Reacting Fluids Laboratory
Department of Chemical Engineering
Louisiana State University
Baton Rouge, Louisiana

STATUS REPORT

on

NON-EQUILIBRIUM FLOW AND THE KINETICS OF CHEMICAL REACTIONS IN THE CHAR ZONE

N.A.S.A. Grant NGR 19-001-016

Evaluation of the Energy Transfer
in the Char Zone During Ablation

by

Ralph W. Pike, Associate Professor
Principal Investigator
Gary C. April, Graduate Associate
Eduardo G. del Valle, Graduate Associate

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I SUMMARY

In the temperature range from 500°F to 2500°F non-equilibrium flow analysis predicted only a small change in degradation product composition as the gases flow through the char zone. Essentially all of the reaction took place in the temperature range from 2000°F to 2500°F. Comparing non-equilibrium flow with the two limiting cases the energy absorbed in the char zone for frozen flow was one half of that of non-equilibrium flow, and equilibrium flow was two and one half times that of non-equilibrium flow.

Experimental results were obtained simulating the char zone during ablation in the temperature range from 900°F to 1650°F using the Char Zone Thermal Environment Simulation System. The data showed that the flow was essentially frozen, and this was accurately predicted by the non-equilibrium flow analysis. The limiting case of equilibrium flow incorrectly predicted significant changes in degradated product composition in this temperature range.

Details are given concerning the criteria used for selecting the chemical reactions that were important in the char zone, the generalized reaction kinetics analysis, the computer solutions of the equations and the experimental system.

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II. INTRODUCTION

The primary objective of this research program is to determine accurately the energy absorbed in the char zone of a charring ablator, and how this is affected by the chemical reactions that take place in the char zone. Presently, there are two methods available to describe the limits on the heat transfer in the char zone. These are referred to as the frozen flow and equilibrium flow cases.

The minimum amount of energy that can be absorbed in the char zone can be computed by considering the flow to be frozen. This refers to the situation where the degradation products flowing through the char do not undergo any chemical reactions (the composition is constant). The amount of energy absorbed is given by the change in sensible heat of the gases.

The maximum amount of energy that can be absorbed in the char zone is obtained by considering the chemical species in the flow field to be in thermodynamic equilibrium. This refers to the situation where the degradation products undergo reaction at an infinitely fast rate, and the amount of energy absorbed is computed by considering the species to be in thermodynamic equilibrium. This gives the maximum energy absorbed since the reactions are nearly all endothermic.

The limits on the energy transfer established by these two cases have been previously reported (1, 2). It was found that the amount of energy that could be absorbed was almost an order of magnitude greater for equilibrium flow than for frozen flow for the same front and back surface temperatures on the char. Due to the high mass flux of gases from the plastic decomposition the actual amount of energy that is absorbed lies somewhere between these two limiting cases and is determined by the rates of chemical reaction among the species present.

In this report the necessary equations are developed to compute the energy absorbed in the char zone. These equations are solved for non-equilibrium flow in the char and for the two limiting cases of frozen and equilibrium flow. Comparisons are made between the computed results and experimental data obtained on the Char Zone Thermal Environment Simulator System which is also described. Details are given for the generalized reaction kinetics analysis and the criteria used for solution of the reactions that are important in the char zone. Also included are descriptions, flow diagrams and print-outs of the computer programs used in the computations.

III. ENERGY AND MOMENTUM TRANSFER IN NON-EQUILIBRIUM FLOW

To compute the energy transferred and the pressure distribution in the char zone, it is necessary to solve the energy equation and momentum equation with appropriate boundary conditions. For steady flow of degradation products in a char zone of constant thickness, the energy equation has the following form:

$$W_g \cdot \bar{C}_p \cdot \epsilon \cdot \frac{dT}{dz} - \frac{d}{dz}\left[k_e \cdot \frac{dT}{dz}\right] + \sum_{i=1}^{K+1} H_j r_j = 0 \qquad (1)$$

The first term represents the convective heat transfer, the second term represents conductive heat transfer and the third term represents the heat absorbed by chemical reactions. The derivation of this equation and a description of the numerical solution is given in Appendix A.

To describe the pressure distribution a modified form of Darcy's equation was used which accounts for inertial effects that are important due to the high mass flux of degradation products. For the steady flow of an ideal gas in the char with varying mass flux, the following integral equation was obtained to predict the pressure distribution:

$$P = \left\{P_L^2 + 2R\left[\epsilon/\gamma \int_z^L (W_g \mu\, T/\bar{M})\, dz + \beta \int_z^L (W_g^2 T/\bar{M})\, dz\right]\right\}^{1/2} \qquad (2)$$

The first term on the right hand side is the pressure on the high temperature surface of the char, the second and third terms represents the pressure loss due to viscous and inertial effects respectively.

The energy absorbed in the char zone is equal to the difference between the heat flux at the high temperature surface and the heat flux at the low temperature surface. As also shown in Appendix A the energy absorbed

for non-equilibrium flow in the char is given by:

$$q_{cz} = \epsilon \sum_{i=1}^{K} \int_{T_o}^{T_L} W_g x_j C_{p_j} dT + \sum_{j=1}^{K+1} \int_{T_o}^{T_L} \frac{dN_j}{dT} \cdot M_j \cdot H_j dT \qquad (3)$$

The first term on the right hand side represents the heat absorbed due to the change in enthalpy of the gases and the second term represents the heat absorbed by chemical reactions.

Equations (1), (2) and (3) were solved numerically using programs written in FORTRAN IV on an IBM 7040 computer. This is described in detail in Appendix C where flow diagrams of the sub-programs are given with a print-out of the programs. A subsequent section (Generalized Reaction Kinetics Analysis) discusses the method used to compute the reaction rates of the simultaneous chemical reactions as they occur in the char zone.

However before the calculations can be performed two additional pieces of information must be known. These are the specific chemical reactions that occur in the char with their associated kinetic constants and the initial composition of the degradation products when they enter the char zone. The ten specific chemical reactions that are thought to occur in the char zone are listed in Table 1, and the method of arriving at these reactions is discussed in the following section entitled "Criteria for Reactions Selection." Also discussed in this section are the methods for establishing the initial compositions which were based on the compositions predicted by thermodynamic equilibrium calculations and pyrolysis gas chromotography experiments.

In Figure 1 a comparison is shown of the temperature distribution for non-equilibrium, equilibrium and frozen flow from the solution of the equations of change (continuity, momentun and energy) for a surface temperature

TABLE 1

IMPORTANT CHEMICAL REACTIONS IN THE CHAR ZONE IN THE TEMPERATURE RANGE FROM 500 TO 2500°F

1. $CH_4 = 1/2\ C_2H_6 + 1/2\ H_2$

2. $C_2H_6 = C_2H_4 + H_2$

3. $C_2H_4 = C_2H_2 + H_2$

4. $C_2H_2 = 2C + H_2$

5. $CH_4 = 1/2\ C_2H_2 + 3/2\ H_2$

6. $CH_4 = C + 2H_2$

7. $C_6H_6 = 3C_2H_2$

8. $C + CO_2 = 2CO$

9. $NH_3 = 1/2\ N_2 + 3/2\ H_2$

10. $CH_4 + 3/2\ O_2 = CO_2 + H_2O$

