reactor.

Fuel: Propane/air

Equivalence ratio	$\phi = 0.2$
Mixture flowrate	$\dot{m} = 0.0394$ g/s
Preheat temperature	$T_{in} = 800$K
Pressure	$P = 3 \times 10^5$ Pa

Geometry:

Cell diameter	$D_{Tub} = 0.32$ cm
Reactor length	$\ell = 2.0$ cm
Void fraction	$V_F = 0.87$

```
    SAMPLE PROBLEM - ASSIGNED TEMP. OPTION
  5 15  1  2  0  0  0
0.15675    0.67       0.17       0.0005     0.8
0.0359     600.0      3.0
800.       1200.
0.0        0.05       0.10       0.15       0.2        0.25       0.3        0.35
0.4        0.45       0.5        0.75       1.0        1.5        1.75       2.0
1200.      1200.      1200.      1200.      1200.      1200.      1200.      1200.
1200.      1200.      1200.      1200.      1200.      1200.      1200.      1200.
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
N2         .78334     .77686     1.05475
O2         .20833     .16529     1.14045
C3H8       .00833     2.0   E-031.2758
H2O        1.0   E-10 .03306     .844069
CO2        1.0   E-10 .02479     1.27446
  2  1
C3H8 O2                    C3H8 O2   H2O  CO2        4.1    E+9            40.61
.25  1.04                                  -.75 -3.964.0  3.0
C3H6                       O2   H2O  CO2             1.1    E+09 0.        17.6
1.0                                       -5.0 4.0  3.0
```

SAMPLE PROBLEM - ASSIGNED TEMP. OPTION

* INTEGRAL PARAMETERS *

IS (NUMBER OF SPECIES)	= 5
MI (GRID POINTS)	= 15
NIT (NUMBER OF OVERALL ITERATIONS)	= 1
ILOSS (HEAT LOSS OPTION)	= 2
IGEOM (PROBLEM GEOMETRY OPTION)	= 0
ICCEFF (HEAT TRANSFER INPUT OPTION)	= 0
KR7 (PRINT OPTION)	= 0

* NONINTEGRAL PARAMETERS *

*** REACTOR DATA ***

MONOLITH HONEYCOMB CATALYTIC COMBUSTOR

NUMBER OF TUBES	= 1.00
VOID FRACTION	= .870
DIAMETER OF COMBUSTOR	= .17 (CM)
EFFECTIVE CELL DIAMETER	= .16 (CM)

INLET TEMPERATURE	= 800.00 (K)
PRESSURE	= 3.00 (ATM)
MASS FLOW RATE	= .394-001 (G/S)
CONDUCTIVITY	= .500-003 (CAL/S-CM-K)
EMISSIVITY	= .80

*** RESERVOIR TEMPERATURES ***

UPSTREAM	= 800.00
DOWNSTREAM	= 1200.0

GRID POINTS CHOSEN (S)

.0000	.5000-001	.1000+000	.1500	.2000	.2500	.3000	.3500	.4000	.4500
.5000	.7500	1.000	1.500	1.750					

INITIAL GUESSED WALL TEMPERATURES (TL)

1200.	1200.	1200.	1200.	1200.	1200.	1200.	1200.	1200.	1200.
1200.	1200.	1200.	1200.						

* SPECIES INITIAL MOLE FRACTIONS,FIRST GUESSES,AND DIFFUSION FACTORS *

SPECIE	ALPF	ALPL	DIFFUSION FACTOR
N2	.783+000	.777+000	1.0347
O2	.208+000	.165+000	1.1004
CARB	.833-002	.200-002	1.2758
H2O	.100-009	.334-001	.8441
CO2	.100-009	.248-001	1.2745

* THERMOCHEMISTRY DATA *

CURVE FIT OF DATA IN FORM CP=RB+RC*T+RD/(T*T) (CAL/(MOLE*K)

HF(CAL/MOL)	H(CAL/MOL)	RB	RC	RD	S(CAL/MOL/K)	TU(K)		NAME
N2	28.000							
.79000+000	.23993+005	.61391+001	.16415-002	.29727+005	.64548+002	300.	1000.	N2
.79000+000	.22188+005	.83049+001	.23357-003	-.74806+006	.63774+002	1000.	2500.	N2
O2	32.000							
.00000	.25541+005	.67044+001	.16795-002	-.19419+005	.68908+002	300.	1000.	O2
.00000	.23450+005	.80725+001	.50513-003	-.21519+006	.67976+002	1000.	2500.	O2
H2O	18.000							
-.57798+005	.31716+005	.68290+001	.29575-002	.27843+005	.69022+002	300.	1000.	H2O
-.57798+005	.30303+005	.99698+001	.12774-002	-.14328+007	.68463+002	1000.	2500.	H2O
CO2	44.000							
-.94054+005	.41438+005	.95778+001	.36020-002	-.16589+006	.81997+002	300.	1000.	CO2
-.94054+005	.36573+005	.13972+002	.38449-003	-.13412+007	.79867+002	1000.	2500.	CO2
C3H8	44.000							
-.24820+005	.10888+006	.32090+002	.11928-001	-.20372+007	.15940+003	300.	2500.	C3H8
-.24820+005	.10888+006	.32090+002	.11928-001	-.20372+007	.15940+003	2500.	6000.	C3H8

* KINETIC REACTION DATA *

TOTAL NUMBER OF REACTIONS 2
NUMBER OF GAS PHASE REACTIONS 1

N	TYPE	REACTION	PRE EXP FACTOR (MOLE-CM-S)	TEMP EXP	ACTIVATION (KCAL/MOLE)
1	GAS	5.0 O2 + 1.0 C3H8--=4.0 H2O + 3.0 CO2	.4100+010	.000	40.6100
2	SURF	5.0 O2 + 1.0 C3H8--=4.0 H2O + 3.0 CO2	.1100+010	.000	17.6000

	AXIAL DISTANCE ALONG MONOLITH , CYLINDER OR PLATE S (CM)									
	.050	.100	.150	.200	.250	.300	.350	.400	.450	.500
BULK TEMP (K)	813.4	823.2	831.3	838.4	844.8	850.7	856.2	861.4	866.3	870.9
WALL TEMP (K)	1200.0	1200.0	1200.0	1200.0	1200.0	1200.0	1200.0	1200.0	1200.0	1200.0
MOLE FRACTION										
BULK SPECIES										
N2	.78314	.78299	.78287	.78276	.78266	.78257	.78249	.78241	.78233	.78226
O2	.20698	.20600	.20518	.20446	.20382	.20322	.20266	.20214	.20164	.20116
C3H8	.00807	.00788	.00772	.00758	.00746	.00734	.00723	.00713	.00703	.00694
H2O	.00104	.00179	.00242	.00297	.00347	.00393	.00435	.00476	.00514	.00550
CO2	.00078	.00134	.00181	.00223	.00260	.00294	.00326	.00357	.00385	.00413
WALL SPECIES										
N2	.77687	.77687	.77687	.77687	.77687	.77687	.77687	.77687	.77687	.77687
O2	.16531	.16531	.16531	.16530	.16530	.16530	.16530	.16530	.16530	.16530
C3H8	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
H2O	.03304	.03304	.03304	.03304	.03304	.03304	.03304	.03304	.03304	.03304
CO2	.02478	.02478	.02478	.02478	.02478	.02478	.02478	.02478	.02478	.02478

	AXIAL DISTANCE ALONG MONOLITH , CYLINDER OR PLATE S (CM)			
	.750	1.000	1.500	1.750
BULK TEMP (K)	890.3	907.2	935.3	948.4
WALL TEMP (K)	1200.0	1200.0	1200.0	1200.0
MOLE FRACTION				
BULK SPECIES				
N2	.78196	.78170	.78127	.78106
O2	.19919	.19744	.19453	.19317
C3H8	.00656	.00622	.00566	.00540
H2O	.00702	.00836	.01059	.01164
CO2	.00527	.00627	.00795	.00873
WALL SPECIES				
N2	.77687	.77687	.77687	.77687
O2	.16530	.16530	.16530	.16530
C3H8	.00000	.00000	.00000	.00000
H2O	.03304	.03304	.03304	.03304
CO2	.02478	.02478	.02478	.02478

SAMPLE PROBLEM NO. 6
CATALYTIC REACTOR WITH UP- AND DOWNSTREAM HEAT EXCHANGER

Description: In this problem, two banks of heat exchanger tubes are located up- and downstream of a monolith catalytic reactor to remove radiant heat transmitted from the reactor. Additionally, convective heat transfer between the reactive gas and the coolant is also permitted when the reactive gas flows pass the tube banks.

Fuel:	Propane/air	
	Equivalence ratio	$\phi = 0.8$
	Mixture flowrate	$\dot{m} = 5.75$ g/s
	Preheat temperature	$T_{in} = 644$K
	Pressure	$P = 1 \times 10^5$ Pa
Coolant:	Hydrogen	
	Inlet temperature	$T_c = 700$K
	Pressure	$P = 100 \times 10^5$ Pa
	Flowrate	$\dot{m}_c = 1.19$ g/s
Geometry:	Reactor diameter	$D = 5.00$ cm
	Reactor length	$\ell = 5.75$ cm
	Void fraction	$V_F = 0.87$
	Cell diameter	$D_{Tub} = 0.32$ cm
	Coolant tube diameter	$d_c = 0.70$ cm
	Coolant tube thickness	$t_c = 0.06$ cm
	Coolant tube bank center to center distance	$\Delta d = 0.80$ cm

```
SAMPLE PROBLEM E- MONOLITH BETWEEN HEAT EXCHANGERS
  5 22  3  0  3  0  0
0.3175     0.87       5.0        0.0005      0.8
5.75       644.       1.0
700.       1000.
0.0        0.02       0.04       0.06        0.08        0.10        0.15        0.20
0.25       0.30       0.40       0.50        0.70        1.0         1.5         2.0
2.5        3.         3.5        4.          4.5         5.25
1800.      1800.      1800.      1800.       1800.       1800.       1800.       1800.
1800.      1800.      1800.      1800.       1800.       1800.       1800.       1800.
1800.      1800.      1800.      1800.       1800.       1800.       1800.       1800.
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1333.      1.185      700.       100.        2.
0.055      0.065        0.7        0.8       .0.1
673.       1073.      0.000756 0.00108
2.827      59.7       6.52       0.00078     12000.0
N2         .764       .7401      1.03475
O2         .203       .0394      1.10045
C3H8       .0325      5.    E-051.2758
H2O        1.0    E-10 .126      .844069
CO2        1.0    E-10 .0945     1.27446
  2  1
C3H8 O2                     C3H8 O2   H2O  CO2        4.1    E+9          40.61
.25  1.04                                  -.75 -3.964.0  3.0
C3H8                        O2   H2O  CO2             1.1    E+09 0.      17.6
1.0                                       -5.0 4.0  3.0
```

SAMPLE PROBLEM 1 - MONOLITH BETWEEN HEAT EXCHANGERS

* INTEGRAL PARAMETERS *

IS (NUMBER OF SPECIES)	= 5
NL (GRID POINTS)	= 22
NIT (NUMBER OF OVERALL ITERATIONS)	= 3
ILOSS (HEAT LOSS OPTION)	= 0
IGEOM (PROBLEM GEOMETRY OPTION)	= 3
ICCEFF (HEAT TRANSFER INPUT OPTION)	= 0
KR7 (PRINT OPTION)	= 0

* NONINTEGRAL PARAMETERS *

*** REACTOR DATA ***

MONOLITH HONEYCOMB CATALYTIC COMBUSTOR

NUMBER OF TUBES	= 54.94
VOID FRACTION	= .870
DIAMETER OF COMBUSTOR	= 5.00 (CM)
EFFECTIVE CELL DIAMETER	= .32 (CM)

INLET TEMPERATURE	= 644.00 (K)
PRESSURE	= 1.00 (ATM)
MASS FLOW RATE	= .575+001 (G/S)
CONDUCTIVITY	= .500-003 (CAL/S-CM-K)
EMISSIVITY	= .80

*** RESERVOIR TEMPERATURES ***

UPSTREAM	= 700.00
DOWNSTREAM	= 1000.0

GRID POINTS CHOSEN (S)

.0000	.2000-001	.4000-001	.6000-001	.8000-001	.1000+000	.1500	.2000	.2500	.3000
.4000	.5000	.7000	1.000	1.500	2.000	2.500	3.000	3.500	4.000
4.500	5.250								

INITIAL GUESSED WALL TEMPERATURES (TL)

1800.	1800.	1800.	1800.	1800.	1800.	1800.	1800.	1800.	1800.
1800.	1800.	1800.	1800.	1800.	1800.	1800.	1800.	1800.	1800.
1800.									

*** COOLANT PROPERTIES ***

COOLANT
INLET TEMPERATURE = 700.00 (K)
PRESSURE = 100.00 (ATM)
MASS FLOW RATE = .119+001 (G/S)
APPROACH VELOCITY =1333.00 (CM/S)
MOLECULAR WEIGHT = 2.00

FOR COOLANT TUBE:
TUBE DIAMETER = .70 (CM)
TUBE THICKNESS = .065 (CM)
CONDUCTIVIY = .550-001 (CAL/S-CM-K)

CENTER TO CENTER DISTANCE (TUBE BANK) = .80 (CM)
DISTANCE BETWEEN MONOLITH AND TUBE BANK = .100 (CM)

* THERMOCHEMICAL DATA FOR COOLANT

TEMPERATURE	THERMAL CONDUCTIVITY
673.00	.756-003
1073.00	.108-002

HEAT CAPACITY CPH = C1 + C2 * T + C3 / T**2 (CAL/G-MOLE - K)

C1 = .652+001 (CAL/G-MOLE - K)
C2 = .780-003 (CAL/G-MOLE - K**2)
C3 = .120+005 (CAL-K/G-MOLE)

VISCOSITY PARAMETERS
SIGMA = 2.827 (A)
E/K = 59.700 (K)

* SPECIES INITIAL MOLE FRACTIONS,FIRST GUESSES,AND DIFFUSION FACTORS *

SPECIE	ALPF	ALPL	DIFFUSION FACTOR
N2	.764+000	.740+000	1.0347
C2	.203+000	.394-001	1.1004
C3H8	.325-001	.500-004	1.2758
H2O	.100-009	.126+000	.8441
CO2	.100-009	.945-001	1.2745

* THERMOCHEMISTRY DATA *

CURVE FIT OF DATA IN FORM CP=RB+RC*T+RD/(T*T) (CAL/(MOLE*K)

HF(CAL/MOL)	H(CAL/MOL)	RB	RC	RD	S(CAL/MOL/K)	TU(K)		NAME
N2	28.000							
.79000+000	.23993+005	.61391+001	.16415-002	.29727+005	.64548+002	300.	1000.	N2
.79000+000	.22188+005	.83049+001	.23357-003	-.72806+006	.63774+002	1000.	2500.	N2
O2	32.000							
.00000	.25541+005	.67044+001	.16795-002	-.19419+005	.68908+002	300.	1000.	O2
.00000	.23450+005	.80725+001	.50513-003	-.21319+006	.67976+002	1000.	2500.	O2
H2O	18.000							
-.57798+005	.31716+005	.68290+001	.29575-002	.27843+005	.69022+002	300.	1000.	H2O
-.57798+005	.30303+005	.99698+001	.12774-002	-.14328+007	.68463+002	1000.	2500.	H2O
CO2	44.000							
-.94054+005	.41438+005	.95778+001	.36020-002	-.16389+006	.81997+002	300.	1000.	CO2
-.94054+005	.36573+005	.13972+002	.38449-003	-.13412+007	.79867+002	1000.	2500.	CO2
C3H8	44.000							
-.24820+005	.10888+006	.32090+002	.11928-001	-.20372+007	.15940+003	300.	2500.	C3H8
-.24820+005	.10888+006	.32090+002	.11928-001	-.20372+007	.15940+003	2500.	6000.	C3H8

* KINETIC REACTION DATA *

TOTAL NUMBER OF REACTIONS 2
NUMBER OF GAS PHASE REACTIONS 1

M	TYPE	REACTION	PRE EXP FACTOR (MOLE-CM-S)	TEMP EXP	ACTIVATION (KCAL/MOLE)
1	GAS	5.0 O2 + 1.0 C3H8--=4.0 H2O + 3.0 CO2	.4100+010	.000	40.6100
2	SURF	5.0 O2 + 1.0 C3H8--=4.0 H2O + 3.0 CO2	.1100+010	.000	17.6000

	AXIAL DISTANCE ALONG MONOLITH , CYLINDER OR PLATE S (CM)									
	.020	.040	.060	.080	.100	.150	.200	.250	.300	.400
BULK TEMP (K)	663.0	677.7	689.9	700.7	710.5	731.1	749.4	766.1	781.6	809.3
WALL TEMP (K)	1814.6	1885.5	1898.0	1904.4	1912.7	1926.8	1949.5	1969.7	1987.4	2009.2
MOLE FRACTION										
BULK SPECIES										
N2	.76403	.76378	.76356	.76338	.76321	.76286	.76255	.76227	.76202	.76157
O2	.20072	.19898	.19753	.19625	.19511	.19272	.19063	.18875	.18702	.18398
C3H8	.03204	.03170	.03141	.03116	.03093	.03046	.03004	.02967	.02942	.02872
H2O	.00183	.00317	.00429	.00526	.00615	.00798	.00958	.01103	.01237	.01470
CO2	.00137	.00238	.00321	.00395	.00461	.00598	.00719	.00828	.00927	.01102
WALL SPECIES										
N2	.74031	.74031	.74031	.74031	.74031	.74031	.74031	.74031	.74031	.74031
O2	.03925	.03925	.03925	.03925	.03925	.03925	.03925	.03925	.03925	.03925
C3H8	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
H2O	.12596	.12597	.12597	.12597	.12597	.12597	.12597	.12597	.12597	.12597
CO2	.09447	.09447	.09447	.09447	.09448	.09448	.09448	.09448	.09448	.09448

	AXIAL DISTANCE ALONG MONOLITH , CYLINDER OR PLATE S (CM)									
	.500	.700	1.000	1.500	2.000	2.500	3.000	3.500	4.000	4.500
BULK TEMP (K)	834.6	878.5	935.1	1013.4	1081.3	1141.8	1196.8	1247.4	1294.1	1336.2
WALL TEMP (K)	2032.1	2057.5	2083.7	2104.2	2112.7	2114.3	2111.9	2102.7	2079.9	2026.0
MOLE FRACTION										
BULK SPECIES										
N2	.76117	.76048	.75961	.75841	.75736	.75641	.75555	.75474	.75397	.75323
O2	.18125	.17656	.17062	.16242	.15527	.14885	.14296	.13746	.13223	.12718
C3H8	.02818	.02725	.02607	.02444	.02302	.02175	.02058	.01949	.01845	.01745
H2O	.01680	.02040	.02497	.03128	.03677	.04170	.04623	.05046	.05448	.05837
CO2	.01260	.01530	.01873	.02346	.02758	.03128	.03467	.03785	.04086	.04378
WALL SPECIES										
N2	.74031	.74031	.74031	.74031	.74031	.74031	.74031	.74031	.74031	.74031
O2	.03925	.03925	.03924	.03924	.03924	.03924	.03924	.03924	.03924	.03924
C3H8	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
H2O	.12597	.12597	.12597	.12597	.12597	.12597	.12597	.12597	.12597	.12597
CO2	.09448	.09448	.09448	.09448	.09448	.09448	.09448	.09448	.09448	.09448

AXIAL DISTANCE ALONG MONOLITH , CYLINDER OR PLATE S (CM)

5.250

BULK TEMP (K) 1385.1

WALL TEMP (K) 1878.7

MOLE FRACTION

BULK SPECIES

N2	.75217
O2	.12000
C3H8	.01603
H2O	.06389
CO2	.04792

WALL SPECIES

N2	.74031
O2	.03924
C3H8	.00000
H2O	.12597
CO2	.09448

** FOR HEAT EXCHANGER PROBLEM OPTION 2

		EXCHANGER 1	EXCHANGER 2
COOLANT TEMPERATURE IN (K)	=	700.00	709.51
COOLANT TEMPERATURE OUT (K)	=	709.51	740.54
TOTAL HEAT TRANSFERED TO COOLANT (CAL/S)	=	.400+002	.131+003
TEMPERATURE OF FUEL/AIR (K):			
UPSTREAM OF HEAT EXCHANGER	=	637.93	1385.05
DOWNSTREAM OF HEAT EXCHANGER	=	644.00	1325.34

SECTION 5

PROGRAM AND SUBROUTINES

Brief descriptions of the main program and subroutines are given in this section. The code consists of the main program, MAIN1, and eighteen subroutines. A cross reference between these routines is given in Table 5-1 and a simplified flow chart is shown in Figure 5-1.

5.1 MAIN1 MAIN PROGRAM

The main program, MAIN1, has a number of functions and serves as the driver for the entire program. Primarily, MAIN1 initializes some constants and reads a variety of input parameters. Subroutines READIN, OBTAIN and KINKIN are called by MAIN1 to read in initial species concentration, thermochemical and kinetic reaction data, respectively. Following this operation, the main program loop on grid solution iterations is entered. In this loop, space step quantities and terms necessary for the governing equations are constructed. The FLAME subroutine is then called to calculate the change in concentrations and temperatures due to chemical reactions. Following this loop, the solution is checked for convergency, and the loop is repeated until the solution is converged.

BEES Subroutine

This subroutine sets up the initial terms for solving the 2-D heat conduction problem when the traverse heat loss option is invoked.

COEF Subroutine

This subroutine calculates the reactor film transfer coefficient based on specified catalytic reactor geometries and flowrates.

TABLE 5-1. SUBROUTINE CROSS REFERENCE

Routine/ Subroutine	Calls Routine/ Subroutine	Called by Routine/ Subroutine
BEES	CPROP	MAIN1
COEF	--	MAIN1
COND2	--	FLAME
CPROP		BEES FLAME OPT2
FLAME	CPROP COND2 RERAY	MAIN1
GETDAT	--	OBTAIN
KINKIN		MAIN1
MAIN1	READIN OBTAIN KINKIN VIEW1 VIEW BEES FLAME TRIDM PROP COEF STNPRT OPT2	
OBTAIN	GETDAT	MAIN1
OPT2	CPROP PROP	MAIN1
PROP	--	MAIN1
READIN	--	MAIN1
RERAY	--	FLAME
STNPRT	--	MAIN1
TRIDM	TRID	MAIN1
VIEW	--	MAIN1
VIEW1	--	MAIN1

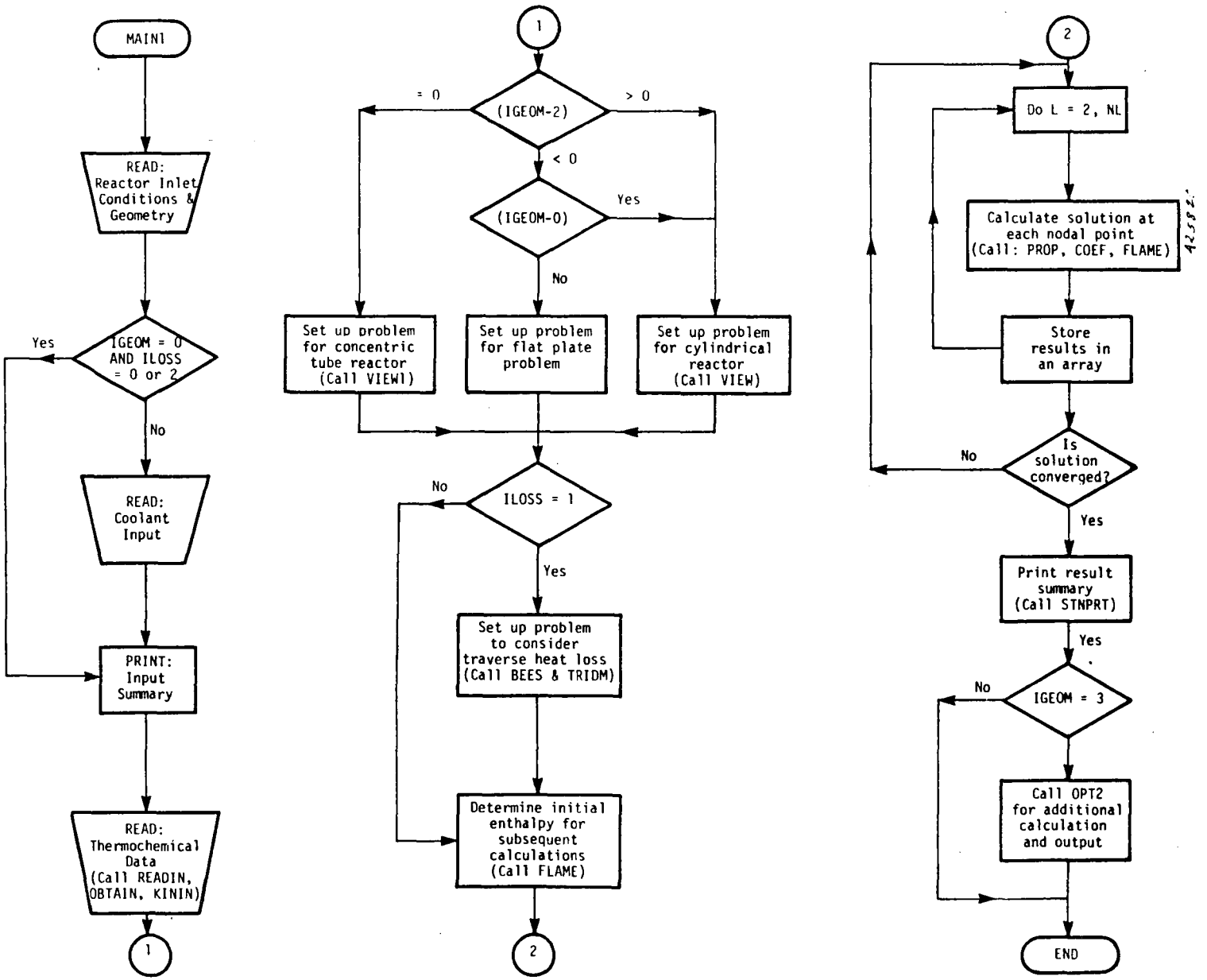

Figure 5-1. Program flow chart.

COND2 Subroutine

This subroutine solves the heat conduction term in the surface energy balance based on the information obtained in the TRIDM subroutine.

CPROP Subroutine

This subroutine calculates the coolant heat transfer coefficient.

FLAME Subroutine

This is the program's key subroutine which solves the species and energy equations including the effects of chemical kinetics. The routine begins by setting up the individual species thermochemical properties. Utilizing current solution estimates, errors and their derivatives with respect to the variables are formed for the enthalpy, total pressure and species mass balance equations. The resulting equation errors are then checked for convergence. If convergence is not achieved the matrix of error derivatives is inverted and multiplied by the errors to obtain the corrections to the variables needed to drive the equation errors to zero. If the corrections exceed a certain multiple of the variables, all of the corrections are uniformly damped so as not to overcorrect the variables. Corrections are then made and the solution procedure cycles to the top of the subroutine to repeat the above process until either a converged solution is found or the allowed number of iterations is exceeded.

READIN Subroutine

This subroutine reads the species names, initial species concentrations and diffusion factors.

OBTAIN Subroutine

This subroutine scans the curve fit thermochemical data file for the species of interest. Once the proper species thermochemical data file is found, subroutine GETDAT is called to extract and store the data.

GETDAT Subroutine

This subroutine extracts curve fit thermochemical data from input/output unit 11 and stores the data for use during a calculation.

KINKIN Subroutine

This subroutine reads in the kinetic reactions and their associated rates. It then develops the stoichiometric coefficients for the reactions and checks to see if the reactions balance. The stoichiometric coefficients are applied in the FLAME subroutine.

RERAY Subroutine

This subroutine is a generalized matrix inversion routine which either gives a set of solution vectors or the solution vectors plus the full matrix inversion.

OPT2 Subroutine

This subroutine sets up the computer code to perform the problem with a catalytic reactor radiating to up- and downstream heat exchangers.

PROP Subroutine

This subroutine calculates the transport properties for the reacting gas given the gas composition, temperature, and pressure.

STNPRT Subroutine

This subroutine sets up the computer code to print out the results as well as the input information of the specified problem.

TERMS Subroutine

This subroutine further reduces the terms set up by the BEES subroutine into a smaller set.

TRID Subroutine

This subroutine is a general routine which solves a set of tridiagonal linear equations.

TRIDM Subroutine

This subroutine uses the terms set up for the 2-D heat conduction problem by the TERMS subroutine and rearranges them into a set of tridiagonal linear equations. It then calls the TRID subroutine to solve the equations and uses the subsequent result to calculate reactor wall temperatures.

VIEW Subroutine

This subroutine calculates the view factors for monolith reactors given the monolith cell geometry.

VIEW1 Subroutine

This subroutine calculates the view factors for reactors with concentric tube configurations.

SECTION 6

SYMBOLS AND COMMON BLOCKS

Variables are contained in COMMON blocks and INCLUDE statements which represent a set of COMMON blocks. The COMMON'S in each INCLUDE statement are shown in Table 6-1 and the COMMON blocks and INCLUDE statements in each routine are shown in Table 6-2. A list of symbols in these COMMONS blocks and INCLUDE statements is given in Table 6-3 and local variables in the routines are given in Table 6-4.

TABLE 6-1. COMMONS BLOCKS IN INCLUDE STATEMENTS

INCLUDE	COMMON Blocks
BASIC	
ENERGY	ENERGY, VFA, SAVE
HEAT	HEAT, TRANS, PROPS, CHEAT, F2, AMB, TWS, BBB
HEAT1	HEATL, MEAN
PROC1	F1, F3
PROC2	F4, F5
PROC3	F6
PROF	CARD1, IUNIT, LIN, WANTS

TABLE 6-2. COMMON BLOCK CROSS REFERENCE

	INCLUDE								COMMON												
	BASIC	ENERGY	HEAT	HEAT1	PROC1	PROC2	PROC3	PROF	BLK1	BLK2	BLK6	BLK7	BLK8	BLK9	BLK11	BLK19	BLK21	BK1	BK2	BK4
BEES	X		X		X	X				X					X			X		
COEF	X		X	X	X												X			
COND2	X		X		X	X										X				
CPROP	X		X		X					X			X	X	X					
FLAME	X	X	X		X	X	X		X	X	X	X	X			X	X	X	X	X
GETDAT	X				X		X	X												
KINKIN	X				X	X	X	X												
MAIN1	X	X	X	X	X	X	X	X	X	X	X	X	X	X				X		X
OBTAIN	X				X			X												
OPT2	X	X	X		X		X			X	X		X							
PROP	X		X		X	X	X	X												
READIN	X				X	X		X												
RERAY	X																			
STNPRT	X		X		X	X	X			X	X								X	X
TRIDM	X		X		X	X														
VIEW	X																			
VIEW1	X	X	X						X											

TABLE 6-3. SYMBOLS IN COMMON STATEMENTS

Variable	Common	Description
$\bar{A}$(,)	F6	Basic matrix of coefficients set up in FLAME, fully inverted on last iteration in FLAME, and used to set up linearized corrections in ACEF. Equivalenced to DAA for storage economy only.
ADSM	F5	Composite term used for integration
AEM1	F2	Iteration variable
AEM2	F2	Iteration variable
AH	F5	Not used
AHH	F5	Composite term used for integration
AK	F2	Thermal conductivity of reactor (cal/s/cm-K)
AKT	BLK2	Thermal conductivity for coolant tube (cal/s/cm-K)
ALPF( )	F3	Assigned initial or frozen values of the α_i's which are input to the code. These values are assigned to station one and are never varied.
ALPHI( )	F6	The current set of α_i's at a given station as generated by the FLAME subroutine. Entering FLAME these variables contain the terms α_i introduced in Eq. 44.
AM	ENERGY	Mass flowrate of reactants (gm/s)
AMH	BLK2	Coolant flowrate (gm/s)
A1	TRANS	Interation variable
A2	TRANS	Iteration variable
A3	TRANS	Not used
A4	TRANS	Not used

TABLE 6-3. CONTINUED

Varible	Common	Description
$\bar{B}$	BLK8	Radiation variable σT^4
BF( )	F3	Not used
BIN(JS)	TRANS	Not used
BP3(J)	BBB	Variables defined in Subroutine BEES
BP5(J)	BBB	
BP6(J)	BBB	
BP7(J)	BBB	
B1(J)	BBB	
B16(J)	BBB	
C	F5	Perimeter of reactor cells (cm)
CC	BLK8	Distance between monolith and tube bank (cm)
CH	HEAT	Nondimensional heat transfer coefficient
CHH	F5	Composite term used for integration
CHM	HEAT	Mass transfer coefficient (gm/cm^2-s)
CHT	BLK21	Same as CH
CM	HEAT	Nondimensional mass transfer coefificient
CMH	HEAT	$Le^{0.667}$
CMSTG	TRANS	Not used
CMT	BLK21	Same as CM
CPF( )	F6	Molal heat capacity of each species (cal/mole/K)

TABLE 6-3. CONTINUED

Variable	Common	Description
$\bar{CPG}$( )	F6	Heat capacity of gas mixture in cal/gm-K. Within FLAME, CPG is heat capacity times PM.
CPPH	BLK2	Specific heat capacity (cal/gmole-K).
C1	BLK9	Specific heat coefficients (Eq. 50)
C2	BLK9	Specific heat coefficients (Eq. 50)
C3	BLK9	Specific heat coefficients (Eq. 50)
DBTW	TRANS	Not used
DC	BLK8	Diameter of combustor (cm)
DIAM	F5	Reactor diameter (cm)
DQCON	BLK19	Conduction term defined in Subroutine COND2
DR	BLK2	Coolant tube thickness (cm)
DS(I)	F2	One-half of the distance S(I)-S(I-2)
DT	BLK2	Coolant tube diameter (cm)
DY	F2	Same as DR
EAK( )	F4	Activation energy (Kcal/gmole-k)
EK	BLK9	Viscosity parameter ε/k (Eq. 46-48) (K)
EMIV	VFA	Emissivity of reactor
EMIVT	BLK2	Coolant tube emissivity
EXK( )	F4	Temperature exponent
F(,)	VFA	View factor
FC	F5	Not used

TABLE 6-3. CONTINUED

Variable	Common	Description
FKF( )	F4	Pre-exponential factor (mole, cm, s)
FL(,)	BLK1	View factor
FT	F1	Not used
GKT	BLK3	Thermal conductivity (cal/cm-s-K)
GKT1	BLK9	Coolant thermal conductivity at TK1 (cal/cm-s-K)
GKT2	BLK9	Coolant thermal conductivity at TK2 (cal/cm-s-K)
H	F1	Enthalpy of gas mixture as input to FLAME. In FLAME solution the parameter includes other input terms (h^0).
HAMB(J)	AMB	External heat transfer coefficient (cal/cm^2-s-K)
HEW( )	SAVE	Enthalpy based on wall composition and bulk
HHO( )	BK4	Stored local value of HO
HI( )	F6	Molal enthalpy of each species
HN	BLK2	Heat transfer coefficient on the coolant side (cal/cm^2-s-K)
HNN( )	BK1	Convective heat transfer coefficient for external cooling (cal/cm^2-s-K)
HO	BLK2	Heat transfer coefficient on the hot gas side (cal/cm^2-s-K)
HOS( )	F6	Product of molal enthalpy and partial pressure of each species; modified to include heat transfer terms for computational efficiency
HW	ENERGY	Enthalpy based on wall composition and temperature
ICC	F1	Value of ITC as carried by program with regard to heat loss operations (see Section 5.1)
ICOEF	BK1	Input external heat transfer coefficient flag

TABLE 6-3. CONTINUED

Variable	Common	Description
ICON	F1	Flag indicating convergence (=0) or nonconvergence (=1) of FLAME routine
IGEOM	F1	Reactor geometry option
IKIN( )	BLK7	Noncatalytic (0) or catalytic (1) node
ILOSS	F1	Heat loss option
INMAS	IUNIT	Mass storge unit
IS	F1	Number of species
ISP	F1	IS+1
ISPECI(2)	CARD1	Species name
ISS	F5	Number of species x 2
ITER	F1	Iteration count in FLAME
ITURB	HEAT1	Not used
IWANT(3,)	WANTS	Flat (IWANT (,) and species name (IWANT ( )) of desired species.
KR	F1	Kinetics flag in FLAME
KR7	F1	Diagnostic output option
L	F1	Axial station number
MGAS	F1	Number of gas phase reactions
MT	F1	Total number of reactions
N	F1	Number of species
NAMA( )	F6	First four characters of species name
NAMB( )	F1	Second four characters of species name

TABLE 6-3. CONTINUED

Variable	Common	Description
NL	F2	Number of grid points
NWANT	WANTS	Number of species in input list. Must equal IS.
P	F1	Pressure in atmospheres
PHI(,)	F4	Not used
PLN	F1	Log of pressure
PLP( )	F6	Log of partial pressure of each species
PM	F6	Product of pressure and molecular weight
PMS1	SAVE	Saved value for pressure molecular weight
PMS2	SAVE	Saved value for pressure molecular weight
PMU(,)	F4	Stoichiometric coefficient of each product species in each reaction
PP( )	F6	Partial pressure of each species
PPM( )	BLK6	Local value of PM(1)
PR	PROPS	Prandtl number
PS(,)	BLK6	PP(I)/PM(1)
PT	BLK8	Coolant pressure (atm)
PX	BLK3	Not used
QCHEM	ENERGY	Chemical energy term in Eq. (6)
QCON	BLK11	Conduction term defined in Subroutine COND2
QCOND	ENERGY	Conduction energy term in Eq. (5)
QCONV	ENERGY	Convective energy term
QLOSS	ENERGY	Total heat loss

TABLE 6-3. CONTINUED

Variable	Common	Description
QRAD	ENERGY	Radiation loss, Eq. (8)
QRADIN	ENERGY	Radiation from up- and downstream reservoirs
QR1( )	BLK1	Radiation terms defined in Subroutine VIEW1
QR2( )	BLK1	Radiation terms defined in Subroutine VIEW1
RB( ) RC( ) RD( ) RE( ) RF( ) RDS( )	F6	Curve fit constants for enthalpy, entropy and Cp of each species. See page 5.14. RB = F_1 + F_2, RC = F_3, RD = F_4, RE = F_5 and RF = F_6
RMU(,)	F4	Stoichiometric coefficient of each reactant species in the reaction
RU	PROPS	Variable defined in MAIN1
RUD	PROPS	Variable defined in MAIN1
RT(2)	F3	Product of gas constant and temperature
S(JS1)	F2	Grid point locations (cm)
SB( )	F6	Entropy/R of each species at pressure (not standard state). Later modified to be log K_p of formation log p (free energy of formation at pressure.
SG	BLK9	Viscosity parameter (Eq. 46-48)
SNSM	F5	Not used
SPLP( )	SAVE	Saved value for log partial pressure
SS	BLK11	Mid-point between S_i and S_{i-1}

TABLE 6-3. CONTINUED

Variable	Common	Description
ST	PROP	Not used
SUMH	F5	Summation of products of partial pressure and enthalpy
SUMP(2)	F3	Summation of partial pressures
T( )	F6	Temperature (K)
TAMBI	AMB	Not used
TAMBO	AMB	Not used
TAU	VFA	Stefan Boltzman constant
TCOND	PROPS	Thermal conductivity (cal/s-cm-K)
THMU (,)	F4	Not used
TI	F2	Inlet temperature (K)
TK1	BLK9	Lower coolant reference temperature (K)
TK2	BLK9	Upper coolant reference temperature (K)
TL(JS1)	F2	Wall temperature (K)
TRES(2)	F2	Upstream (1) and downstream (2) reservoir temperature
TSQ(t)	F3	Temperature to the square power
TS1	SAVE	Saved value for gas temperature
TS2	SAVE	Saved value for wall temperature
TT( )	BK2	Coolant temperature (K)
TTI	BLK2	Coolant inlet temperature on the coolant side (K)
TTW( )	BLK4	Stored local value of TTW1

TABLE 6-3. CONTINUED

Variable	Common	Description
TU( )	F6	Temperature at which switch is made from low temperature to high temperature thermodynamic data curve fits (see page 5-14).
TW(J)	TWS	Iterative value for temperatures
TWT	F5	Not used
TW1(J)	TWS	Iterative value for temperatures
TW2(J)	TWS	Iterative value for temperatures
TZ	BLK6	Average temperature for property calculation
VG	CHEAT	Void fraction of monolith
VISC	PROPS	Viscosity (gm/cm-s)
VL	BLK8	Coolant inlet velocity (cm/sec)
VNU(,)	F1	Stoichiometric coefficients for equilibrium reactions
W	BLK6	Constant = 1.0
WM( )	IUNIT	Molecular weight of each species as input
WT	BLK9	Coolant molecular weight (gm/mole)
X(JS)	PROPS	Distance normalized to tube diameter
XALPF( )	WANTS	ALPF( ) as read
XHRF	CARD1	Heat of formation (cal/gmole)
XMW	CARD1	Molecular weight
XNU	PROPS	Not used

TABLE 6-3. CONCLUDED

Variable	Common	Description
XNUB	MEAN	Heat transfer correlation variable
XNUI	CHEAT	Heat transfer correlation variable
XP	CHEAT	Defined in Subroutine COEF
XPPS	MEAN	Not used
XTP	CHEAT	Not used

TABLE 6-4. SYMBOLS IN ROUTINES/SUBROUTINES

Variable	Subroutine	Description
AA	FLAME	Inverse of A loaded into AA and corrected for rearrangements in kinetics package of FLAME
AAK	BEES	Temporary value for reactor thermal conductivity
AAN( )	VIEW1	Locally defined variable
AA1	FLAME	Locally defined variables for Newton-Raphson coefficients
AA2	FLAME	
AA3	FLAME	
AC	OPT2	Locally defined constant
ADSM	MAIN1	Locally defined variable
AEMN	MAIN1	Locally defined variable
AFF( )	FLAME	Affinity of given kinetic reaction (= $T\Delta S$)
AHM( )	OPT2	Same as AMH
AKK	MAIN1	Temporary value of AK
ALFA	FLAME	Normalize coolant tube conductance $h_H \Delta r/k$
ALPSV( )	MAIN1	Saved value of ALPHI( )
AM	MAIN1	Mass flowrate (gm/s) for IGEOM $\neq$ 1 Mass flux (gm/cm^2-s) for IGEOM = 1
AMU( )	KININ	μ_i for reactants
AN	VIEW1	Locally defined variables
ANK	CPROP	Exponential n in Eq. (49)
ANP	VIEW1	Locally defined variables
AR	OPT2	Locally defined constant

TABLE 6-4. CONTINUED

Variable	Subroutine	Description
ARAT	VIEW1	Locally defined variable
AREA	MAIN1	Cross sectional area (cm^2)
ARG( )	TERMS	Call list function
AS	MAIN1	Locally defined variable
AV	MAIN1	Surface area to volume ratio (1/cm)
AVS	CPROP	Eq. (46)
AX	OPT2	Locally defined constant
B	TRID	-Tw(I+1) x B6(I+1) - B7(I+1)
BB	VIEW1	Locally defined variable
BB( )	OPT2	Locally defined variable
BIG( )	FLAME	Largest positive contribution to each mass balance. After kinetics package becomes largest absolute contribution.
BMU( )	KININ	μ_1 for products
BR1	MAIN1	Locally defined variable
BR2	MAIN1	Locally defined variable
BUST	FLAME	Value assigned to BUMP
C	OPT2	Locally defined variable
C1	VIEW1	Locally defined variable
C2	VIEW1	Locally defined variable
C3	VIEW1	Locally defined variable

TABLE 6-4. CONTINUED

Variable	Subroutine	Description
C4	VIEW1	Locally defined variable
C5_	VIEW1	Locally defined variable
CONST	FLAME	Locally defined iteration variable
CPDF	FLAME	Local summation
CPDW	FLAME	Local summation
CPEW	FLAME	Local summation
CPEWW( )	OPT2	Specific heat capacity of edge gases at wall
CPH( )	OPT2	Same as CPPH
CPP	OPT2	Average gas specific heat capacity (cal/gmole-K)
CPTIL	PROP	Locally defined variables for thermodynamics properties calculations
CT	FLAME	π times coolant tube diameter
CT	OPT2	Pi times coolant tube diameter
D(,)	VIEW	Locally defined variable
DAMP	FLAME	Damping factor
DCHM	FLAME	Zero
DCTW	FLAME	Zero
DENS	CPROP	Density (gm/cc)
DERR	FLAME	Derivation of error

TABLE 6-4. CONTINUED

Variable	Subroutine	Description
DIAG( )	TRID	-B4 (I+1)
DIAM	VIEW	Same as DTUB, effective cell diameter (cm)
DIAMC	VIEW1	Same as DTUB, effective cell diameter (cm)
DIAMS	MAIN1	Diameter/height of reactor (cm)
DKPT( )	FLAME	The partial of log K with respect to log T for each kinetic reaction
DLNTW	FLAME	Temperature correction
DLTX	MAIN1	Temporary value for inlet temperature (K)
DM1	FLAME	Locally defined variable
DM2	FLAME	Locally defined variable
DNE	FLAME	Number of reactants in a kinetic reaction
DOM	FLAME	Log of mole fraction of a species
DS	VIEW	Locally defined variable
DSS	VIEW	Locally defined variable
DTT	CPROP	Same as DT, coolant tube diameter (cm)
DTTWI	FLAME	Normalized temperature correction
DTUB	MAIN1	Effective cell diameter (cm)
DTW	COND2	Local variable
DTWDT	FLAME	Temporary value for hot order wall temperature; derivatives for iteration corrections
DTWDTH	FLAME	
DTWDTW	FLAME	
DTWI	FLAME	Locally defined variable
DTWII	FLAME	Locally defined variable

TABLE 6-4. CONTINUED

Variable	Subroutine	Description
DUM	FLAME	Locally defined temporary values
DUM1	FLAME	
DUM2	FLAME	
DUMN	FLAME	
DUMQRA	FLAME	
DY2	BEES	0.25 x square of coolant tube thickness (cm^2)
E	FLAME	Prior to inversion in FLAME, equal to error of mass balance and equilibrium equations; after inversion equal to corrections in log partial pressures of species
E	OPT2	Locally defined variable
EMAX	FLAME	Maximum correction in species partial pressure on a given iteration
EMIVV	MAIN1	Temporary value of emissivity
EMXP	FLAME	EMAX from prior iteration
ERR	FLAME	Iteration error
ESUM	FLAME	Locally defined variable
ETW	FLAME	Not used
ETWW	FLAME	Not used
FCC( )	FLAME	Temporary storage for PP( )
FF	OPT2	Locally defined variable
FF1	OPT2	Locally defined variable
FIB	MAIN1	Locally defined variable

TABLE 6-4. CONTINUED

Variable	Subroutine	Description
FM( )	VIEW1	Locally defined variable
FP	OPT2	Local radiation variable
FP( )	VIEW1	Locally defined variable
FQ( )	VIEW1	Locally defined variable
FZ	FLAME	Locally defined variable
GMAX	OPT2	Mass flux (gm/cm^2-s)
HH	BEES	Locally defined variable
HH( )	OPT2	Same as HN
HO( )	OPT2	Heat transfer coefficient (cal/cm^2-s-K)
HSV	MAIN1	Locally defined variable
HT	FLAME	Total conductance
IB	MAIN1	Iteration control integer
IBGN	STNPRT	Locally defined output counters
ICB	FLAME	Count of iterations with BUMP activated
ICP	KININ	Local counters
ICR	KININ	Local counters
IDENT	KININ	Output alphanumeric
IDUM	OBTAIN	Dummy integer
IEND	STNPRT	Locally defined output counters
IEOF	OBTAIN	End-of-species-file indicator

TABLE 6-4. CONTINUED

Variable	Subroutine	Description
IFLAG	KININ	Stop program if there is a problem with kinetic data
IFRZ	FLAME	Local control integer
IHDG	OBTAIN	Dummy integer
IMXP	FLAME	Index for maximum iterations
ISL	FLAME	Local control integer
ISPEC( )	READIN	Same as NAMA, NAMB
ISS	FLAME	Number of species plus 2
ISS	READIN	Number of species times 2
ISW	KININ	Flag on whether a species name in a reaction can be matched with the species input names
ITDR	MAIN1	Iteration counter
ITEMS	STNPRT	Locally defined output counters
ITERZ	FLAME	Interaction counter
ITMX	FLAME	Maximum number of iterations allowed
IX	FLAME	Reaction equation index
IX	KININ	Local index
J	READIN	Locally defined integer
JMAX	READIN	Same as PARAMETER JP (see BASIC PROG)
KIN	KININ	Input unit
KNY	READIN	Unused integer
KOUT	KININ	Output integer
KR7S	MAIN1	Stored value of KR7

TABLE 6-4. CONTINUED

Variable	Subroutine	Description
KS	FLAME	1 or IS+1
JSS	FLAME	IS or 2+IS
M	FLAME	Local index
MATCH	OBTAIN	Local counter
MGP	FLAME	Identity of first surface reaction
NA( )	KININ	Reactant names
NASYM( )	KININ	Output alphanumeric
NB( )	KININ	Product names
NBSYM( )	KININ	Output alphanumeric
NEQ	FLAME	Total number of equations used in corrector step.
NEQU	TRIDM	Number of grid points minus 1
NI	OPT2	Temporary index
NIT	OPT2	Iteration counter
NI1	FLAME	Reray control integers
NI2		
NI3		
NLL	MAIN1	Number of grid points minus 1
NLNGTH	OBTAIN	Same as NLNGTH
NLP	MAIN1	Number of grid points plus 1
NMA	KININ	Temporary alphanumeric
NP( )	KININ	Output alphanumeric
NR( )	KININ	Output alphanumeric

TABLE 6-4. CONTINUED

Variable	Subroutine	Description
NT - NTUB	OPT2 MAIN1	Locally defined integer Locally defined variable
NUMNA	KININ	Maximum value of ICR for each reaction
NUMNB	KININ	Maximum value of ICP for each reaction
OMG	CPROP	Eq. (47)
OK	OBTAIN	Local counter
PAGES	STNPRT	Locally defined output counter
PCM	FLAME	Locally defined variable
PI	VIEW1	Constant 3.1416
PKP( )	FLAME	Reverse rate of kinetic reaction
PKPE( )	FLAME	Natural log of PKP
PKR( )	FLAME	Forward rate of kinetic reaction
PKRE( )	FLAME	Natural log of PKR
PLIM	FLAME	Maximum allowed change in log partial pressures
PLN	MAIN1	ℓn P
PLPSV( )	MAIN1	Saved value of log partial pressure
PMR( )	FLAME	Net forward rate of each reaction as used in FLAME
PMSV1	MAIN1	Locally defined variable
PMSV2	MAIN1	Locally defined variable
PMV1 PMV2 PMV3 PMV5 PMV6	PROP PROP PROP PROP PROP	Locally defined variables for thermodynamics properties calculations

TABLE 6-4. CONTINUED

Variable	Subroutine	Description
PP	VIEW1	Locally defined variable
PPSV( )	MAIN1	Saved value of partial pressure
PRMU(,)	FLAME	Net stoichiometric product coefficient for each species in each reaction subsequently multiplied by CKIN (JE) for computational convenience
PRT	CPROP	Prandtl number
PSUM	KININ	Used in reaction balance check
QC( )	OPT2	Total heat transferred to coolant (cal/s)
QDIFF	FLAME	Diffusion energy
QQ( )	MAIN1	Locally defined variable
QQ( )	STNPRT	Variable dfined in MAIN1
QR( )	FLAME	Local Radiation variable
QRAT	FLAME	Local radiation variable
QRR	FLAME	Iterative value of radiation loss
QRR( )	OPT2	Not used
QRSAVE	FLAME	Saved value of radiation flux
QTOT	OPT2	Not used
QTOTAL	MAIN1	Total energy transferred to coolant (cal/s)
R	VIEW	Effective cell radius
RAT( )	FLAME	Maximum of PKP (JX) and PKR (JX). Basis of ordering reactions
RATIO	TRID	Locally defined variable
RE	COEF	Reynolds number

TABLE 6-4. CONTINUED

Variable	Subroutine	Description
RET	CPROP	Reynolds number
REY	OPT2	Reynolds number
RH	MAIN1	Locally defined variable
RR	CPROP	Reynolds number per unit length (1/cm)
RR	VIEW1	Ratio of effective cell diameter to coolant tube diameter
RSUM	KININ	Used in reaction balance check
SIGN	FLAME	Locally defined variable
SL	VIEW1	Locally defined variable
SR	VIEW1	Locally defined variable
STEP	MAIN1	Iteration step size
STP( )	KININ	Net stoichiometric coefficient for products
STPR( )	KININ	Difference between stoichiometric coefficients for each species in each reaction equation
STR( )	KININ	Net stoichiometric coefficient for reactants
SUB( )	TRID	B3(I+1)
SUM( )	OPT2	Local summation
SUMD	FLAME	Locally defined summation variables
SUMHEW	FLAME	
SUMK	FLAME	
SUMHW	FLAME	
SUMR	FLAME	
SUP	TRID	B5(I+1)

TABLE 6-4. CONTINUED

Variable	Subroutine	Description
T11	MAIN1	Temporary value of T(1)
TAV̄	OPT2	Temporary value of TAVR
TAVG( )	OPT2	Locally defined variable
TC( )	FLAME	-HI (JP)/RT = -d(log K_p)/d(log T)
TDIF	MAIN1	Temperature difference control value
TFZ( )	FLAME	Fixed values of temperature (data statements)
TG( )	OPT2	Temperature upstream of heat exchanger (°K)
TG( )	STNPRT	Variable defined in MAIN1
TG( )	MAIN1	Locally defined variable
TGAS	FLAME	Temporary value for gas temperature
TGI	OPT2	Temperature of fuel/air mixture (°F)
TGNLP	OPT2	Temperature downstream of heat exchanger (°K)
TII	OPT2	Iterative temperature
TKE	CPROP	Eq. (48)
TPMU	PROP	Locally defined variables for thermodynamics properties calculations
TRES1	MAIN1	Stored value of upstream reservoir temperature (K)
TRES2	MAIN1	Stored value of downstream reservoir temperature (K)
TSV	MAIN1	Temporary value for inlet temperature (K)
TTF( )	OPT2	Coolant temperature out (°K)

TABLE 6-4. CONTINUED

Variable	Subroutine	Description
TTP	FLAME	T(1)
TTWA( )	OPT2	Locally defined variable
TTW1	FLAME	Temporary value for coolant wall temperature
TTW2	FLAME	Temporary value for hot side wall temperature
TWSI	FLAME	Locally defined variable
TWSII	FLAME	Locally defined variable
TX	BEES	Same as TTI, coolant inlet temperature (K)
U	OPT2	
V( )	FLAME	Not used
VA,VB,VC VD,VE	FLAME	Locally defined variables used in thermodynamics calculations
VF	MAIN1	Void fraction of monolith
VFF	FLAME	Locally defined variables used in thermodynamics calculations
VLK	FLAME	Log of k_f (see Eq. (12))
VMU	PROP	Locally defined variables for thermodynamics properties calculations
WMM	MAIN1	Locally defined variable
WM1	MAIN1	Molecular weight of gas at inlet (gm/gmole)
WM2	MAIN1	Molecular weight of gas at outlet (gm/gmole)

TABLE 6-4. CONCLUDED

Variable	Subroutine	Description
XA	OPT2	Locally defined variable
XB	OPT2	Locally defined variable
XBP	READIN	Diffusion factors
XC	OPT2	Locally defined variable
XF	READIN	Species initial mole fraction
XE	READIN	Species first guesses, mole fractions
XLE	COEF	Lewis number, Pr/Sc
XNUBM	MAIN1	Local summation value
XSUM	MAIN1	Local summation value
XX	FLAME	Saved values of FKF (JX) prior to pressure and third body modifications
Y	OPT2	Locally defined radiation variable
Z	OPT2	Locally defined variable
Z1,Z2,Z3	FLAME	Locally defined iteration variables
ZDS	VIEW1	Locally defined variables
ZZ	FLAME	Unused variable

SECTION 7

CODE LISTING

```
      SUBROUTINE BEES
      REAL HH
      INCLUDE BASIC
      INCLUDE HEAT
      INCLUDE PROC1
      INCLUDE PROC2
      COMMON/BLK2/TT(JS1),AKT,DR,DT,EMIVT,AMH,CPPH,TTI,HN,HO
      COMMON/BLK11/SS
     -COMMON/BK1/HNN(JS1),ICOEF
C------
      TX=TTI
      DY2 = DY * DY / 4.0
      DO 100 I = 2, NL
      SS=(S(I)-S(I-1))/2.+S(I-1)
      IF(ICOEF.NE.1) CALL CPROP(TX)
      AAK=AK
      HNN(I)=HN
      AK=AKT
      HH=HN
      IF(ICOEF.EQ.1)GO TO 1
      GO TO 2
    1 HH=HAMB(I)
      HNN(1)=HH
    2 SSN=S(I)-S(I-1)
C
         B1(I) = DY2 / (DS(I) * SSN)
         B2(I) = DY2 / (DS(I+1) * SSN)
         B3(I) = AK * DY / 4.0 / DS(I)
         B4(I) = SSN * (HH + 2.*AK/DY) + AK*DY/4.*(1./DS(I+1)+1./DS(I))
         B5(I) = AK * DY / 4.0 / DS(I+1)
         B6(I) = 2.*AK / DY * SSN
         B7(I) = HH * TX * SSN
         B8(I) = 2.*AK * C / DY * SSN
         B9(I) = AK * C * DY / (4.*DS(I+1))
         B10(I) = AK * C * DY / (4.*DS(I))
C
         BP7(I) = B7(I) / B4(I)
         BP3(I) = B3(I) / B4(I)
         BP5(I) = B5(I) / B4(I)
         BP6(I) = B6(I) / B4(I)
C
         B11(I) = 2.0 + B1(I) + B2(I) - BP6(I)
         BM = 1. - BP3(I)
         B12(I) = BP7(I) / BM
         B13(I) = BP5(I) / BM
         B14(I) = BP6(I) / BM - 2. - B2(I)
         B15(I) = BP3(I) / BM
         B16(I) = BP6(I) / BM - 2. - B1(I)
C
  100 CONTINUE
      AK=AAK
C
      RETURN
      END
```

```
      SUBROUTINE COEF
      INCLUDE BASIC
      INCLUDE HEAT
      INCLUDE HEAT1
      INCLUDE PROC1
      COMMON/BLK21/CHT,CMT
C------
      RE=RUD/VISC
      XLE = PR / SC
      XP=RE*PR/X(L)
       XNUI=.81*PR**.4*SQRT(RE*4./(1./VF-1.))
      IF(XNUI.LE.3.66) XNUI=3.66
      CMH=(XLE)**.667
      IF (IGEOM .NE. 1) GO TO 10
C---------FLAT PLATE LAMINAR FLOW CORRELATION---------
      XNUB = .332 * PR ** .333 * SQRT(RE)
      GO TO 40
   10 IF (RE .GT. 10000.) GO TO 20
      XNUB = 3.66 * (1.0 + .095 * XP * RUD / RU) ** .45
      GO TO 30
   20 XNUB = .023 * RE ** .8 * PR ** .4
   30 IF (L .GT. 2) GO TO 40
      IF (XNUB .GT. XNUI) XNUB = XNUI
   40 CONTINUE
      CH=RU*XNUB/PR/RE
      CM=CH*CMH
      CHT=CH
      CMT=CM
   90 FORMAT(8X,10E10.5)
      RETURN
      END
```

```
      SUBROUTINE COND2(NN)
      INCLUDE BASIC
      INCLUDE HEAT
      INCLUDE PROC1
      INCLUDE PROC2
      COMMON/BLK19/QCON,DQCON
C-----
         IF(NN .NE. 2)  GO TO 100
            TW(NN) = (B12(NN) + B13(NN) * TW2(NN+1) + TW1(NN) +
     $                 B2(NN) * TW(NN+1)) / (-B14(NN))
            TW(NN-1) = TW(NN)
      TW1(NN-1)=TW1(NN)
      TW2(NN-1)=TW2(NN)
      DTW=-TW1(NN)/B14(NN)
            GO TO 250
  100    CONTINUE
C
         IF(NN .NE. NL)  GO TO 200
            TW(NN) = (B12(NN) + B15(NN) * TW2(NN-1) + TW1(NN) +
     $                 B1(NN) * TW(NN-1) ) / (-B16(NN))
            TW(NN+1) = TW(NN)
      TW1(NN+1)=TW1(NN)
      TW2(NN+1)=TW2(NN)
      DTW=-TW1(NN)/B16(NN)
            GO TO 250
  200    CONTINUE
C
         TW(NN) = (BP7(NN) + TW1(NN) + TW(NN-1) * B1(NN) +
     $             TW(NN+1) * B2(NN) + TW2(NN-1) * BP3(NN) +
     $             TW2(NN+1) * BP5(NN)) / B11(NN)
      DTW=TW1(NN)/B11(NN)
  250    CONTINUE
C
         TW2(NN) = TW(NN) * (2.0 + B1(NN) + B2(NN)) - TW1(NN) -
     $             B1(NN) * TW(NN-1) - B2(NN) * TW(NN+1)
C
      QCON=-(B8(NN)+B9(NN)+B10(NN))*TW1(NN)+B8(NN)*TW(NN)+B9(NN)*TW1(NN+
     $1)+B10(NN)*TW1(NN-1)
      DQCON=-(B8(NN)+B9(NN)+B10(NN))*TW1(NN)+B8(NN)*DTW
      IF(NN.EQ.2) DQCON=DQCON+B10(NN)*TW1(NN)
      IF(NN.EQ.NL) DQCON=DQCON+B9(NN)*TW1(NN)
C
      RETURN
      END
```

```
      SUBROUTINE CPROP(TZ)
      INCLUDE BASIC
      INCLUDE HEAT
      INCLUDE PROC1
      COMMON/BLK11/SS
      COMMON/BLK2/TT(JS1),AKT,DR,DT,EMIVT,AMH,CPPH,TTI,HN,HO
      COMMON/BLK8/VL,PT,WT,B,DC,CC,GKT
      COMMON/BLK9/TK1,TK2,GKT1,GKT2,SG,EK,C1,C2,C3
C***  VISCOSITY
      TKE=TZ/EK
      OMG=1.16/TKE**0.148+0.525/EXP(0.775*TKE)+2.162/EXP(2.438*TKE)
      AVS=26.69*SQRT(WT*TZ)/(OMG*SG*SG)*0.000001
C
C***  THERMAL CONDUCTIVITY
      ANK=ALOG(GKT2/GKT1)/ALOG(TK2/TK1)
      IF(ANK.LT.0.0)GO TO 7
      GKT=GKT1*(TZ/TK1)**ANK
      GO TO 8
    7 ANK=-ANK
      GKT=GKT1/(TZ/TK1)**ANK
C
C***  HEAT CAPACITY
    8 CPPH=C1+C2*TZ+C3/TZ**2
      CPPH=CPPH/WT
C
C**   DENSITY
      DENS=PT/TZ*WT/82.04
C
C***  PRANDTL AND REYNOLDS NUMBER CALCULATIONS
      PRT=AVS*CPPH/GKT
      RET=VL*DENS/AVS
      RR=RET
      RET=DT*RR
      IF(IGEOM.EQ.1)RET=SS*RR
C
C**   HEAT TRANSFER COEFFICIENT CORRELATIONS
      DTT=DT
      IF(IGEOM.GT.1)GO TO 1
      IF(IGEOM.EQ.1)GO TO 2
      HN=1.1*PRT**0.333*GKT/DT
      IF(RET.GT.500.)GO TO 3
      HN=HN*(0.48*SQRT(RET)+0.43)
      GO TO 99
    3 HN=HN*(0.46*SQRT(RET)+0.00128*RET)
      GO TO 99
    1 IF(RET.GT.10000)GO TO 4
      HN=3.66*GKT/DTT
      GO TO 99
    4 HN=0.023*GKT/DTT*RET**0.8*PRT**0.4
      GO TO 99
    2 IF(RET.GT.50000)GO TO 5
      HN = .332 * GKT / SS * PRT ** .333 * SQRT(RET)
      GO TO 99
    5 HN=0.0296*RET**0.8*PRT**0.333*GKT/SS
   99 RETURN
      END
```

```
      SUBROUTINE  FLAME
      INCLUDE BASIC
      INCLUDE HEAT
      INCLUDE ENERGY
      INCLUDE PROC1
      INCLUDE PROC2
      INCLUDE PROC3
      COMMON/BLK1/      FL(JS1,JS1),QR1(JS1),QR2(JS1)
      COMMON/BLK2/TT(JS1),AKT,DR,DT,EMIVT,AMH,CPPH,TTI,HN,HO
      COMMON/BLK6/PS(JS,JP2),PPM(JS1),W,TZ
      COMMON/BLK7/IKIN(JS1)
      COMMON/BLK8/VL,PT,WT,B,DC,CC,GKT
      COMMON/BLK21/CHT,CMT
      COMMON/BLK19/QCON,DQCON
      COMMON/BK1/HNN(JS1),ICOEF
      COMMON/BK3/PX(JS,JP2)
      COMMON/BK4/HHO(JS1),TTW(JS1)
      DIMENSION QR(JS1)
C
      DIMENSION TC(JP2),E(JP2),FCC(JP2),XX(JP2),PRMU(JP2,JX),AFF(JP2)
     $,DKPT(JP2),PKP(JP2),PKR(JP2),PMR(JP2),RAT(JP2),BIG(JP2)
     $,PKPE(JP2),PKRE(JP2)
      DIMENSION V(JY),AA(JY,JY)
      DIMENSION  TFZ(9)
C
      DATA  TFZ/1400.,1300.,1200.,1100.,1000.,900.,800.,700.,600./
      DATA NUL/0/,ICOLD/0/
C------
      NSS=ISS
      DO 1  J=1,ISS
      PP(J)=EXP(PLP(J))
      FCC(J)=PP(J)
    1 SPLP(J)=PLP(J)
      PMS1=PM(1)
      PMS2=PM(2)
      TS1=T(1)
      TS2=T(2)
      IFRZ=0
      ICB=0
      BUST=100.
      ITMX=40
      IMXP=1
      PLIM=2.3025851
      TTP=T(1)
      EMXP=1.E+10
      ITER=1
      DAMP=1.
      ICON=1
      ISL=0
      N=ISS+4
      IF(IGEOM .EQ. 2)  N = N + 1
      NEQ=N
   30 DO 2 K=1,2
      CPG(K)=0.
      VA=ALOG(T(K)/3000.)/1.9865
```

```
      VB=T(K)-3000.
      VC=(T(K)+3000.)*.5
      VD=T(K)*3000.
      VE=VC/(VD*VD)
      VFF=VB/1.9865
      RT(K)=1.9865*T(K)
      TSQ(K)=T(K)*T(K)
      SUMP(K)=0.
      KS=1+(K-1)*IS
      KSS=IS+(K-1)*IS
      DO 2  I=KS,KSS
      M=I-(K-1)*IS
      J=2
      IF(T(K).LT.TU(M,1)) J=1
      CPF(I)=RC(M,J)+T(K)*RD(M,J)+RE(M,J)/TSQ(K)
      HI(I)=RB(M,J)+VB*(RC(M,J)+RD(M,J)*VC+RE(M,J)/VD)
      SB(I)=RF(M,J)+RC(M,J)*VA+VFF*(RD(M,J)+RE(M,J)*VE)-PLP(I)
      CPG(K)=CPG(K)+PP(I)*CPF(I)
      PS(L,I)=PP(I)/PM(1)
      PX(L,I)=PP(I)/P
      PPM(L)=PM(1)
      SUMP(K)=SUMP(K)+PP(I)
      TC(I)=-HI(I)/RT(K)
      E(I)=TC(I)+SB(I)
      SB(I)=E(I)
    2 DCHM=0.
      CHM=CHT*CH
      DCTW=0.0
      DO11 I=1,N
      V(I)=0.
      DO11 J=1,N
   11 A(I,J)=0.
      SUMHW=0.
      SUMH=0.
      SMHEW=0.
      DO 3 I=1,IS
      HOS(I)=HI(I)*PP(I)
      SUMH=SUMH+HOS(I)
      HOS(I+IS)=HI(I+IS)*PP(I+IS)
      SUMHW=SUMHW+HOS(I+IS)
      HEW(I)=HI(I+IS)*PP(I)
      SMHEW=SMHEW+HEW(I)
      IF (KR7 .LE. 3) GO TO 3
      WRITE(6,10330) L
10330 FORMAT(//20X,7HSTATION ,I3)
      WRITE(6,10000 ) HOS(I),HOS(I+IS),HEW(I),SUMH,SUMHW,SMHEW
    3 CONTINUE
10000 FORMAT(25X,4E10.5)
      IF (L .EQ. 1) RETURN
      IF(ILOSS.EQ.0.AND.IGEOM.EQ.0)GO TO 60
      IF(ICOEF.EQ.1)GO TO 201
      TZ=TT(L)
      IF(ITER.EQ.1) CALL CPROP(TZ)
   60 CONTINUE
  201 CONTINUE
      IF (L .EQ. 2) TGAS = TI
      CPDW=0.
```

```
      CPDF=0.
      CPEW=0.
      DO 4 I=1,IS
      CPEW=CPEW+PP(I)*CPF(I+IS)
      CPDW=CPDW+PP(I+IS)*CPF(I+IS)
    4 CPDF=CPDF+PP(I)*CPF(I)
      RHS(1)=-PM(1)*H+SUMH+CHM*(SUMH-SMHEW+CMH*(SMHEW-SUMHW*PM(1)/PM(2))
     *)
      A(1,1)=-(1.+CHM)*T(1)*CPDF
      A(1,1)=A(1,1)-(SUMH-SMHEW+CMH*(SMHEW-SUMHW*PM(1)/PM(2)))*DCHM
      A(1,2)=-CHM*T(2)*((CMH-1.)*CPEW-CMH*CPDW*PM(1)/PM(2))
     *-DCTW*(SUMH-SMHEW+CMH*(SMHEW-SUMHW*PM(1)/PM(2)))
      A(1,3)=PM(1)*H +CHM*SUMHW*PM(1)/PM(2)
      A(1,4)=-PM(1)/PM(2)*CHM*SUMHW
      DO 5 I=1,IS
      A(1,I+4)=-HOS(I)-CHM*(HOS(I)-HEW(I)*(1.-CMH))
    5 A(1,I+IS+4)=CHM*HOS(I+IS)*PM(1)/PM(2)
      DUMQRA=EMIV*(1.-F(L,L))*TAU*T(2)**4
      QRAT=(QRADIN+DUMQRA)*AHH*C
      IF(ILOSS .LT. 2)  GO TO 32
      QCON=0.0
      DQCON=0.0
      DO 31 I=1,N
   31 A(2,I)=0.0
      A(2,2)=1.0
      RHS(2)=0.0
      GO TO 39
   32 IF (ILOSS.GT.0) GO TO 33
      IF(L-2) 7,6,7
    6 TWSI= CHH*(TL(L+1)-T(2))/DS(L+1)
      TWSII=AEM1*(T(2)**4.-TRES(1)**4.)
      DTWI=-CHH*T(2)/DS(L+1)
      DTWII=4.*AEM1*T(2)**4.
      GO TO 10
    7 IF(L-NL) 9,8,8
    8 TWSI=AEM2*(T(2)**4.-TRES(2)**4.)
      TWSII=CHH*(T(2)-TL(L-1))/DS(L)
      DTWI=4.*AEM2*T(2)**4.
      DTWII=CHH*T(2)/DS(L)
      GO TO 10
    9 TWSI= CHH*(TL(L+1)-T(2))/DS(L+1)
      TWSII=CHH*(T(2)-TL(L-1))/DS(L)
      DTWI=-CHH*T(2)/DS(L+1)
      DTWII=CHH*T(2)/DS(L)
   10 QCON=TWSI-TWSII
      DQCON=DTWI - DTWII
      GO TO 34
   33 TW1(L) = T(2)
      CALL COND2(L)
   34 RHS(2)=PM(1)*H-SUMH+PM(1)*QCON-PM(1)*QRAT
      A(2,2)=-PM(1)*(DQCON-AHH*C*4.*DUMQRA)
      A(2,3)=-PM(1)*(H+QCON-QRAT)
      A(2,1)=T(1)*CPDF
   39 CONTINUE
      DO 410 I=1,IS
      A(2,4+I) = PP(I)*HI(I)
      A(3,4+I)=PP(1)
```

```
  410 A(4,4+IS+I)=PP(I+IS)
  411 RHS(3)=P-SUMP(1)
      RHS(4)=P-SUMP(2)
      DO 720 I=1,IS
       A(4+I,1)=A(4+I,1)+(PP(I)-PP(I+IS)*PM(1)/PM(2))*DCHM*CMH
      A(4+I,2)=A(4+I,2)+(PP(I)-PP(I+IS)*PM(1)/PM(2))*DCTW*CMH
      A(4+I,3)=-PM(1)*ALPHI(I)-CHM*PP(I+IS)*PM(1)/PM(2)*CMH
      A(I+4,4)=CHM*PP(I+IS)*PM(1)/PM(2)*CMH
      A(4+I,4+I)=PP(I)+CHM*PP(I)*CMH
      A(4+I,4+IS+I)=-CHM*CMH    *PP(I+IS)*PM(1)/PM(2)
  720 RHS(4+I)=+PM(1)*ALPHI(I)-PP(I)-CHM*(PP(I)-PP(I+IS)*PM(1)/PM(2))*
     *CMH
      DO 420 I=1,IS
      A(4+IS+I,3)=-PM(1)/PM(2)*PP(I+IS)
      A(4+IS+I,4)=PM(1)/PM(2)*PP(I+IS)
      A(4+IS+I,4+I)=PP(I)
      A(4+IS+I,4+IS+I)=-PP(I+IS)*PM(1)/PM(2)
  420 RHS(4+IS+I)=-PP(I)+PP(I+IS)*PM(1)/PM(2)
C
      IF(IGEOM .NE. 2)  GO TO 422
      CT=3.1416*DT
      TT(1)=TTI
      IF(ITER.EQ.1) HO=CHT*CPG(1)/PM(1)
      ALFA=HN*DR/(AKT)
      HT=HO-AKT/DR*(1./(1+ALFA)-1.)
      Z1=CT*HO/AM*PM(1)*(S(L)-S(L-1))
      Z2=AKT*ALFA/(DR*(1.+ALFA))
      Z3=CT*HN/AMH/CPPH*(S(L)-S(L-1))
      QRR=0.0
      DO 104 K=2,NL
      IF(K.EQ.L)GO TO 105
      QRR=QRR+FL(K,L)*TL(K)**4
      GO TO 104
  105 QRR=QRR+FL(K,L)*T(2)**4
  104 CONTINUE
      EMIVT=EMIV
      QR(L)=-EMIVT*TAU*(QRR+QR1(L)*TRES(1)**4+QR2(L)*TRES(2)**4)
      CONST=HO*T(1)+Z2*TT(L)-QR(L)
      TTW1=TT(L)
      ITERZ=1
  107 ERR=EMIVT*TAU*TTW1**4+HT*TTW1-CONST
      DERR=4.*EMIVT*TAU*TTW1**3+HT
      DLNTW=-ERR/DERR
      TTW1=TTW1+DLNTW
      DTTW1=DLNTW/TTW1
      IF(ABS(DTTW1).LE..002) GO TO 109
      ITERZ=ITERZ+1
      IF(ITERZ.LE.30) GO TO 107
      WRITE(6,108) ERR,DLNTW
  108 FORMAT(//10X,'COOLANT TUBE ENERGY BALANCE EXCEEDS ITERATION LIMIT
     *ERROR= ',E10.5,1X,'DLNTW= ',E10.5)
      STOP
  109 CONTINUE
      CONST=4.*EMIVT*TAU*TTW1**3+HT
      TTW2=(ALFA*TT(L)+TTW1)/(1.+ALFA)
      DTWHT=HO*T(1)/CONST
      DTWGTW=4.*EMIVT*TAU*FL(L,L)*T(2)**4/CONST
```

```
      DTWDTH=Z2*TT(L)/CONST
      AA1=Z1*(T(1)-DTWDT)
      AA2=Z1*DTWDTW
      AA3=Z1*(T(1)-TTW1)
      A(1,1)=A(1,1)-AA1
      A(1,2)=A(1,2)+AA2
      A(1,3)=A(1,3)-AA3
      A(1,N)=Z1*DTWDTH
      RHS(1)=RHS(1)+AA3
      A(2,1)=A(2,1)+AA1
      A(2,2)=A(2,2)-AA2
      A(2,3)=A(2,3)+AA3
      A(2,N)=-A(1,N)
      RHS(2)=RHS(2)-AA3
      A(N,1)=-Z3*DTWDT/(1.+ALFA)
      A(N,2)=-Z3*DTWDTW/(1.+ALFA)
      A(N,N)=TT(L)+Z3/(1.+ALFA)*(TT(L)-DTWDTH)
      RHS(N)=-TT(L)+TT(L-1)-Z3*(TT(L)-TTW2)
      HHO(L)=HO
      TTW(L)=TTW1
      QRSAVE=QR(L)
      QH2=AMH*CPPH*(TT(L)-TT(L-1))
  422 CONTINUE
C
      IF (KR7 .LE. 3) GO TO 255
      WRITE(6,502)
      DO501 I=1,N
  501 WRITE(6,500) (A(I,J),J=1,N), RHS(I)
  500 FORMAT(1X,12E10.4/(2X,12E10.4))
  502 FORMAT(1X,20HA(I,J),RHS(I),BEFORE)
  255 IF(KR-5) 334,333,334
  333 DO 332 M=1,MT
      IX = 0.
      IF(M.GT.MGAS) IX=IS
      DNE=0.0
      DO 327 I=1,IS
  327 DNE=DNE-RMU(IX+I,M)
      FKF(M)=FKF(M)*82.056**DNE
      EXK(M)=EXK(M)+DNE
      XX(M)=FKF(M)
  332 CONTINUE
      KR=4
      MGP=MGAS+1
  334 DO 337 M=MGP,MT
  337 FKF(M)=XX(M)*PM(1)/CM
      IF(ICB.LE.( BUMP=1.
      DO 340 M=1,MT
      SUMD=0.
      SUMK=0.
      SUMR=0.
      K=1
      IF(M.GT.MGAS) K=2
      DO 315 I=1,ISS
      PRMU(I,M)=PMU(I,M)-RMU(I,M)
      SUMK=SUMK+PRMU(I,M)*SB(I)
      SUMR=SUMR+RMU(I,M)*PLP(I)
      SUMD=SUMD+PRMU(I,M)*HI(I)
```

```
      PRMU(I,M)=PRMU(I,M)*BUMP
  315 CONTINUE
      AFF(M)=SUMK*RT(K)
      DKPT(M)=SUMD/RT(K)
      VLK=ALOG(FKF(M))+EXK(M)*ALOG(T(K))-EAK(M)/RT(K)
      IF(K.EQ.1) VLK=ALOG(FKF(M))+EXK(M)*ALOG(TGAS)-EAK(M)/1.9865/TGAS
      PKPE(M)=AMIN1(SUMR-SUMK+VLK,80.)
      PKRE(M)=AMIN1(SUMR+VLK,80.)
      PKP(M)=EXP(PKPE(M) )
      PKR(M)=EXP(PKRE(M) )
      PMR(M)=PKR(M)-PKP(M)
      RAT(M)=AMAX1(PKP(M),PKR(M))
      IF (KR7 .LT. 3) GO TO 340
      WRITE(6,903)
      WRITE(6,902) (PRMU(I,M),I=1,ISS)
      WRITE(6,341) M,FKF(M),SUMK,SUMR,DKPT(M),VLK,EXK(M),EAK(M),
     *   PKR(M),PKP(M),PMR(M)
  902 FORMAT(1X,12E10.3)
  903 FORMAT(1H0,49HPRMU,M,FKF,SUMK,SUMR,DKPT,VLK,EXK,EAK,PKR,PKP,PMR /)
  341 FORMAT(I3,2X,11E11.5)
  340 CONTINUE
      DO 379 M=1,MT
      SIGN=IKIN(L)
      IF(M.LE.MGAS) SIGN=-PM(1)*ADSM
      DO 375 I=1,ISS
      SUMD=RMU(I,M)*PKR(M)-PMU(I,M)*PKP(M)
      DO 375 J=1,ISS
  375 A(J+4,I+4)=A(J+4,I+4)+SUMD*PRMU(J,M)*SIGN
      SUMD=PMR(M)*(EXK(M)+EAK(M)/RT(2))+PKP(M)*DKPT(M)
      DO 380 I=1,IS
      IF (M.GT.MGAS) GO TO 328
      DUM1=PM(1)*ADSM*PMR(M)* PRMU(I,M)
      A(I+4,1)=A(I+4,1)-DUM1*PKP(M)*DKPT(M)
      A(I+4,3)=A(I+4,3)-DUM1
      RHS(I+4)=RHS(I+4)+DUM1
      GO TO 380
  328 DUM1=PMR(M)*PRMU(I+IS,M)*IKIN(L)
      A(I+IS+4,1)=A(I+IS+4,1)-DUM1*DCHM/CHM
      A(I+IS+4,2)=A(I+IS+4,2)+SUMD*PRMU(I+IS,M)*IKIN(L)-DUM1*DCTW/CHM
      A(I+IS+4,3)=A(I+IS+4,3)+DUM1
      RHS(I+IS+4)=RHS(I+IS+4)-DUM1
  380 CONTINUE
  379 CONTINUE
      IF(IGEOM .NE. 1)  GO TO 498
C  FLAT PLATE PROBLEM
      RHS(2) = RHS(1) + RHS(2)
      DO 50 I=1,NEQ
         A(2,I) = A(2,I) + A(1,I)
         A(1,I) = 0.0
      A(3,I)=0.0
      A(I,1)=0.
      A(I,3)=0.
   50 CONTINUE
      RHS(1) = 0.0
      A(1,1) = 1.0
      RHS(3)=0.0
      A(3,3)=1.0
```

```
C
      DO 52 I=1,IS
         DO 51 J=1,NEQ
            A(I+4,J) = 0.0
      A(J,I+4)=0.
   51    CONTINUE
         A(I+4,I+4) = 1.0
         RHS(I+4) = 0.0
   52 CONTINUE
C
  498 CONTINUE
C
      IF (KR7 .LE. 3) GO TO 905
      WRITE(6,499)
  499 FORMAT(1H0,43HA(I,J),RHS(I),AFTER KINET AND BEFORE INVERT)
      DO 904 I=1,N
  904 WRITE(6,500)(A(I,J),J=1,N),RHS(I)
  905 CONTINUE
      FZ=1.0
      IF(IFRZ.EQ.0) GO TO 7114
      ETWW=RHS(2)
      RHS(2)=0.
      FZ=100.
      IF(IFRZ.LT.0) FZ=1.0
 7114 IF(BUMP.GT.1.) GO TO 101
      DUM=T(1)/A(1,1)
      DUM1=T(1)/A(2,1)
      IF (ICOEF .EQ. 1) DUM1 = T (2) / A(2,2)
      IF(ABS(RHS(1)*DUM).GT..2) GO TO 101
      IF(ABS(RHS(2)*DUM1) .GT. .1*FZ) GO TO 101
      IF(ABS(RHS(3))/P.GT..00001*FZ) GO TO 101
      IF(ABS(RHS(4))/P.GT..00001*FZ) GO TO 101
C
      IF(IGEOM .NE. 2)  GO TO 322
      DUMN=TT(L)/A(N,N)
      IF(ABS(DUMN*RHS(N)).GT.0.2)GO TO 101
  322 CONTINUE
      ESUM=0.
      DO 301 I=1,ISS
      PCM=PM(1)*ALPHI(I)
      IF(I .GT. IS) PCM=AMAX1(PP(I-IS),PM(1)*PP(I)/PM(2))
      BIG(I)=AMAX1(PCM,PP(I))
  301 ESUM=AMAX1(ESUM,ABS(RHS(I+4))/(BIG(I)+1.E-30))
      IF(ABS(ESUM).GT..00001*FZ) GO TO 101
      ICON=0
      IF(IFRZ.LE.0) GO TO 7115
      ICON=1
      IFRZ=0
      ITER=0
 7115 DO 102 I=1,N
      DO 102 J=1,N
  102 AA(I,J)=A(I,J)
  101 NEQ=ISS+4
      IF(IGEOM .EQ. 2)  NEQ = NEQ + 1
      IF(IFRZ.EQ.0) GO TO 7113
      DO 7111   I=1,N
      J=2
```

```
 7111 A(J,I)=0.
       J=2
      A(J,J)=1.0
 7112 RHS(J)=0.
 7113 CONTINUE
      NI1=0
      NI2=0
      NI3=0
      CALL RERAY(NEQ,A,NI1,RHS,1,NI2,NI3)
      ETW=-1./(A(2,2)*T(2))
      DO 190 I=5,N
  190 E(I-4)=RHS(I)
      ISS=NSS
      IF(KR7.LE.3) GO TO 40
      WRITE(6,504)
      DO 503 I=1,N
  503 WRITE(6,500)(A(I,J),J=1,N),RHS(I)
  504 FORMAT(1H0,19HA(I,J),RHS(I),AFTER )
   40 DAMP=1.
      EMAX=1.E-30
      DO 15 I=1,ISS
      IF(ABS(EMAX).GT.ABS(E(I)))GO TO 42
      EMAX=E(I)
      IMAX=I
   42 DOM=PLP(I)-PLN
      IF(E(I)) 20,15,18
   18 DUM=(4.+4.*DOM)/(3.-DOM)
      GO TO 13
   20 DUM=(3.*DOM-4.)/(4.+DOM)
      IF(DUM) 13,15,15
   13 CONTINUE
   19 DAMP=AMIN1(DAMP,(DUM-DOM)/E(I))
   15 CONTINUE
      IF(E(IMXP)/EMXP.LT.-0.33) PLIM=PLIM/2.
      IF(MOD(ITER,2).EQ.0) EMXP=EMXP/EXP(PLIM)
      IF(ABS(1.-E(IMXP)/EMXP) .LT. .25) PLIM=AMIN1(PLIM*2.,9.2103404)
      EMXP=EMAX
      IMXP=IMAX
      DAMP=AMIN1(DAMP,PLIM/(ABS(EMXP)))
      DM1=AMAX1(ABS(RHS(1)),ABS(RHS(2)))
      IF(IGEOM .EQ. 2)  DM1 = AMAX1(DM1,ABS(RHS(N)))
      DM2=AMAX1(ABS(RHS(3)),ABS(RHS(4)))
      DAMP=AMIN1(DAMP,0.4/AMAX1(DM1,DM2))
      IF(DAMP.GT..99) GO TO 21
      DO 27 I=1,ISS
   27 E(I)=DAMP*E(I)
C     MAKE CORRECTIONS
   21 DO 28 I=1,ISS
      PLP(I)=PLP(I)+E(I)
      PP(I)=EXP(PLP(I))
   28 CONTINUE
      IF(IGEOM .EQ. 2)  TT(L) = TT(L) / (1.0-RHS(N)*DAMP)
      DO 600 K=1,2
      T(K)=T(K)/(1.-RHS(K)*DAMP)
  600 PM(K)=PM(K)*(1.+RHS(K+2)*DAMP)
 1401 QCONV=AM*(SUMH/PM(1)-H)
      QDIFF=CHM*AM*(SUMH-SMHEW)/PM(1)
```

```
      QCHEM=CHM*CMP*AM*(SMHEW/PM(1)-SUMHW/PM(2))
      QCOND=AM*(TWSI-TWSII)
      QRAD=-QRAT*AM
      IF (KR7 .LT. 3) GO TO 48
      WRITE(6,505) DAMP,T(1),PM(1),T(2),PM(2)
  505 FORMAT(1H ,6HDAMP= ,E10.5,4H T= ,E10.5, 5H PM= ,E10.5,4HT2= ,E10.5
     *,5HPM2= ,E10.5)
      WRITE(6,506) (PLP(I),I=1,ISS)
  506 FORMAT(5X,10E10.5)
      WRITE(6,510) QCONV,QDIFF,QCHEM,QCOND,QRAD
  510 FORMAT(8X,'ENERGY TERMS'/10X,'CONVECTION ='E10.5,2X,'DIFFUSION ='
     *E10.5,2X,'QCHEM ='
     *E10.5,2X,'BED CONDUCTION ='E10.5,2X,'WALL RADIATION ='E10.5)
      WRITE(6,512) QH2,TT(L),TTW1,TTW2,AMH,CPPH,HO,HN
      WRITE(6,512)DT,DR,AKT,HT,ALFA,CT,QRSAVE
  512 FORMAT(5X,8E10.5)
   48 IF (ICON .GT. 0) GO TO 45
      IF(IFRZ.LT.0.AND.L.NE.2) GO TO 1721
      GO TO 1708
 1721 T(2) = TFZ(-IFRZ)
      IFRZ = IFRZ + 1
      ITER = 0
      ICON = 1
      GO TO 30
 1708 DO 55 I=1,IS
      ALPHI(I+IS)=PP(I+IS)/PM(2)
   55 ALPHI(I)=PP(I)/PM(1)
 1414 CONTINUE
      H=SUMH/PM(1)
      HW=SUMHW/PM(2)
      QLOSS=QLOSS+QCOND+QRAD
      TGAS=T(1)
      RETURN
   45 ITER=ITER+1
C
      IF(ITER.GT.ITMX-10) KR7=4
      IF(ITER.LT.ITMX) GO TO 30
      WRITE(6,47)
   47 FORMAT(1H0,27HALLOWED ITERATIONS EXCEEDED)
 4700 IF(IFRZ.GT.0) GO TO 46
      IFRZ=1
      ITER=0
      T(1)=TS1
      T(2)=TL(L)
      IF(ISL.GT.2) GO TO 46
      IF(ISL.EQ.1) T(2)=TL(NL)
      IF(ISL.EQ.2) T(2)=TL(2)
      ISL=ISL+1
      PM(1)=PMS1
      PM(2)=PMS2
      DO 1413 I=1,IS
      PP(I)=FCC(I)
      PP(I+IS)=PP(I)
      PLP(I+IS)=SPLP(I)
 1413 PLP(I)=SPLP(I)
      GO TO 30
   46 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE GETDAT(J)
      INCLUDE BASIC
      INCLUDE PROF
      INCLUDE PROC1
      INCLUDE PROC3
C
         DIMENSION ZZ(JP,2)
C------
      NAMA(J) = ISPECI(1)
      NAMB(J) = ISPECI(2)
      ALPF(J) = XALPF(J)
      ALPF(J+IS) = XALPF(J+IS)
C     READ CURVE FIT DATA
      WM(J)=XMW
      DO 220 K=1,2
         READ (INMAS,20220) RA, RB(J,K), RC(J,K), RD(J,K), RE(J,K),
     *   RF(J,K), ZZ(J,K), TU(J,K)
20220    FORMAT (6E9.6, 2F6.0)
  220 CONTINUE
      WRITE (6,20140) NAMA(J), NAMB(J),WM(J)
20140 FORMAT(10X,2A4,2(2X,F10.3))
      DO 240 K=1,2
         WRITE (6,20240) RA, RB(J,K), RC(J,K), RD(J,K), RE(J,K)
     *  ,RF(J,K), ZZ(J,K), TU(J,K), NAMA(J), NAMB(J)
20240    FORMAT(5X, 6(E12.5,1X), 2(F6.0,1X), 2X, 2A4)
         RB(J,K) = RB(J,K) + RA
         RF(J,K) = RF(J,K) / 1.9865
  240 CONTINUE
  300 RETURN
      END
```

```
      SUBROUTINE KININ
      INTEGER BLANK
      INCLUDE BASIC
      INCLUDE PROF
      INCLUDE PROC1
      INCLUDE PROC2
      INCLUDE PROC3
C
      DIMENSION  NA(5), NB(5), AMU(5), BMU(5)
      DIMENSION NASYM(5), NBSYM(5)
      DIMENSION NR(5),NP(5),STR(5),STP(5),STPR(JP)
C
      DATA BLANK /4H    /
      DATA NASYM / 4H    , 4*4H +   /
      DATA NBSYM / 4H--= , 4*4H +   /
      DATA NGAS/4HGAS /
      DATA NSUR/4HSURF/
C
C-----
      KIN = 5
      KOUT = 6
C
C     READ TOTAL NO. OF REACTIONS AND NO. OF GAS PHASE REACTIONS
  100 READ(KIN,20100)  MT, MGAS
         WRITE(KOUT,20110)  MT, MGAS
         WRITE(KOUT,20120)
         IFLAG = 0
C
C  DO FOR EACH REACTION
         DO 400 M = 1, MT
            ISW = 0
            RSUM = 0.
            PSUM = 0.
C
            READ(KIN,20400) NA,NB,FKF(M),EXK(M),EAK(M)
         READ(KIN,20410) AMU, BMU
C
C
            IX = 0
            IF(M .GT. MGAS)  IX = IS
C
            DO 300 I = 1, IS
             NMA = NAMA(I)
               THMU(I,M) = 0.
               RMU (I,M) = 0.
               PMU (I,M) = 0.
               RMU(I+IS,M) = 0.
               PMU(I+IS,M) = 0.
C
      STPR(I)=0.
               DO 200 J = 1, 5
C
                  IF(NA(J).NE.NMA)  GO TO 150
                     RMU(I+IX,M) = AMU(J)
                     NA(J) = BLANK
```

```
  150              IF(NB(J).NE.NMA)  GO TO 200
                      PMU(I+IX,M) = BMU(J)
                      NB(J) = BLANK
  200           CONTINUE
C
      STPR(I)=PMU(I+IX,M)-RMU(I+IX,M)
C
                RSUM = RMU(I+IX,M) * WM(I) + RSUM
                PSUM = PMU(I+IX,M) * WM(I) + PSUM
C
  300       CONTINUE
      ICR=0
      ICP=0
      DO 310 J=1,5
      STR(J)=0.
      STP(J)=0.
      NR(J)=BLANK
  310 NP(J)=BLANK
      DO 340 I = 1, IS
      IF (STPR(I)-0.) 320,340,330
  320 ICR=ICR+1
      NR(ICR)=NAMA(I)
      STR(ICR)=-STPR(I)
      GO TO 340
  330 ICP=ICP+1
      NP(ICP)=NAMA(I)
      STP(ICP)=STPR(I)
  340 CONTINUE
      NUMNA=ICR
      NUMNB=ICP
      IDENT=NGAS
      IF(M.GT.MGAS) IDENT=NSUR
      WRITE(KOUT,20420) M,IDENT,(NASYM(J),STR(J),NR(J),J=1,NUMNA)
     $,       (NBSYM(J),STP(J),NP(J),J=1,NUMNB)
      WRITE(KOUT,20425) FKF(M),EXK(M),EAK(M)
      EAK(M)=1000.*EAK(M)
C
           IF(ABS(RSUM-PSUM) .LE. 1.E-04 * RSUM) GO TO 400
              WRITE(KOUT,20300)  M
              IFLAG = 1
              STOP
C
  400    CONTINUE
C  END DO
C
20100 FORMAT(2I3)
20110 FORMAT(1H1, 30X, 25H* KINETIC REACTION DATA *
     $,//          15X,30HTOTAL NUMBER OF REACTIONS      , I3
     $,/           15X,30H NUMBER OF GAS PHASE REACTIONS, I3 ,/)
20120 FORMAT(7X,1HM,4X,4HTYPE,T28,8HREACTION,T80,14HPRE EXP FACTOR
     $       T96, 8HTEMP EXP,T110, 10HACTIVATION
     $,/     T81, 11H(MOLE-CM-S),T110, 11H(KCAL/MOLE)  /)
20300 FORMAT(66H SUM OF MOLECULAR WEIGHTS INDICATES IMBALANCE IN KINETIC
     $ EQUATION ,I3)
20400 FORMAT(10(A4,1X),     3E10.4)
20410 FORMAT( 5F5.0, T41, 5F5.0 )
20420 FORMAT(5X,I3,4X,A4,6(A3,F3.1,1X,A4))
20425 FORMAT(1H+, T82, E10.4, T96, F8.3, T110, F10.4 )
C
      RETURN
      END
```

```
      MAIN1
      INCLUDE BASIC
      INCLUDE HEAT
      INCLUDE HEAT1
      INCLUDE ENERGY
      INCLUDE PROF
      INCLUDE PROC1
      INCLUDE PROC2
      INCLUDE PROC3
      REAL NTUB
      COMMON/BLK1/      FL(JS1,JS1),QR1(JS1),QR2(JS1)
      COMMON/BLK2/TT(JS1),AKT,DR,DT,EMIVT,AMH,CPPH,TTI,HN,HO
      COMMON/BLK6/PS(JS,JP2),PPM(JS1),W,IZ
      COMMON/BLK7/IKIN(JS1)
      COMMON/BLK8/VL,PT,WT,B,DC,CC,GKT
      COMMON/BLK9/TK1,TK2,GKT1,GKT2,SG,EK,C1,C2,C3
      COMMON/BK1/HNN(JS1),ICOEF
      COMMON/BK4/HHO(JS1)
C
      DIMENSION AMF(JS),TG(JS),QQ(JS1)
      DIMENSION ALPSV(JY), PPSV(JY), PLPSV(JY)
      DIMENSION TITLE(20)
C
C-------
      TAU=1.356E-12
      KR=5
C
  120 READ(5,460)TITLE
      WRITE (6,470) TITLE
      READ(5,500) IS,NL,NIT,ILOSS,IGEOM,ICOEF,KR7
C
      IF(NIT .EQ. 0)  NIT = 20
      KR7S = KR7
C
      WRITE(6,520) IS, NL, NIT, ILOSS, IGEOM, ICOEF, KR7
  520 FORMAT(/, T10,23H* INTEGRAL PARAMETERS *
     $,     //, T15,40HIS ( NUMBER OF SPECIES )                    =, I3
     $,      /, T15,40HNL ( GRID POINTS )                         =, I3
     $,      /, T15,40HNIT ( NUMBER OF OVERALL ITERATIONS )       =, I3
     $,      /, T15,40HILOSS ( HEAT LOSS OPTION )                 =, I3
     $,      /, T15,40HIGEOM ( PROBLEM GEOMETRY OPTION )          =, I3
     $,      /, T15,40HICOEFF ( HEAT TRANSFER INPUT OPTION )      =, I3
     $,      /, T15,40HKR7 ( PRINT OPTION )                       =, I3  )
      READ (5,660) DTUB, VF, DIAMS, AK, EMIV
      AS=(1.-VF)*3.1416*DIAMS*DIAMS/4.
      NTUB = VF * DIAMS * DIAMS / DTUB / DTUB
      IF (IGEOM .EQ. 0 .AND. NTUB .GT. 1) ILOSS = 0
      IF(IGEOM .NE. 3)  GO TO 34
         AS=(1.-VF)*DIAMS
         NTUB = VF * DIAMS / (3.1416*DTUB*DTUB/4.)
   34 CONTINUE
      READ (5,660) AM, TI, P
      READ (5,660) TRES
      C=3.1416*DTUB*NTUB
      AV=4./DTUB
C
```

```
      READ (5,730) (S(I),I=1,NL)
      READ(5,700)(TL(I),I=2,NL)
      READ(5,830)(IKIN(I),I=2,NL)
      IF (ILOSS .EQ. 0 .AND. IGEOM .EQ. 0)GO TO 32
      IF(ICOEF.EQ.1)GO TO 20
      READ(5,30)VL,AMH,TTI,PT,WT
      READ(5,30)AKT,DR,DT,DC,CC
      READ(5,30)TK1,TK2,GKT1,GKT2
      READ(5,30)SG,EK,C1,C2,C3
      DY=DR
   20 CONTINUE
   30 FORMAT(8F10.5)
      IF(ICOEF.NE.1)GO TO 32
      READ(5,30)(HAMB(I),I=2,NL)
      READ(5,30)TTI,AKT,DR
      DY=DR
   32 CONTINUE
C
      WRITE(6,680)
  680 FORMAT(   ///, T10,26H* NONINTEGRAL PARAMETERS *
     $,       //, T45,20H*** REACTOR DATA ***        )
      IF(IGEOM .NE. 1)  WRITE(6,681) NTUB, VF, DIAMS, DTUB
  681 FORMAT(//, T15,38HMONOLITH HONEYCOMB CATALYTIC COMBUSTOR
     $,       /, T15,26HNUMBER OF TUBES            =, F7.2
     $,       /, T15,26HVOID FRACTION              =, F7.3
     $,       /, T15,26HDIAMETER OF COMBUSTOR      =, F7.2 , 5H (CM)
     $,       /, T15,26HEFFECTIVE CELL DIAMETER    =, F7.2 , 5H (CM)
     $)
      IF(ILOSS.EQ.0.OR. IGEOM.EQ.0)GO TO 40
      WRITE(6,690)
  690 FORMAT(//, T15,52HFOR CYLINDER COOLED EXTERNALLY OR FLAT PLATE PRO
     $BLEM  )
      WRITE(6,692) DR
  692 FORMAT( /, T15,26HTHICKNESS OF CYLINDER OR
     $,       /, T15,26HTHICKNESS OF PLATE         =,F5.3, 5H (CM)    )
   40 CONTINUE
      WRITE(6,694)TI,P,AM,AK,EMIV
  694 FORMAT(//, T15,26HINLET TEMPERATURE          =,F7.2,4H (K)
     $,       /, T15,26HPRESSURE                   =,F7.2, 6H (ATM)
     $,       /, T15,26HMASS FLOW RATE             =,E9.3, 6H (G/S)
     $,       /, T15,26HCONDUCTIVITY               =,E9.3,13H (CAL/S-CM-K)
     $,       /, T15,26HEMISSIVITY                 =, F7.2 )
      DUM1 = ABS(TRES(1))
      DUM2 = ABS(TRES(2))
      WRITE(6,670) DUM1, DUM2
      WRITE(6,725) (S(I),I=1,NL)
      WRITE(6,715) (TL(I),I=2,NL)
  715 FORMAT(//,T10,'INITIAL GUESSED WALL TEMPERATURES (TL)'
     $,       /,T10,10G10.4,/,T11,10G10.4,/,T12,10G10.4,/,T13,10G10.4 )
  725 FORMAT(//,T10,'GRID POINTS CHOSEN (S)'
     $,       /,T10,10G10.4,/,T11,10G10.4,/,T12,10G10.4,/,T13,10G10.4 )
      IF(IGEOM.EQ.0.AND.ILOSS.EQ.0)GO TO 45
      WRITE(6,20500) TTI, PT, AMH, VL, WT, DT, DR,AKT
      IF (IGEOM .EQ. 3) WRITE(6,20505) DC, CC
20500 FORMAT(1H1,//, T45,26H*** COOLANT PROPERTIES ***
     $,       //, T15,19HCOOLANT
     $,       /, T15,19HINLET TEMPERATURE =, F7.2, 4H (K)
```

```
     $,       /, T15,19HPRESSURE           =, F7.2, 6H (ATM)
     $,       /, T15,19HMASS FLOW RATE     =, E9.3, 6H (G/S)
     $,       /, T15,19HAPPROACH VELOCITY =, F7.2, 7H (CM/S)
     $,       /, T15,19HMOLECULAR WEIGHT  =, F7.2
     $,      //, T10,21H    FOR COOLANT TUBE:
     $,       /, T15,19HTUBE DIAMETER      =, F7.2, 5H (CM)
     $,       /, T15,19HTUBE THICKNESS     =, F7.3, 5H (CM)
     $,       /, T15,19HCONDUCTIVIY        =, E9.3,13H (CAL/S-CM-K)
     $)
20505 FORMAT(
     $       //, T15,41HCENTER TO CENTER DISTANCE (TUBE BANK)   =, F7.2
     $, 5H (CM)
     $,       /, T15,41HDISTANCE BETWEEN MONOLITH AND TUBE BANK =, F7.3
     $, 5H (CM)        )
      WRITE(6,20600)  TK1, GKT1, TK2, GKT2, C1, C2, C3, SG, EK
20600 FORMAT(//,T10,35H  * THERMOCHEMICAL DATA FOR COOLANT
     $,      //,T15,37HTEMPERATURE      THERMAL CONDUCTIVITY
     $,     2(/,T17,F7.2, T37,E10.3)
     $,      //,T15,65HHEAT CAPACITY  CPH = C1 + C2 * T + C3 / T**2
     $(CAL/G-MOLE - K)
     $,      //,T20, 4HC1 =, E10.3,17H (CAL/G-MOLE - K)
     $,       /,T20, 4HC2 =, E10.3,20H (CAL/G-MOLE - K**2)
     $,       /,T20, 4HC3 =, E10.3,15H (CAL-K/G-MOLE)
     $,      //,T15,20HVISCOSITY PARAMETERS
     $,       /,T20, 7HSIGMA =, F7.3, 4H (A)
     $,       /,T20, 7HE/K   =, F7.3, 4H (K)       )
   45 CONTINUE
C
      CALL READIN
C
      CALL OBTAIN
C
      CALL KININ
C
      DO 190 I=1,NL
  190   X(I)=S(I)/DTUB
      IF (IGEOM - 2) 196, 197, 198
  196 IF (IGEOM .EQ. 0) GO TO 198
      C = 1.0
      RU = AM
      AS = DY
      DO 192 I = 1, JS1
      DO 191 J = 1, JS1
  191 F(I,J) = 0.0
  192 F(I,1) = 1.0
      GO TO 195
  197 AREA = 3.1416 / 4.0 * (DTUB*DTUB - DT * DT)
      RU = AM / AREA
      RUD = RU * (DTUB - DT)
      CALL VIEW1(DTUB,DT)
      GO TO 195
  198 AREA = 3.1416 / 4.0 * DTUB * DTUB
      RU = AM / AREA / NTUB
      RUD = RU * DTUB
      CALL VIEW(DTUB,NL,S,F)
  195 CONTINUE
C
```

```
      NLL=NL-1
      NLP=NL+1
      BR1=TAU*TRES(1)**4
      IF (TRES(1).GT.0.) GO TO 210
      BR1=0.
      TRES1 = TRES(1)
      TRES(1) = - TRES(1)
      DO 200 J=2,NL
  200   F(J,2)=F(J,2)+F(J,1)
  210 BR2=TAU*TRES(2)**4
      IF (TRES(2).GT.0.) GO TO 230
      BR2=0.
      TRES2 = TRES(2)
      TRES(2) = - TRES(2)
      DO 220 J=2,NL
  220   F(J,NL)=F(J,NL)+F(J,NLP)
  230 AEMN=AS*EMIV*TAU/AM
      EMIVV=EMIV
      AKK=AK
      DO 240 L=3,NL
  240   DS(L)=(S(L)-S(L-2))/2.
      DS(2) = DS(3)
      DS(NL+1) = DS(NL)
C
      IF(ILOSS .EQ. 1)  CALL BEES
C
      IF(ILOSS.EQ.0.AND.IGEOM.EQ.0)GO TO 245
         DO 241 L=1,NLP
  241    TT(L) = TTI
  245 CONTINUE
      TL(1)=TL(2)
      DO 255 L=2,NL
         TW(L)= TL(L)
  255 CONTINUE
      TW(1) = TW (2)
      TW(NL+1) = TW(NL)
  260 PLN=ALOG(P)
      DO 270 J=1,ISS
        PP(J)=ALPF(J)*P
  270   PLP(J)=ALOG(PP(J))
      PM(1)=0.
      DO 280 I=1,IS
  280   PM(1)=PM(1)+ALPF(I)*WM(I)
      PM(1)=P*PM(1)
      PM(2)=PM(1)
      TG(1) = TI
      T(1)=TI
      T(2)=TL(1)
      L=1
      CALL FLAME
      IF(ILOSS .EQ. 1)  CALL TRIDM
      TSV=TI
      DO 290 I=1,ISS
        ALPHI(I)=PP(I)/PM(1)
        PPSV(I)=PP(I)
        PLPSV(I)=PLP(I)
  290   ALPSV(I)=ALPHI(I)
```

```
      PMSV1=PM(1)
      PMSV2=PM(2)
      HSV=SUMH/PM(1)
      H=HSV
      WMM=PM(1)/P
      RH=PM(1)/(82.056*T(1))
      ITDR=0
  300 DLTX=0.
      AEM1=AEMN
      AEM2=-AEM1
      EMIV=EMIVV
      AK=AKK
      IF (TRFS1 .LT. 0.) AEM1=0.
      IF (TRFS2 .LT. 0.) AEM2=0.
      H=HSV
      T(1)=TSV
      T(2)=TL(2)
      PM(1)=PMSV1
      PM(2)=PMSV2
      QLOSS=0.
      DO 310 I=1,ISS
        ALPHI(I)=ALPSV(I)
        PLP(I)=PLPSV(I)
  310   PP(I)=PPSV(I)
      STEP=1.
      IB=1
      DO 420 L=2,NL
  320   KR7=KR7S
      IF(ILOSS.EQ.0.AND.IGEOM.EQ.0)GO TO 41
      TT(L)=TT(L-1)
   41 CONTINUE
        IF (ITDR.GT.0) T(1)=TG(L)
      T11=T(1)
      IF(IGEOM.EQ.1)RUD=RU*S(L)
      IF(IGEOM.EQ.1)T(1)=(T(1)+T(2))/2.
        CALL PROP
        CALL COEF
      T(1)=T11
        FIB=IB-1.
        DUM=1.-FIB*STEP
        AHH=(S(L)-S(L-1))/AM*DUM
      ADSM = AHH * AM / RU
        CHH=AS*AK/AM*DUM
        CH=AHH*C
        A1=A1*C*AHH
        A2=A2*C*AHH
        QRADIN=-EMIV*(F(L,1)*BR1+F(L,NLP)*BR2)
        DO 330 I=2,NL
          IF (I.EQ.L) GO TO 330
          B=TAU*TL(I)**4
          QRADIN=QRADIN-F(L,I)*B*EMIV
  330     CONTINUE
        CALL FLAME
        IF (ICON.EQ.0) GO TO 350
        GO TO 450
C
C
```

```
  350   IF (IB.EQ.1) GO TO 360
        IB=IB-1
        IF (MOD(IB,2).EQ.1) GO TO 320
        IB=IB/2
        STEP=STEP*2.
        GO TO 320
  360   TDIF=ABS(1.-T(2)/TL(L))
        IF (TDIF.GT.DLTX) DLTX=TDIF
        IF (L.GT.2) GO TO 380
        PMSV1=PM(1)
        PMSV2=PM(2)
        TSV=T(1)
        DO 370 I=1,ISS
          PLPSV(I)=PLP(I)
  370     PPSV(I)=PP(I)
  380   CONTINUE
        TG(L)=T(1)
        TL(L)=T(2)
      IF(ILOSS.EQ.0.AND.IGEOM.EQ.0)GO TO 42
      QQ(L)=(TT(L)-TT(L-1))*AMH*CPPH
      IF(IGEOM .EQ. 1 .OR. (IGEOM .EQ. 0 .AND. ILOSS .EQ. 1) )
     $              QQ(L)=HNN(L)*(T(2)-TTI  )*(S(L)-S(L-1))
   42 CONTINUE
        XSUM=0.
        DO 390 I=2,L
  390     XSUM=XSUM+XNUBXP(I)
        XNUBM=XSUM/XPP
        WM1=PM(1)/P
        WM2=PM(2)/P
        DO 400 J=1,ISS
  400     AMF(J)=PP(J)/P
        RH=PM(1)/(82.056*T(1))
        RH2=PM(2)/(82.056*T(2))
  410   CONTINUE
        IF (ICON.GT.0) GO TO 450
  420   CONTINUE
C
      IF(DLTX.LT..001) GO TO 52
      IF(ITDR.GE.NIT)GO TO 52
      GO TO 425
   52 CONTINUE
      IF(IGEOM .EQ. 3 .OR. (IGEOM .EQ. 0 .AND. ILOSS.EQ. 0) )  GO TO 421
      QTOTAL = 0.0
      DO 51 JJ = 2, NL
   51 QTOTAL = QTOTAL + QQ(JJ)
      WRITE(6,20700)  TTI, TT(NL), QTOTAL
  421 CONTINUE
20700 FORMAT(1H1,//,T15,36H**  OVERALL HEAT TRANSFER RESULTS **
     $,           /,T20,26HCOOLANT TEMPERATURE  IN  =, F7.2 , 4H (K)
     $,           /,T20,26HCOOLANT TEMPERATURE OUT  =, F7.2 , 4H (K)
     $,           /,T20,26HTOTAL HEAT TRANSFERED TO
     $,           /,T20,26HCOOLANT                  =, E10.3, 7H(CAL/S)
     $)
C
      CALL STNPRT(TG,QQ)
      IF(IGEOM.EQ.3)TZ=TTI
      IF(IGEOM .EQ. 3) CALL OPT2 (DIAMS,NTUB,TG,AS,DTUB)
```

```
      IF(KR7.LT.3)GO TO 425
      IF(IGEOM.EQ.3)GO TO 425
      IF(IGEOM.EQ.0.AND.ILOSS.EQ.0)GO TO 425
      WRITE(6,54)(HNN(L),L=2,NL)
      WRITE(6,55)(HHO(L),L=2,NL)
   54 FORMAT(/,5X,52HHEAT TRANSFER COEFFICIENT COOLANT SIDE (CAL/S-K-CM2
     $),/,5X,8(2X,E10.3,2X),/)
   55 FORMAT(/,5X,52HHEAT TRANSFER COEFFICIENT FUELAIR SIDE (CAL/S-K-CM2
     $),/,5X,8(2X,E10.3,2X),/)
  425 CONTINUE
      IF(DLTX.LT..001) GO TO 110
      IF(ITDR.GE.NIT)GO TO 110
      ITDR=ITDR+1
      GO TO 300
  110 WRITE(6,810)ITDR,DLTX
  450 STOP
C
  460 FORMAT (20A4)
  470 FORMAT(1H1,//,T15,20A4,/ )
  500 FORMAT (12I3)
  510 FORMAT (8F10.0)
  530 FORMAT (10X,6HALPF  ,8E10.4/21X,8E10.4)
  540 FORMAT (E10.5)
  550 FORMAT (1H,I4,7E14.5,2A4)
  560 FORMAT (6E9.6,6X,F6.0,6X,2A4)
  570 FORMAT (I3)
  580 FORMAT (10X,21HKINETC REACTION DATA//15X,20HNUMBER OF REACTIONS=I3
     $         /)
  590 FORMAT (20F4.1)
  600 FORMAT (10X,20F4.1)
  610 FORMAT (5(A4,1X),5X,3E10.4)
  620 FORMAT (5X,I3,3X,A4,1H+,A4,1H+,A4,3H--=,4X,A4,1H+,A4,6X,E10.4,6X,F
     $         8.3,6X,F10.4)
  630 FORMAT (8E10.3)
  640 FORMAT (10X,8HDIFF FAC,10E10.5)
  650 FORMAT (I5,5X,7F10.0)
  660 FORMAT (8F10.0)
  670 FORMAT(//,T10,'*** RESERVOIR TEMPERATURES ***'
     $,       //,T15,'UPSTREAM   =',G12.5
     $,        /,T15,'DOWNSTREAM =',G12.5       )
  700 FORMAT (8E10.5)
  710 FORMAT (10X,10F10.4/15X,10F10.4/20X,10F10.4/25X,10F10.4//)
  720 FORMAT (10X,10F10.4/15X,10F10.4/20X,10F10.4/25X,10F10.4//)
  730 FORMAT (8E10.5)
  740 FORMAT (10X,9HENTHALPY=,E10.5,8X,6HMOLWT=,E10.5,8X,4HRHO=,E10.5
     $,/       4HALP=,10E10.5)
  750 FORMAT (1X,'XNUB = ',E10.5,10X,'XPP = ',E10.5)
  760 FORMAT (1X,'MEAN NUSSELT NUMBER = ',E10.5)
  770 FORMAT (1H0,34HBULK AND WALL PROPERTIES ALONG BED)
  780 FORMAT (10X,9HDISTANCE=,E10.5,5X,5HNODE=,I4,5X,5HDLTX=,E10.5)
  790 FORMAT (10X,6HBULK  ,3HT= ,E10.5,4HMW= ,E10.5,3HH= ,E10.5,5HRHO= ,
     $         E10.5/10E10.5)
  800 FORMAT (10X,6HWALL  ,3HT= ,E10.5,4HMW= ,E10.5,4HHW= ,E10.5,5HRHO=
     $,        E10.5/10E10.5)
  810 FORMAT(///,T15,25(1H*)
     $,        //,T15,'ITERATIONS =',I5, '     TEMP ERROR =', G13.5
     $,        //,T15,25(1H*))
  830 FORMAT(40I2)
C
      END
```

```
      SUBROUTINE OBTAIN
      INCLUDE BASIC
      INCLUDE PROF
      INCLUDE PROC1
      DIMENSION LNGTH(2)
      DATA LNGTH/ 2, 30 /
      DATA IEND/3HEND/
C------
      OK = 0
      DO 9 I=1,NWANT
      IWANT(1,I)=0
    9 CONTINUE
C  CURVE FIT DATA ASSIGNED TO UNIT 11
C  TABULAR   DATA ASSIGNED TO UNIT 12
      ICC = -1
      INMAS =12
      IF(ICC.LT.0) INMAS=11
      REWIND INMAS

C     ORIGINALLY COMPAR

      NLNGTH = LNGTH(2)
      IF(ICC.LT.0) NLNGTH=LNGTH(1)
      MATCH = 0
      IEOF = 0
         WRITE(6, 300)
  300 FORMAT(1H1,30X,24H* THERMOCHEMISTRY DATA *  ,/)

      IF(INMAS.EQ.11) WRITE (6,10)
   10 FORMAT(1H0,15X,59HCURVE FIT OF DATA IN FORM CP=RB+RC*T+RD/(T*T) (C
     *AL/(MOLE*K)//7X,12H HF(CAL/MOL),2X, 10HH(CAL/MOL),5X,2HRB,11X,2HRC
     *,11X,2HRD,7X,12HS(CAL/MOL/K),6X,5HTU(K),4X,4HNAME    /)
      IF(INMAS.EQ.12) WRITE (6,11)
   11 FORMAT(1H0,15X,12HTABULAR DATA/12X, 4HNAME, 8X, 2HMW,6X,11HHF(CAL/
     *MOL)/15X,   78HCP(CAL/(MOL*K)),H(CAL/MOL),F(CAL/(MOL*K) GIVEN EVER
     *Y 100K FROM 100 TO 5000K     )
C     ORIGINALLY GETSPE(IEOF)

      READ(INMAS,4) IHDG
    4 FORMAT(A2)
    3 READ(INMAS,1) ISPECI,XMW,XHRF
    1 FORMAT(10X,2A4,2X,2F10.0)
      IF (ISPECI(1) .EQ. IEND) IEOF = 1

      IF (IEOF .NE. 0) GO TO 200
  150 DO 160 I=1,NWANT
         IF (IWANT(1,I) .NE. 0) GO TO 160
            DO 120 J=1,2
               IF(IWANT(J+1,I).NE.ISPECI(J)) GO TO 160
  120       CONTINUE
            MATCH = MATCH + 1
            IWANT(1,I) = MATCH
            CALL GETDAT(I)
            IF (MATCH .EQ. NWANT) GO TO 200
      GO TO 3
```

```
  160 CONTINUE

C     ORIGINALLY GETDUM(NLNGTH)

      DO 8 I=1,NLNGTH
         READ (INMAS,20100) IDUM
20100    FORMAT (A1)
    8 CONTINUE

      GO TO 3

C     ORIGINALLY CHECK(OK)

  200 DO 5 I=1,NWANT
      IF(IWANT(1,I).NE.0) GO TO 5
      WRITE(6,6)(IWANT(J,I),J=2,3)
    6 FORMAT(1HO, 39H*** NO DATA IN SPECIES MASTER FILE FOR , 2A4,
     $           4H ***
     $)
         OK = OK + 1
    5 CONTINUE

      IF(OK.EQ.0) GO TO 7
         WRITE (6,20120)
20120    FORMAT (1HO, 47H*** PROGRAM STOPPED IN OBTAIN - UNKNOWN SPECIES
     $,          14H REQUESTED ***
     $)
         STOP
    7 RETURN
      END
```

```
      SUBROUTINE OPT2  (DIAMS,NTUB,TG,AS,UTUB)
      REAL NT, NTUB
      INCLUDE BASIC
      INCLUDE HEAT
      INCLUDE ENERGY
      INCLUDE PROC1
      INCLUDE PROC3
      COMMON/BLK6/PS(JS,JP2),PPM(JS1),W,TZ
      COMMON/BLK2/TT(JS1),AKT,DR,DT,EMIVT,AMH,CPPH,TTI,HN,HO
      COMMON/BLK8/VL,PT,WT,B,DC,CC,GKT
      DIMENSION TG(JS1)
      DIMENSION TII(2),AHM(2),HH(2),CPH(2),HO(2),C(2)
      DIMENSION U(2),E(2),SUM(2),XA(2),XB(2),XC(2),TAVG(2),TTWA(2)
      DIMENSION BB(2),TTF(2),QC(2),CPEWW(2),QRR(2)
      W = 1.
      AREA=DIAMS*W
      B=DIAMS
      CT=3.1416*DT
      Y = CC / B
      Z=DC/DT
      NT = 1. / DC
      TAV=200.
      TF=500.
      TII(1)=TTI
      TII(2)=TTI
      FF = SQRT(1.+Y*Y) - Y
      IF(Z.GT.2.)GO TO 2
      FF1=1.01+0.049*Z-0.059*Z**2
      GO TO 3
    2 FF1=1.26-0.224*Z+0.0145*Z**2
    3 FF=FF*FF1
      FP=(FF*EMIV*TAU*NTUB)/(NT*B*CT)
      NIT=1
      DO 99 K=1,2
      GMAX=AM/B*DC/CC
      TZ=TII(K)
   34 CALL CPROP(TZ)
      PM(1)=PPM(1)
      T(1)=TI
      IF(K.EQ.2)T(1)=TG(NL)
      IF(K.EQ.2)PM(1)=PPM(NL)
      TAVG(K)=T(1)
   32 J=2
      IF(TAVG(K).LT.TU(M,1)) J=1
      CPEWW(K)=0.0
      DO 6 M=1,IS
      CPP=RC(M,J)+TAVG(K)*RD(M,J)+RE(M,J)/TAVG(K)**2
      NI=NL
      IF(K.EQ.1)NI=2
    6 CPEWW(K)=CPEWW(K)+PS(NI,M)*CPP
      CPG(1)=CPEWW(K)*PM(1)
      CALL PROP
      REY=DT*GMAX/VISC
      IF(REY.GT.500.)GO TO 30
      AK=0.8
```

```
      AX=0.5
      AC=1.5
      GO TO 31
   30 AR=0.3
      AX=0.4
      AC=0.65
      IF(REY.LT.3000.)AC=1.0
   31 HO(K)=AR/REY**AX*CPEWW(K)*GMAX/PR**0.667*AC
      AHM(K)=AMH
      HH(K)=HN
      CPH(K)=CPPH
      U(K)=1./(1./HH(K)+DR/AKT+1./HO(K))
      E(K)=U(K)*CT/(AHM(K)*CPH(K))
C***  CALCULATE RADIATION TERM
      SUM(K)=0.0
      N=1
      IF(K.EQ.2)N=NL+1
      DO 1 I=2,NL
    1 SUM(K)=SUM(K)+(S(I)-S(I-1))*F(I,N)*TL(I)**4
      IF(K.EQ.1)N=3
      SUM(K)=(NTUB*3.1416*DTUB*SUM(K)+AS*TL(N-1)**4)*FP/NTUB
      C(K)=CT/(AHM(K)*CPH(K))
      XA(K)=(B-U(K)*C(K)/E(K)*(B-(1.-EXP(-E(K)*B))/E(K)))
      XB(K)=(B-XA(K))*SUM(K)/U(K)+TII(K)*(1.-EXP(-E(K)*B))/E(K)
      XC(K)=2.*AM*CPEWW(K)/(CT*NT*U(K))
      IF(K.EQ.2)GO TO 4
      TAVG(K)=(XB(K)-XC(K)*TI)/(XA(K)-XC(K))
      TGI=TAVG(K)*2.-TI
      TTWA(K)=TAVG(K)-AM*CPEWW(K)*(TGI-TI)/(HO(K)*B*CT*NT)
      GO TO 20
    4 TAVG(K)=(XB(K)+XC(K)*TG(NL))/(XA(K)+XC(K))
      TGNLP=TAVG(K)*2.-TG(NL)
      TTWA(K)=TAVG(K)-AM*CPEWW(K)*(TG(NL)-TGNLP)/(HO(K)*B*CT*NT)
   20 IF(ABS(TAVG(K)-TAV).LT.1.0)GO TO 55
      TAV=TAVG(K)
      NIT=NIT+1
      GO TO 32
   55 BB(K)=(SUM(K)*U(K)/HO(K)+U(K)*TAVG(K))*CT/(AHM(K)*CPH(K))
C **  CALC. WORKING FLUID EXIT TEMP AND HEAT REMOVAL RATE
C **
      TTF(K)=(BB(K)*(1.-EXP(-E(K)*B))/E(K)+TII(K)*EXP(-E(K)*B))
      TII(2)=TTF(1)
      IF(ABS(TTF(K)-TF).LT.1.0)GO TO 33
      TF=TTF(K)
      TZ=(TTF(K)+TII(K))/2.
      GO TO 34
   33 QRR(K)=SUM(K)*CT*B
      QC(K)=AHM(K)*CPH(K)*(TTF(K)-TII(K))
   99 CONTINUE
C
      QTOT = (TTF(1)-TII(1))*AHM(1)*CPH(1)+(TTF(2)-TII(2))*AHM(2)*CPH(2)
      WRITE(6,20800)  TII(1), TII(2), TTF(1), TTF(2), QC(1), QC(2)
     $,                TGI, TG(NL), TI, TGNLP
      IF(KR7.LT.3)GO TO 50
      WRITE(6,51)HH(1),HH(2),HO(1),HO(2)
   51 FORMAT(//5X,7HHH(1)= ,E10.3,3X,7HHH(2)= ,E10.3,3X,7HHO(1)= ,E10.3,
     $3X,7HHO(2)= ,/)
```

```
   50 CONTINUE
20800 FORMAT(1H1,//,T10,38H** FOR HEAT EXCHANGER PROBLEM OPTION 2
     $,           //,T46,25HEXCHANGER 1   EXCHANGER 2
     $,            /,T15,30HCOOLANT TEMPERATURE  IN (K)  =,T47,2(F7.2,8X)
     $,            /,T15,30HCOOLANT TEMPERATURE OUT (K)  =,T47,2(F7.2,8X)
     $,            /,T15,30HTOTAL HEAT TRANSFERED TO
     $,            /,T15,30HCOOLANT (CAL/S)              =,T47,2(E9.3,6X)
     $,            /,T15,30HTEMPERATURE OF FUEL/AIR (K):
     $,            /,T15,30HUPSTREAM OF HEAT EXCHANGER   =,T47,2(F7.2,8X)
     $,            /,T15,30HDOWNSTREAM OF HEAT EXCHANGER =,T47,2(F7.2,8X)
     $)
      RETURN
      END
```

```
PROCS
BASIC PROC
      PARAMETER JP = 12
      PARAMETER  JP2 = 2 * JP
      PARAMETER  JD = JP + 1
      PARAMETER JS = 40
      PARAMETER JS1 = JS + 1
      PARAMETER  JY = 2 * JP + 4
      PARAMETER  JX = 5
 END
HEAT PROC
      REAL HAMB
      COMMON/HEAT/CH,CHM,CMH,CM
      COMMON/TRANS/ A1,A2,A3,A4,DBTW,CMSTG,BIN(JS)
      COMMON/PROPS/X(JS),PR,SC,TCOND,VISC,XNU,ST,RUD,RU
      COMMON/CHEAT/XP,XTP,VF,XNUI
      COMMON / F2 / AEM1, AEM2, DS(JS1), NL, TI, TL(JS1)
     $,             TRES(2)
     $,             S(JS1), AK, DY
      COMMON/ AMB /  HAMB(JS1), TAMBO, TAMBI
      COMMON/ TWS / TW(JS1), TW1(JS1), TW2(JS1)
      COMMON / BBB / B1 (JS1), B2 (JS1), B3 (JS1), B4 (JS1), B5 (JS1)
     $,              B6 (JS1), B7 (JS1), B8 (JS1), B9 (JS1), B10(JS1)
     $,              B11(JS1), B12(JS1), B13(JS1), B14(JS1), B15(JS1)
     $,              B16(JS1), BP3(JS1), BP5(JS1), BP6(JS1), BP7(JS1)
 END
ENERGY PROC
      COMMON/ENERGY/QCONV,QCOND,QCHEM,QRAD,QRADIN,QLOSS,AM,HW
      COMMON/VFA/EMIV,TAU,F(JS1,JS1)
      COMMON/SAVE/HEW(JP2),SPLP(JP2),PMS1,PMS2,TS1,TS2
 END
HEAT1 PROC
      COMMON/HEAT1/ITURB
      COMMON/MEAN/      XNUBXP(100),XNUB,XPP,XPPS
 END
PROF PROC
      COMMON /CARD1/   ISPECI(2), XMW, XHRF
      COMMON /IUNIT/   INMAS
      COMMON/LIN/ WM(JP)
      COMMON /WANTS/   IWANT( 3,JP), NWANT,  XALPF(JP2)
 END
PROC1 PROC
      COMMON / F1 /  FT, H, ICON, IS, ISP, ITER, KR, KR7
     $,              L, MT, MGAS, N, P, PLN
     $,              ICC, NAMB(JP), VNU(JP,JP)
     $,              ILOSS, IGEOM
      COMMON / F3 /  ALPF(JP2), BF(JP)
     $,              RT(2), SUMP(2), TSQ(2)
C
 END
PROC2 PROC
      COMMON / F4 / EAK(JX), EXK(JX), FKF(JX), PMU(JP2,JX)
     $,             RMU(JP2,JX), PHI(JP2,JX), THMU(JD,JX)
      COMMON / F5 / AH, AHH, C, CHH, DIAM, FC, ISS, SNSM
     $,             SUMH, TWT
     $,             ADSM
 END
PROC3 PROC
      COMMON / F6 /  A(JY,JY), ALPHI(JY), CPF(JP2), CPG(2)
     $,              HI(JP2), HOS(JP2), NAMA(JP), PLP(JP2)
     $,              PM(2), PP(JP2), RB(JP,2), RC(JP,2)
     $,              RD(JP,2), RE(JP,2), RF(JP,2), RHS(JY)
     $,              SB(JP2), T(2), TU(JP,2)
 END
```

```
      SUBROUTINE PROP
      INCLUDE BASIC
      INCLUDE HEAT
      INCLUDE PROF
      INCLUDE PROC1
      INCLUDE PROC3
C-----
      PMU1=0.
      PMU2=0.
      PMU3=0.
      PMU5=0.
      PMU6=0.
      CPTIL=0.
      DO 1 I=1,IS
      PMU1=PMU1+PP(I)*BF(I)
      VA=PP(I)/BF(I)
      PMU2=PMU2+VA*WM(I)
      PMU3=PMU3+VA
    1 CPTIL=CPTIL+VA*CPF(I)
      DO 2 I=1,IS
      VA=PP(I)/BF(I)
      VB=VA*WM(I)
      VC=PP(I)*BF(I)
      PMU5=PMU5+VB/(1.385-0.029*VC/PMU1)
    2 CONTINUE
      PMU6=CPTIL/1.9869+.29*PMU3
      TPMU=T(1)**.659/PMU1
      VMU=2.096E-7*TPMU*PMU5
      VISC=VMU
      TCOND=4.165E-7*TPMU*PMU6
      PR=VMU*CPG(1)/TCOND/PM(1)
      SC=PMU5/PMU2
    3 FORMAT(///' MOLECULAR TRANSPORT PROPERTIES'/10X,'TEMP =',E10.5,'K'
     *,2X,'VISC =',E10.5,' GM/CM-S',2X,'ICOND =',E10.5,' CAL/CM-S-K',2X,
     *'PR =',E10.5,2X,'SC =',E10.5)
      RETURN
      END
```

```
      SUBROUTINE PRTLIN(NAME,ARRAY,NVALS)
      DIMENSION ARRAY(1)
C------
C
      WRITE(6,20000) NAME, NVALS, (ARRAY(I),I=1,NVALS)
-20000 FORMAT(2X, A6, I4, 3X, 10E11.4, / 16X, 10E11.4)
      RETURN
      END
```

```
      SUBROUTINE READIN
C             READS IN THE CARD(S) INDICATING THE SPECIES AND
C             THE ALPF AND ALPE VALUES THE PROGRAM WILL USE
      INCLUDE BASIC
      INCLUDE PROF
      INCLUDE PROC1
      INCLUDE PROC2
      DIMENSION     ISPEC(2)
      DATA     IEND /3HEND/
C------
      JMAX = JP
      J = 1
C
      IF(IS .GT. JMAX)  GO TO 200
         WRITE(6, 10)
   10 FORMAT(1H1,15X,70H* SPECIES INITIAL MOLE FRACTIONS,FIRST GUESSES,A
     *ND DIFFUSION FACTORS *  ,/)
      WRITE (6,20090)
20090 FORMAT(/, 15X, 6HSPECIE,18X, 4HALPF, 16X, 4HALPE, 10X
     *,16HDIFFUSION FACTOR/)
      DO 160 J = 1, IS
         READ (5,20100)ISPEC,KNY,XF,XE,XBP
20100    FORMAT(2A4,I2,2E10.3,F10.4)
         WRITE(6,20120) ISPEC,XF,XE,XBP
20120    FORMAT(16X,2A4,12X,E10.3,10X,E10.3,10X,F10.4)
         DO 140 I=1,2
            IWANT(I+1,J) = ISPEC(I)
  140    CONTINUE
         XALPF(J) = XF
         XALPF(J+IS) = XE
         BF(J)=XBP
  160 CONTINUE
C
  180 NWANT = IS
      ISP = IS + 1
      ISS = 2 * IS
      GO TO 220
C
C             MORE THAN JMAX SPECIES REQUESTED
C
  200 WRITE (6,20200) JMAX
20200 FORMAT (43H0*** PROGRAM STOPPED IN READIN -- MORE THAN, I5,
     $        22H SPECIES REQUESTED ***
     $)
      STOP
  220 RETURN
      END
```

```
      SUBROUTINE RERAY(N,C,NN,D,NNN,LS,IS)
C     DIRECT INVERSION PROCEDURE  --  C IS REPLACED BY C**-1
      INCLUDE BASIC
      DIMENSION D(JY,1),SD(JY),C(JY,1),L(JY),S(JY),LL(JY),LLL(JY),LS(1)
C------
      KOUT=6
      N1=N+1
      NP=N+NN
      DO 11 I=1,NP
      LLL(I)=I
      IF(LS(1)) 113,113,112
  112 L(I)=LS(I)
      GO TO 11
  113 L(I)=I
   11 CONTINUE
      IX=-1
      IF(IS+2) 111,109,111
  106 FORMAT(11H  L(I),I=1,I3,5X,(30I3))
  107 FORMAT(15H  ((C(I,J),J=1,I3,12H),(D(J),J=1,I3, 6H),I=1,I3,15H)  BE
     1FORE RERAY)
  108 FORMAT(2X, 11E10.3/(12X, 10E10.3))
  109 WRITE(KOUT,107) NP,NNN,N
      WRITE(KOUT,106)NP,(L(I),I=1,NP)
      IX=0
      DO 110 I=1,N
  110 WRITE(KOUT,108)(C(I,J),J=1,NP),(D(I,J),J=1,NNN)
  111 IS=-1
C     TRIANGULATE MATRIX
      DO 15 I=1,N
      DO 160 M=1,NP
  160 S(M)=ABS(C(I,M))
      IF(IS) 18,16,16
   18 IS=0
      SD(1)=1.
      GO TO 12
C     REDUCE ROW I BY PRECEEDING ROWS
   16 DO 17 J=2,I
      K=L(J-1)
      DIV=-C(I,K)
      IF(DIV) 161,17,161
  161 C(I,K)=0.
      DO162 M=1,NP
      DIVC=DIV*C(J-1,M)
      S(M)=AMAX1(S(M),ABS(DIVC))
  162 C(I,M)=C(I,M)+DIVC
      IF(NNN) 17,17,163
  163 DO 164 M=1,NNN
  164 D(I,M)=D(I,M)+DIV*D(J-1,M)
   17 CONTINUE
C     SEEK MAXIMUM PIVOT
   12 DIV=0.
      K=L(I)
      J=I
      DO 13 JJ=I,N
      M=L(JJ)
```

```
      IF(ABS (C(I,M))-DIV)13,13,121
  121 DIV=ABS (C(I,M))
      K=M
      J=JJ
   13 CONTINUE
      SD(I)=DIV/S(K)
      L(J)=L(I)
      L(I)=K
      IF(SD(I)-1.E-8) 131,131,14
C     SINGULAR MATRIX RETURN
  131 IS=-I
      WRITE(KOUT,132) I,K
      C(I,K)=1.E+30
      S(K)=1.0
      GO TO 12
  132 FORMAT(115X,2I3)
   14 DIV=C(I,K)
      C(I,K)=1.0
      K=LLL(J)
      LLL(J)=LLL(I)
      LLL(I)=K
      LL(K)=I
C     NORMALIZE ROW
      IF(NNN) 143,143,141
  141 DO 142 J=1,NNN
  142 D(I,J)=D(I,J)/DIV
  143 DO 15 J=1,NP
   15 C(I,J)=C(I,J)/DIV
      IF(IX) 152,150,152
  151 FORMAT(24H PIVOT ROW/COL/RES,RATIO 5(I4,1H/I3,1H/E9.2,1H,))
  150 WRITE(KOUT,151) (I,L(I),SD(I),I=1,NP)
C     DIAGONALIZE MATRIX
  152 NM=N-1
      DO 20 I=1,NM
      K=L(I+1)
      DO 20 J=1,I
      DIV=-C(J,K)
      IF(DIV)19,20,19
   19 C(J,K)=0.
      IF(NNN) 191,191,192
  192 DO 193 M=1,NNN
  193 D(J,M)=D(J,M)+DIV*D(I+1,M)
  191 DO 201 M=1,NP
  201 C(J,M)=C(J,M)+DIV*C(I+1,M)
   20 CONTINUE
C     INTERCHANGE COLUMNS
      DO 30 II=1,NP
      I=II
   21 J=L(I)
      L(I)=I
      IF(J-I)22,30,22
   22 IF(IS)25,23,25
   23 DO 24 M=1,N
      S(M)=C(M,I)
   24 C(M,I)=C(M,J)
      IS=I
      I=J
```

```
      GO TO 21
   25 IF(IS-J)26,28,26
   26 DO 27 M=1,N
   27 C(M,I)=C(M,J)
      I=J
      GO TO 21
   28 DO 29 M=1,N
   29 C(M,I)=S(M)
      IS=0
   30 CONTINUE
C     INTERCHANGE ROWS
      DO 40 II=1,N
      I=II
   31 J=LL(I)
      LL(I)=I
      IF(J-I)32,40,32
   32 IF(IS)35,33,35
   33 DO 34 M=1,NP
      S(M)=C(I,M)
   34 C(I,M)=C(J,M)
      IF(NNN) 343,343,341
  341 DO 342 M=1,NNN
      SD(M)=D(I,M)
  342 D(I,M)=D(J,M)
  343 IS=I
      I=J
      GO TO 31
   35 IF(IS-J)36,38,36
   36 DO 37 M=1,NP
   37 C(I,M)=C(J,M)
      IF(NNN) 373,373,371
  371 DO 372 M=1,NNN
  372 D(I,M)=D(J,M)
  373 I=J
      GO TO 31
   38 DO 39 M=1,NP
   39 C(I,M)=S(M)
      IF(NNN) 393,393,391
  391 DO 392 M=1,NNN
  392 D(I,M)=SD(M)
  393 IS=0
   40 CONTINUE
      IF(IX) 411,409,411
  407 FORMAT(15H  ((C(I,J),J=1,I3,12H),(D(J),J=1,I3, 6H),I=1,I3,15H)  AF
     1TER RERAY  )
  409 WRITE(KOUT,407) NP,NNN,N
      DO 410 I=1,N
  410 WRITE(KOUT,108)(C(I,J),J=1,NP),(D(I,J),J=1,NNN)
  411 RETURN
      END
```

```
      SUBROUTINE STNPRT(TG,QQ)
      INTEGER PAGES
      INCLUDE BASIC
      INCLUDE HEAT
      INCLUDE PROC1
      INCLUDE PROC2
      INCLUDE PROC3
      COMMON/BLK2/TT(JS1),AKT,DR,DT,EMIVT,AMH,CPPH,TTI,HN,HO
      COMMON/BLK6/PS(JS,JP2),PPM(JS1),W,TZ
      COMMON/BK3/PX(JS,JP2)
      COMMON/BK4/HHO(JS1),TTW(JSI)
      DIMENSION TG(1), QQ(1)
C-----
      ITEMS = 10
      PAGES = (NL + ITEMS - 2) / ITEMS
      DO 300 I = 1, PAGES
         IEND = I * ITEMS + 1
         IBGN = IEND - ITEMS + 1
         IEND = AMIN1(IEND,NL)
         WRITE(6,20100)
         WRITE(6,20120) (S(J),J=IBGN,IEND)
         WRITE(6,20140) (TG(J),J=IBGN,IEND)
         WRITE(6,20145) (TL(J),J=IBGN,IEND)
C
         WRITE(6,20150)
         DO 200 K = 1, IS
         WRITE(6,20160)NAMA(K),(PX(J,K),J=IBGN,IEND)
  200    CONTINUE
C
         WRITE(6,20165)
         DO 250 K = ISP, ISS
         WRITE(6,20160)NAMA(K-IS),(PX(J,K),J=IBGN,IEND)
  250    CONTINUE
C
         IF(IGEOM.EQ.3 .OR. (IGEOM.EQ.0 .AND. ILOSS.EQ.0)) GO TO 300
         WRITE(6,20170) (TT(J),J=IBGN,IEND)
      WRITE(6,20172) (TTW(J),J=IBGN,IEND)
         WRITE(6,20175) (QQ(J),J=IBGN,IEND)
  300 CONTINUE
C
20100 FORMAT(1H1,//, T24,62HAXIAL  DISTANCE  ALONG  MONOLITH , CYLINDER
     $ OR PLATE   S (CM)          )
20120 FORMAT(//,T20, 10(F7.3,3X) )
20140 FORMAT(//,T4,13HBULK TEMP (K), T20, 10(1X,F6.1,3X) )
20145 FORMAT(//,T4,13HWALL TEMP (K), T20, 10(1X,F6.1,3X) )
20150 FORMAT(//,T4,13HMOLE FRACTION
     $       //,T8,12HBULK SPECIES , / )
20160 FORMAT(/,T11,A4,5X,    10(2X,F7.5,1X) )
20165 FORMAT(//,T8,12HWALL SPECIES , / )
20170 FORMAT(//,T4, 7HCOOLANT
     $,       /,T4,10HTEMP   (K), T20, 10(1X,F7.2,2X) )
20172 FORMAT(//,T4,12HCOOLANT TUBE
     *,       /,T4, 10HTEMP   (K),T20, 10(1X,F7.2,2X) )
20175 FORMAT(//,T4,12HHEAT LOSS TO
C             /,T4,15HCOOLANT (CAL/S), T20,10(G10.4))
      RETURN
      END
```

```
      SUBROUTINE TERMS (B3,B4,B5,B6,B7,TW,TW2,I,ARG)
      DIMENSION B3(1), B4(1), B5(1), B6(1), B7(1)
      DIMENSION TW(1), TW2(1), ARG(4)
C
C------
      ARG(1) = B3(I+1)
      ARG(2) = - B4(I+1)
      ARG(3) = B5(I+1)
      ARG(4) = - (TW(I+1) * B6(I+1) + B7(I+1))
C
      IF(I .NE. 1)  GO TO 100
         ARG(1) = 0.
         ARG(2) = ARG(2) + B3(I+1)
         GO TO 200
  100 IF(I .NE. NEQU)  GO TO 200
         ARG(2) = ARG(2) + B5(I+1)
         ARG(3) = 0.
  200 CONTINUE
C
      RETURN
      END
```

```
      SUBROUTINE TRID (SUB,DIAG,SUP,B,N)
C     ******************************************************************
C     *                                                                *
C     *                                                                *
C     * SUBROUTINE TRID SOLVES SYSTEMS OF TRIDIAGONAL LINEAR EQUATIONS *
C     * OF THE FORM                                                    *
C     *           SUB(K)*X(K-1)+DIAG(K)*X(K)+SUP(K)*X(K+1)=B(K)        *
C     * BY THE THOMAS ALGORITHM                                        *
C     *                                                                *
C     * DESCRIPTION OF THE ARGUMENTS                                   *
C     *                                                                *
C     *    SUB      - THE N - 1 SUBDIAGONAL COEFFICIENTS               *
C     *    DIAG     - THE N DIAGONAL COEFFICIENTS                      *
C     *    SUB      - THE N - 1 SUPRADIAGONAL COEFFICIENTS             *
C     *    B        - INPUT - THE N RIGHT-HAND SIDE CONSTANTS          *
C     *               OUTPUT- THE CALCULATED VALUES OF THE N UNKNOWNS  *
C     *    N        - THE NUMBER OF EQUATIONS                          *
C     *                                                                *
C     *                                                                *
C     ******************************************************************
C
      DIMENSION SUB(N),DIAG(N),SUP(N),B(N)
      IF(N.GT.1)GO TO 10
C
C     SOLUTION FOR N = 1 (A SINGLE EQUATION)
C
      B(1)=B(1)/DIAG(1)
      RETURN
C
C     ELIMINATION OF TRIDIAGONAL SYSTEM
C
10    DO 11 K=2,N
      RATIO = -SUB(K)/DIAG(K-1)
      DIAG(K)=DIAG(K)+RATIO*SUP(K-1)
   11 B(K)= B(K) + RATIO*B(K-1)
C
C     BACK SUBSTITUTION
C
      B(N)= B(N)/DIAG(N)
      K=N
      DO 12 I=2,N
      K=K-1
   12 B(K)=(B(K)-SUP(K)*B(K+1))/DIAG(K)
      RETURN
      END
```

```
      SUBROUTINE TRIDM
      INCLUDE BASIC
      INCLUDE HEAT
      INCLUDE PROC1
      INCLUDE PROC2
C
      DIMENSION SUB(JS1), DIAG(JS1), SUP(JS1), B(JS1)
      DIMENSION ARG(4)
C------
      NEQU = NL - 1
C
      DY2 = DY * DY / 4.0
C
      DO 100 I = 1, NEQU
         CALL TERMS(B3,B4,B5,B6,B7,TW,TW2,I,ARG)
         SUB(I) = ARG(1)
         DIAG(I)= ARG(2)
         SUP(I) = ARG(3)
         B(I)   = ARG(4)
C
  100 CONTINUE
C
      CALL TRID(SUB,DIAG,SUP,B,NEQU)
C
      DO 200 I = 1, NEQU
         TW2(I+1) = B(I)
         TW1(I+1) = TW(I+1) * (2.0+B1(I+1)+B2(I+1)) - TW2(I+1) -
     $              B1(I+1) * TW(I) - TW(I+2) * B2(I+1)
  200 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE VIEW (DIAM,NL,S,F)
      INCLUDE BASIC
      DIMENSION S(JS),F(JS1,JS1),D(JS1,JS1)
      NLP=NL+1
      NLL=NL-1
      R=DIAM/2.
      J=1
    1 DO 2 I=J,NL
      Z=((S(I)-S(J))/R)**2+2.
      IF (Z-1000.) 9,9,10
    9 D(I,J)=(Z-SQRT(Z*Z-4.))/2.
      GO TO 7
   10 D(I,J)=1./Z
    7 D(J,I)=D(I,J)
    2 CONTINUE
      J=J+1
      IF (J-NL) 1,1,3
    3 J=2
      F(2,2)=1.0
    4 DS=ABS(S(J)-S(J-1))/DIAM*4.
      DO 5 I=J,NLL
      DSS=ABS(S(I+1)-S(I))/DIAM*4.
      F(J,I+1)=(D(J,I)-D(J,I+1)-D(J-1,I)+D(J-1,I+1))/DS
      F(I+1,J)=F(J,I+1)*DS/DSS
    5 CONTINUE
      J=J+1
      F(J,J)=1.0
      IF (J-NL) 4,6,6
    6 DO 8 I=2,NL
      DS=ABS(S(I)-S(I-1))/DIAM*4.
      F(I,1)=(D(1,I-1)-D(1,I))/DS
      F(I,NLP)=(D(NL,I)-D(NL,I-1))/DS
      DO 8 J=1,NLP
      IF (I.EQ.J) GO TO 8
      F(I,I)=F(I,I)-F(I,J)
    8 CONTINUE
      IF(KR7.LE.3)GO TO 14
      DO 12 I=2,NL
   12 WRITE(6,13) (F(I,J),J=1,NLP)
   13 FORMAT (8X,10E10.5)
   14 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE VIEW1(DIAMC,DT)
      INCLUDE BASIC
      INCLUDE ENERGY
      INCLUDE HEAT
      COMMON/BLK1/      FL(JS1,JS1),QR1(JS1),QR2(JS1)
      DIMENSION FM(JS1),FQ(JS1),FP(JS1),AAN(JS1)
      RR=DIAMC/DT
      PI=3.1416
      DO 40 J=2,NL
      AL=(S(J)-S(J-1))/DT*2.
      SL=AL**2
      SR=RR**2
      AB=AL**2+SR-1.
      BB=SL-SR+1.
      AN=PI*DIAMC*(S(J)-S(J-1))
      ANP=PI*DT*(S(J)-S(J-1))
      AA=PI*(DIAMC**2-DT**2)/4.
      AAN(J)=AN
      CI=1.-1./RR+2./(PI*RR)*ATAN(2./AL*SQRT(SR-1.))
      C2=SQRT(4.*SR+SL)/AL
      C3=(4.*(SR-1.)+(SL/SR)*(SR-2.))/(SL+4.*(SR-1.))
      C4=(SR-2.)/SR
      C5=SQRT((AB+2.)**2-4.*SR)
      F(J,J)=CI-AL/(2.*PI*RR)*(C2*ASIN(C3)-ASIN(C4)+(C2-1.)*PI/2.)
      FL(J,J)=1./RR-1./(PI*RR)*(ACOS(BB/AB)-1./(2.*AL)*(C5*ACOS(BB/(RR*A
     1B))+BB*ASIN(1./RR)-PI*AB/2.))
      FM(J)=0.5*(1.-F(J,J)-FL(J,J))
      FQ(J)=0.5*ANP/AA*(1.-AN/ANP*FL(J,J))
      FP(J)=1.-FM(J)*AAN(J)/AA-FQ(J)
   40 CONTINUE
      DO 41 J=2,NL
      NLP=NL+1
      JJ=J+1
      JM=J-1
      DO 42 K=2,NL
      KP=K+1
      IF(K.EQ.J)GO TO 42
      F(J,K)=FM(J)*FM(K)*AAN(K)/AA
      FL(J,K)=FM(J)*FQ(K)
      IF(K.GT.JJ)GO TO 43
      IF(K.LT.JM)GO TO 44
      GO TO 42
   43 PP=1.0
      KM=K-1
      DO 45 N=JJ,KM
   45 PP=PP*FP(N)
      F(J,K)=F(J,K)*PP
      FL(J,K)=FL(J,K)*PP
      GO TO 42
   44 PP=1.0
      DO 46 N=KP,JM
   46 PP=PP*FP(N)
      F(J,K)=F(J,K)*PP
      FL(J,K)=FL(J,K)*PP
   42 CONTINUE
```

```
      PP=1.0
      IF(J.EQ.NL)GO TO 60
      DO 47 N=JJ,NL
   47 PP=PP*FP(N)
   60 F(J,NLP)=FM(J)*PP
      QR2(J)=FQ(J)*PP
      PP=1.0
      IF(J.EQ.2)GO TO 61
      DO 48 N=2,JM
   48 PP=PP*FP(N)
   61 F(J,1)=FM(J)*PP
      QR1(J)=FQ(J)*PP
   41 CONTINUE
      IF(KR7.LE.3)GO TO 1
      WRITE(6,51)
   51 FORMAT(//10X,'    WALL TO WALL VIEW FACTORS    '//)
      DO 49 J=2,NL
   49 WRITE(6,50) (F(J,K),K=1,NLP)
   50 FORMAT(10X,10F10.3)
      WRITE(6,53)
   53 FORMAT(//10X,'    WALL TO TUBE VIEW FACTORS    '//)
      DO 52 J=2,NL
   52 WRITE(6,50) (FL(J,K),K=1,NLP)
    1 CONTINUE
      ARAT=DIAMC*DIAMC/4.0/DT
      DO 65 J=2,NL
      ZDS=(S(J)-S(J-1))*DIAMC/DT
      DO 64 K=2,NL
   64 FL(J,K)=FL(J,K)*ZDS/(S(K)-S(K-1))
      QR1(J)=QR1(J)*ARAT/(S(J)-S(J-1))
   65 QR2(J)=QR2(J)*ARAT/(S(J)-S(J-1))
      RETURN
      END
```

APPENDIX A

BRIEF DEVELOPMENT AND DEMONSTRATION OF BIFURCATION APPROXIMATIONS TO DIFFUSION COEFFICIENTS

Because the development of the set of transport relations used in this code is not in the readily available combustion literature, it is appropriate to include a brief summary of the development in this report.

The formulation derives much of its utility from the simplification introduced when binary diffusion coefficients are approximated with the bifurcation relations. These are

$$D_{ij} = \frac{\bar{D}}{F_i F_j} \tag{A-1}$$

where the F_i are diffusion factors for individual species which are independent of the system of species involved. They could be temperature dependent but this flexibility is rarely justified. The accuracy of the approximation has been tested for a variety of systems. Two examples taken from Reference 3 are shown in Tables A-1 and A-2. These results are typical when good (and consistent) sets of diffusion data are correlated. Note that these particular correlations have arbitrarily taken F_{O_2} as 1.0 to anchor an otherwise floating correlation.

In order to develop an explicit flux relationship using this approximation, it is appropriate to start with the Stefan-Maxwell relation

$$\frac{\partial x_i}{\partial s} = \sum_j \frac{x_i x_j}{\rho \mathcal{D}_{ij}} \left[\frac{j_j + D_j^T \left(\frac{\partial \ell n\, T}{\partial s} \right)}{K_j} - \frac{j_i + D_i^T \left(\frac{\partial \ell n\, T}{\partial s} \right)}{K_i} \right] \tag{A-2}$$

TABLE A-1. CORRELATION OF BINARY DIFFUSION COEFFICIENTS FOR A HYDROGEN-OXYGEN SYSTEM USING PRESENT METHOD

TEMPERATURE = 12,000°R, PRESSURE = 1 ATM

Species i	Species j	$\mathcal{D}_{ij}$ From Kinetic Theory (ft^2/sec) x 100	F_i	$\mathcal{D}_{ij}$ From Present Correlation (ft^2/sec) x 100	Error Using Present Correlation (Percent)	Error If All $\mathcal{D}_{ij}$ Are Assumed Equal (Percent)
			(a) Diffusion coefficients calculated using Lennard-Jones potential with force data from Svehla (Ref. 14)			
H	H2	36.0260	0.24713	53.1613	47.6	- 63.1
H	H2O	25.9891		23.7639	- 8.6	- 48.9
H	O	26.6238		24.7360	- 7.1	- 50.1
H	O2	22.8038		19.7757	-13.3	- 41.7
H	OH	26.4341		24.3147	- 8.0	- 49.7
H2	H2O	17.3862	0.3720	15.7877	- 9.2	- 23.5
H2	O	17.7166		16.4335	- 7.2	- 24.9
H2	O2	15.0085		13.1381	-12.5	- 11.4
H2	OH	17.5759		16.1537	- 8.1	- 24.4
H2O	O	7.0928	0.8322	7.3461	3.6	87.4
H2O	O2	5.2795		5.8730	11.2	151.6
H2O	OH	6.9078		7.2210	4.5	92.4
O	O2	5.6458	0.7995	6.1132	8.3	135.4
O	OH	7.2643		7.5163	3.5	82.9
O2	OH	5.4946	1.0000	6.0091	9.4	141.9
OH			0.8133			
Average Absolute Error					10.8	68.6
			(b) Diffusion coefficients calculated using values for collision cross-sections suggested by Svehla (Ref. 15)			
H	H2	67.6000	0.2208	74.4024	10.1	- 77.1
H	H2O	28.3200		27.0030	- 4.7	- 45.4
H	O	27.7200		30.8482	11.3	- 44.3
H	O2	24.5500		22.5734	- 8.1	- 37.1
H	OH	29.5900		27.5549	- 6.9	- 47.8
H2	H2O	19.5800	0.3034	19.6568	0.4	- 21.1
H2	O	23.6000		22.4560	- 4.8	- 34.5
H2	O2	17.1900		16.4323	- 4.4	- 10.1
H2	OH	20.1600		20.0586	- 0.5	- 23.3
H2O	O	8.2950	0.8360	8.1500	- 1.7	86.3
H2O	O2	5.7150		5.9638	4.4	170.4
H2O	OH	7.1450		7.2799	1.9	116.3
O	O2	6.8500	0.7317	6.8131	- 0.5	125.6
O	OH	8.6060		8.3166	- 3.4	79.6
O2	OH	5.5520	1.0000	6.0857	9.6	178.3
OH			0.8192			
Average Absolute Error					4.8	73.1

TABLE A-2. CORRELATION OF BINARY DIFFUSION COEFFICIENTS FOR AN OXYGEN-NITROGEN-CARBON-HYDROGEN SYSTEM BASED ON DATA OF SVEHLA (Refs. 14 and 15)

TEMPERATURE = 12,000°R, PRESSURE = 1 ATM

Species i	Species j	$\mathcal{D}_{ij}$ From Kinetic Theory (ft^2/sec) x 100	F_i	$\mathcal{D}_{ij}$ From Present Correlation (ft^2/sec) x 100	Error Using Present Correlation (Percent)	Error If All $\mathcal{D}_{ij}$ Are Assumed Equal (Percent)
O	O2	6.8500	0.7393	6.0528	-11.6	- 4.5
O	N	7.3372		7.6554	4.3	- 10.8
O	N2	5.3995		5.6277	4.2	21.1
O	CO	5.4662		5.6846	4.0	19.7
O	CO2	4.4638		4.6277	3.7	46.5
O	C	8.0754		8.3865	3.9	- 19.0
O	C3	5.1820		5.3597	3.4	26.2
O	CN	5.3620		5.5958	4.4	22.0
O	H	27.7200		29.8130	7.6	- 76.3
O	H2	23.6000		20.4311	-13.4	- 72.2
O	H2O	8.2950		7.5057	- 9.5	- 21.1
O	OH	8.6060		7.7923	- 9.5	- 24.0
O	CH4	5.8190		6.0848	4.6	12.4
O	C2H	4.8947		5.0977	4.1	33.6
O	HCN	4.8625		5.0401	3.7	34.5
O2	N	5.6566	1.0000	5.6595	0.1	15.6
O2	N2	3.9611		4.1604	5.0	65.1
O2	CO	4.0028		4.2025	5.0	63.4
O2	CO2	3.1637		3.4212	8.1	106.7
O2	C	6.3129		6.2000	- 1.8	3.6
O2	C3	3.7100		3.9624	6.8	76.3
O2	CN	3.9623		4.1369	4.4	65.1
O2	H	24.5500		22.0402	-10.2	- 73.5
O2	H2	17.1900		15.1043	-12.1	- 62.0
O2	H2O	5.7150		5.5489	- 2.9	14.5
O2	OH	5.5520		5.7607	3.8	17.8
O2	CH4	4.4735		4.4984	0.6	46.2
O2	C2H	3.6310		3.7686	3.8	80.1
O2	HCN	3.5678		3.7260	4.4	83.3
N	N2	5.4277	0.7907	5.2620	- 3.1	20.5
N	CO	5.4763		5.3153	- 2.9	19.4
N	CO2	4.5136		4.3270	- 4.1	44.9
N	C	7.9727		7.8416	- 1.6	- 17.9
N	C3	5.2069		5.0115	- 3.8	25.6
C	CN	5.3784		5.2323	- 2.7	21.6
N	H	25.5139		27.8700	9.3	- 74.4
N	H2	17.1218		19.1036	11.6	- 61.8
N	H2O	6.9743		7.0181	0.6	- 6.2
N	OH	7.1732		7.2861	1.6	- 8.8
N	CH4	5.7836		5.6895	- 1.6	13.1
N	C2H	4.9083		4.7665	- 2.9	33.3
N	HCN	4.8645		4.7126	- 3.1	34.5

TABLE A-2. Continued

Species i	Species j	$\mathcal{D}_{ij}$ From Kinetic Theory (ft^2/sec) x 100	F_i	$\mathcal{D}_{ij}$ From Present Correlation (ft^2/sec) x 100	Error Using Present Correlation (Percent)	Error If All $\mathcal{D}_{ij}$ Are Assumed Equal (Percent)
N2	CO	3.8943	1.0756	3.9074	0.3	68.0
N2	CO2	3.1114		3.1809	2.2	110.2
N2	C	6.0528		5.7645	- 4.8	8.1
N2	C3	3.6214		3.6840	1.7	80.6
N2	CN	3.8603		3.8463	- 0.4	69.4
N2	H	21.3750		20.4922	- 4.1	- 69.4
N2	H2	14.1671		14.0435	- 0.9	- 53.8
N2	H2O	5.0300		5.1591	2.6	30.0
N2	OH	5.2629		5.3561	1.8	24.3
N2	CH4	4.3182 -		4.1824	- 3.1	51.5
N2	C2H	3.5367		3.5039	- 0.9	84.9
N2	HCN	3.4655		3.4643	- 0.0	84.8
CO	CO2	3.1390	1.0647	3.2131	2.4	99.2
CO	C	6.1194		5.8229	- 4.8	9.9
CO	C3	3.6584		3.7213	1.7	72.0
CO	CN	3.8938		3.8853	- 0.2	64.8
CO	H	21.6122		20.6996	- 4.2	- 66.9
CO	H2	14.2296		14.1856	- 0.3	- 50.4
CO	H2O	5.1001		5.2113	2.2	27.1
CO	OH	5.3305		5.4103	1.5	22.3
CO	CH4	4.3595		4.2248	- 3.1	51.5
CO	C2H	3.5680		3.5394	- 0.8	80.9
CO	HCN	3.5023		3.4994	- 0.1	82.9
CO2	C	4.9902	1.3079	4.7402	- 5.0	35.0
CO2	C3	2.8753		3.0294	5.4	111.3
CO2	CN	3.1245		3.1629	1.2	102.4
CO2	H	18.4881		16.8510	- 8.9	- 59.4
CO2	H2	12.2917		11.5481	- 6.0	- 39.1
CO2	H2O	4.1217		4.2424	2.9	58.7
CO2	OH	4.3441		4.4044	1.4	50.6
CO2	CH4	3.5835		3.4393	- 4.0	82.5
CO2	C2H	2.8685		2.8813	0.4	128.0
CO2	HCN	2.7965		2.8488	1.9	133.9
C	C3	5.7767	0.7218	5.4901	- 5.0	13.2
C	CN	6.0033		5.7319	- 4.5	8.9
C	H	26.1719		30.5380	16.7	- 75.0
C	H2	18.0635		20.9280	15.9	- 63.8
C	H2O	7.5630		7.6883	1.7	- 13.5
C	OH	7.9334		7.9818	0.6	- 17.5
C	CH4	6.3330		6.2328	- 1.6	3.3
C	C2H	5.3831		5.2217	- 3.0	21.5
C	HCN	5.3406		5.1626	- 3.3	22.5

TABLE A-2. Concluded

Species i	Species j	$\mathcal{D}_{ij}$ From Kinetic Theory (ft^2/sec) x 100	F_i	$\mathcal{D}_{ij}$ From Present Correlation (ft^2/sec) x 100	Error Using Present Correlation (Percent)	Error If All $\mathcal{D}_{ij}$ Are Assumed Equal (Percent)
C3	CN	3.6276	1.1293	3.6632	1.0	80.3
C3	H	21.0069		19.5166	- 7.1	- 68.9
C3	H2	13.9792		13.3749	- 4.3	- 53.2
C3	H2O	4.8271		4.9135	1.8	35.5
C3	OH	5.0416		5.1011	1.2	29.7
C3	CH4	4.1210		3.9833	- 3.3	58.7
C3	C2H	3.3265		3.3371	0.3	96.6
C3	HCN	3.2583		3.2994	1.3	100.7
CN	H	20.9403	1.0817	20.3763	- 2.7	- 68.8
CN	H2	13.8853		13.9641	0.6	- 52.9
CN	H2O	4.9948		5.1300	2.7	30.9
CN	OH	5.2299		5.3259	1.8	25.1
CN	CH4	4.2953		4.1588	- 3.2	52.3
CN	C2H	3.5330		3.4841	- 1.4	85.1
CN	HCN	3.4626		3.4447	- 0.5	88.9
H	H2	67.6000	0.2030	74.3967	10.1	- 90.4
H	H2O	28.3200		27.3309	- 3.5	- 76.9
H	OH	29.5900		28.3745	- 4.1	- 78.0
H	CH4	20.3467		22.1568	8.9	- 68.0
H	C2H	18.6611		18.5624	- 0.5	- 64.9
H	HCN	18.8560		18.3525	- 2.7	- 65.3
H2	H2O	19.5800	0.2963	18.7301	- 4.3	- 66.7
H2	OH	20.1600		19.4453	- 3.5	- 67.6
H2	CH4	13.7590		15.1843	10.4	- 52.4
H2	C2H	12.5045		12.7210	1.7	- 47.7
H2	HCN	12.5953		12.5771	- 0.1	- 48.1
H2O	OH	7.1450	0.8064	7.1436	- 0.0	- 8.5
H2O	CH4	5.4665		5.5782	2.0	19.6
H2O	C2H	4.5559		4.6733	2.6	43.6
H2O	HCN	4.5242		4.6205	2.1	44.6
OH	CH4	5.6987	0.7767	5.7912	1.6	14.8
OH	C2H	4.7817		4.8517	1.5	36.8
OH	HCN	4.7388		4.7969	1.2	38.0
CH4	C2H	3.9244	0.9948	3.7886	- 3.5	66.7
CH4	HCN	3.8677		3.7457	- 3.2	69.1
C2H	HCN	3.1729	1.1874	3.1381	- 1.1	106.1
HCN			1.2009			
Average Absolute Error					3.7	50.9

where x_i is the mole fraction of species i, T is the temperature, $\mathcal{D}_{ij}$ is the binary diffusion coefficient for species i and j, and D_i^T is the multicomponent thermal diffusion coefficient for species i. Substituting the approximation for binary diffusion coefficients (Eq. A-1) into the Stefan-Maxwell relation (Eq. A-2) and rewriting in terms of mass fractions, Y_i yields

$$\frac{\partial X_i}{\partial s} = \frac{M^2}{\rho \bar{D}} \left(\frac{Y_i F_i}{M_i} \sum_j \frac{J_j F_j}{M_j} - \frac{F_i J_i}{M_i} \sum_j \frac{Y_i F_j}{M_j} \right) \qquad \text{(A-3)}$$

where, for convenience, a total diffusion mass flux has been defined as the sum of the molecular and thermal diffusional fluxes.

$$J_i = j_i + D_i^T \left(\frac{\partial \ln T}{\partial s} \right) \qquad \text{(A-4)}$$

Multiplying each side of Eq. (A-3) by M_i/F_i, summing over all i, and noting that the sum of the diffusive fluxes is zero and the sum of the mass fractions is unity yields:

$$\sum_J \frac{J_j F_j}{M_j} = \frac{\rho \bar{D}}{M^2} \sum_i \frac{M_i}{F_i} \frac{\partial X_i}{\partial s} \equiv \frac{\rho \bar{D}}{M^2} \sum_j \frac{M_j}{F_j} \frac{\partial X_i}{\partial s} \qquad \text{(A-5)}$$

Substituting Eq. (A-5) into Eq. (A-3) results in

$$\frac{\partial X_i}{\partial s} = \frac{Y_i F_i}{M_i} \sum_j \frac{M_j}{F_j} \frac{\partial X_j}{\partial s} - \frac{M^2}{\rho \bar{D}} \frac{F_i J_i}{M_i} \sum_j \frac{Y_j F_j}{M_j} \qquad \text{(A-6)}$$

At this point is is convenient to define several new quantities.

$$\mu_1 \equiv \sum_j X_j F_j \qquad \text{(A-7)}$$

$$\mu_2 \equiv \sum_j M_j X_j / F_j \qquad \text{(A-8)}$$

$$\mu_4 \equiv \sum_j (Y_i / F_j^2)\ (dF_j/dT) \qquad \text{(A-9)}$$

Taking the derivitor of Eq. A-8 yields

$$\frac{d\mu_2}{ds} = \sum \frac{M_j}{F_j} \frac{dX_j}{ds} = M \sum_M \frac{M_j X_j}{F_j^2} \frac{dF_j}{dT} \frac{dT}{ds} \qquad \text{(A-10)}$$

Introducing Equations A-7 through A-10 into A-6 yields after some rearranging

$$J_i + \frac{D_i^T}{T} \frac{\partial T}{\partial s} = -\frac{\rho \bar{D}}{\mu_1 F_i} \left\{ \frac{dY_i}{ds} + \frac{Y_i}{M} \left[\frac{dM}{ds} - F_i \frac{d\mu_2}{ds} - F_i M \mu_4 \frac{dT}{ds} \right] \right\} \qquad \text{(A-11)}$$

The variation of F_i with temperature as determined with a nine component system over a range from 4000° to 16000°R in Reference 3 were found to rarely exceed 0.1%. Consequently μ_4 has been taken as zero and a universal set of F_i determined for all species. Correlations of these values with molecular weight have been reasonably good as indicated in Figure A-1. The correlating equation

$$F_i = \left(\frac{M_i}{26} \right)^{0.461} \qquad \text{(A-12)}$$

is recommended when specific values of F_i are not available from other correlations. It is apparent that $\bar{D}$ must represent the temperature and pressure dependence of the $\mathcal{D}_{ij}$. Although $\bar{D}$ need have no specific relation to a real diffusion coefficient, the arbitrary choice of F_{O_2} as 1.0 prompts the interpretation of $\bar{D}$ as the self

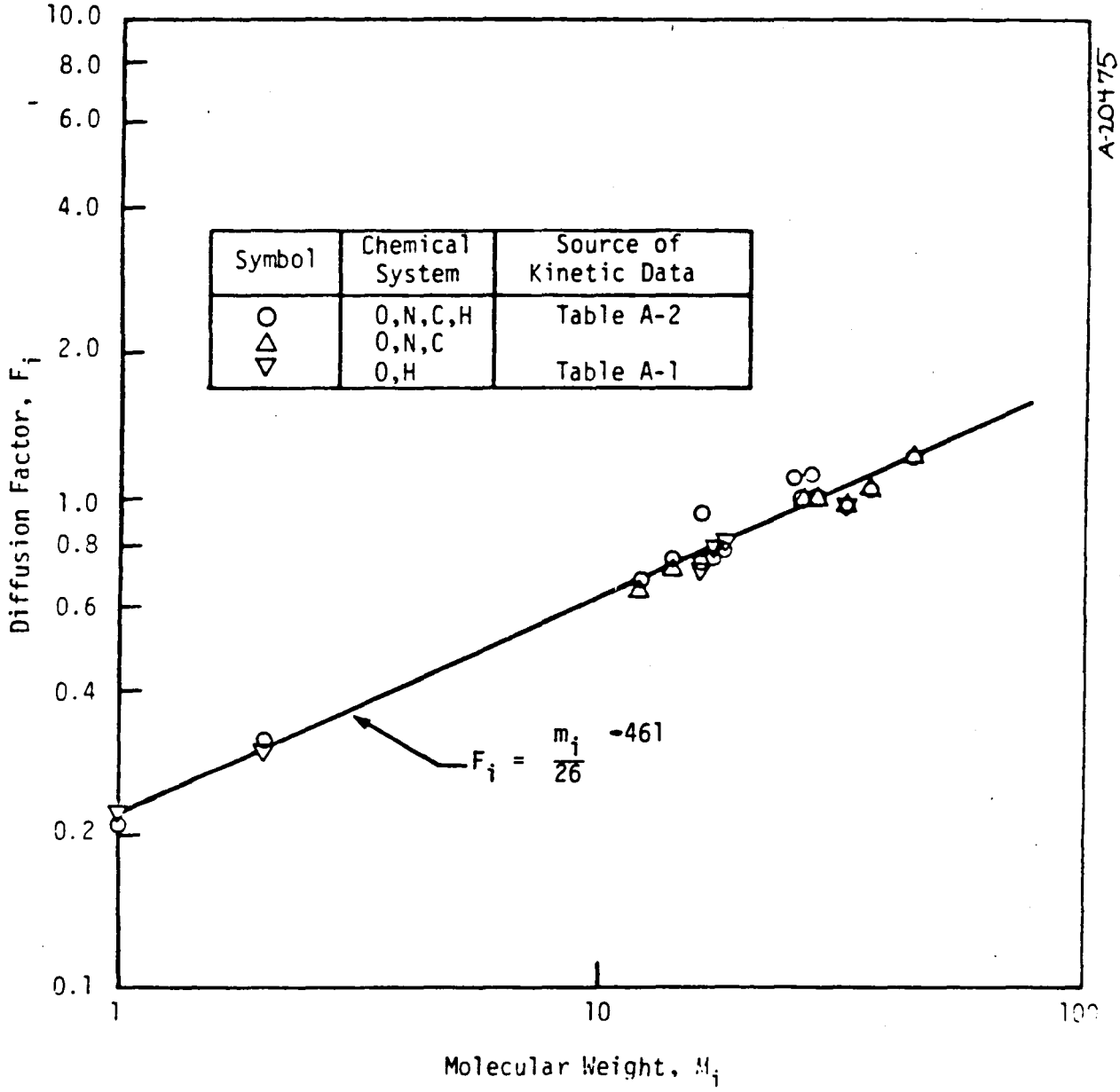

Figure A-1. Correlation of diffusion factors with molecular weight.

diffusion coefficient of O_2, $\mathcal{D}_{O_2,\,O_2}$. This would force a precise fit of the correlation to $\mathcal{D}_{O_2,\,O_2}$ but would not in general provide the best overall correlation. Ignoring this caveat we can evaluate $\mathcal{D}_{O_2,O_2}$ from the equation of Reference 4 as given by Equation 7 of the text:

$$\bar{D} = 2.628 \times 10^{-3} \frac{T(T/M_{ref})^{1/2}}{P\sigma^2_{ref}\Omega_{ij}^{(1,1)*}} \quad (cm^2/sec) \qquad (A\text{-}13)$$

with T in °K, P in atmospheres, and collision cross section, σ in Å. For O_2 as the reference species, σ is equal to 3.467 Å. Using the data from Reference 4, Figure A-2 demonstrates that the integral expression for transport properties is approximated by:

$$\Omega_{ij}^{(1,1)*} \approx 1.07\ [T/(\varepsilon/k)]^{-0.159}$$

where the maximum energy of attraction function, ε/k, for O_2 is 106.7 and thus:

$$\bar{D} = 0.172 \times 10^{-4}\ T^{1.659}/P\ (cm^2/sec) \qquad (A\text{-}14)$$

The extension of this correlation to thermal conductivity is fully developed in the text. However, the system viscosity is also required in PROF for evaluating Reynold's number correlations. Use is made of the correlation suggested by Buddenberg and Wilke (Reference 16) and endorsed by Hirschfelder et al. (Reference 4), namely

$$\mu_{Mix} = \sum_i \frac{X_i \mu_i}{X_i + 1.385 \frac{RT\mu_i}{PM_i} \sum\limits_{\substack{j \\ j\neq i}} \frac{X_j}{\mathcal{D}_{ij}}} \qquad (A\text{-}15)$$

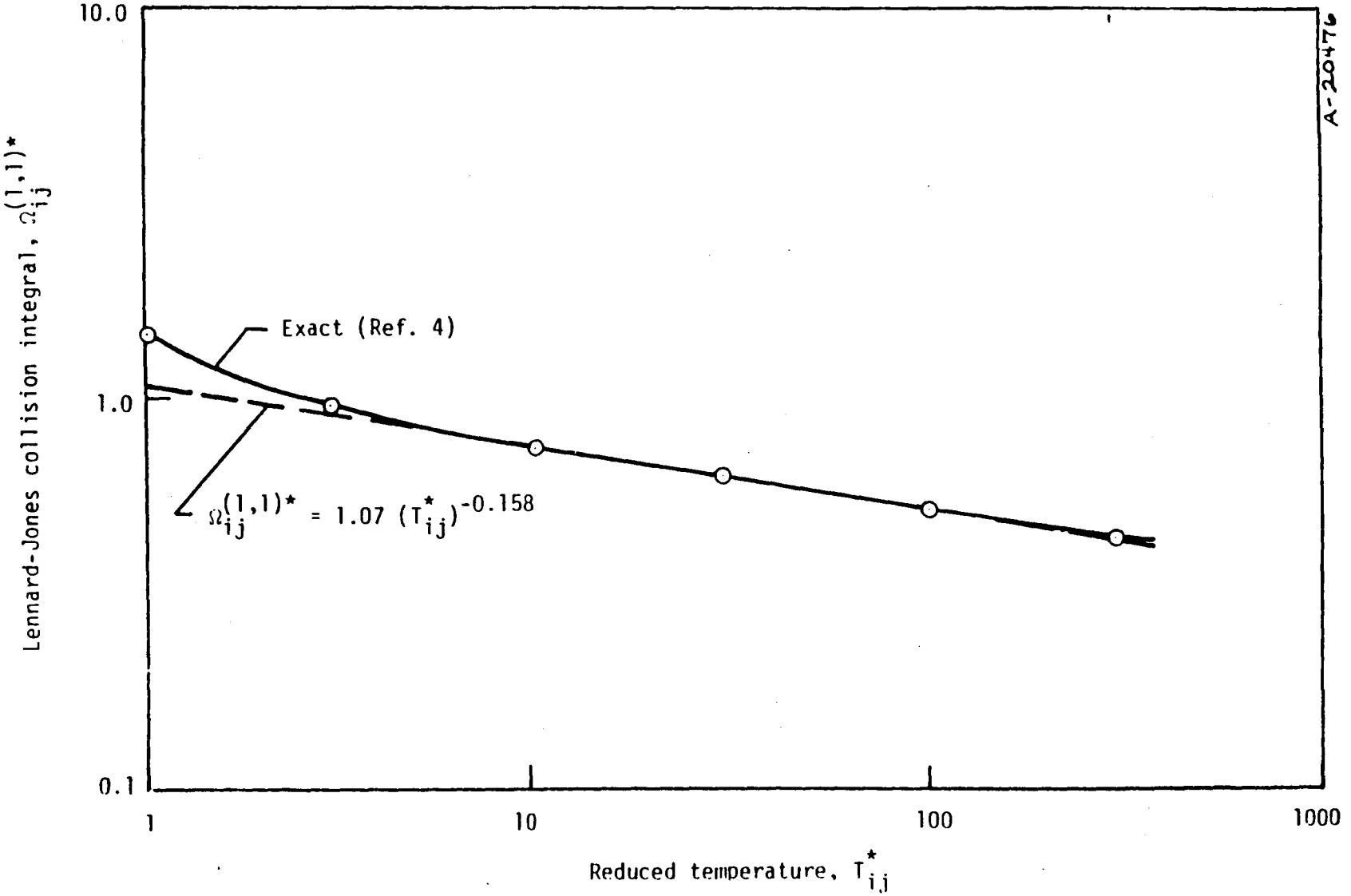

Figure A-2. Collision integral for Lennard-Jones potential.

By introducing the bifurcation relations, taking from Reference 4 the relation for pure component viscosity

$$M_i = \frac{5}{6A_{ii}^*} \rho_i D_{ii}, \qquad \text{(A-16)}$$

assuming $A_{ii}^* \simeq 1.12$ (actually varies from 1.10 to 1.14 in the temperature range of interest), and adjusting 1.385 to 1.344 for simplification, there is obtained

$$\mu_{Mix} = \rho \bar{D} \frac{\mu_2}{1.344 \mu_1 M} \qquad \text{(A-17)}$$

The results presented in this Appendix show that the bifurcation approximation can result in major simplification in transport property evaluations with only minimal loss in accuracy.

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16 Abstract

Under the current program, the basic Acurex HET code has been modified to analyze specific problems for Stirling engine heater head applications. Specifically, the new code will have the following applications:

Adiabatic catalytic monolith reactor

Externally cooled catalytic cylindrical reactor/flat plate reactor

Coannular tube radiatvely cooled reactor

Monolithic reactor radiating to upstream and downstream heat exchangers

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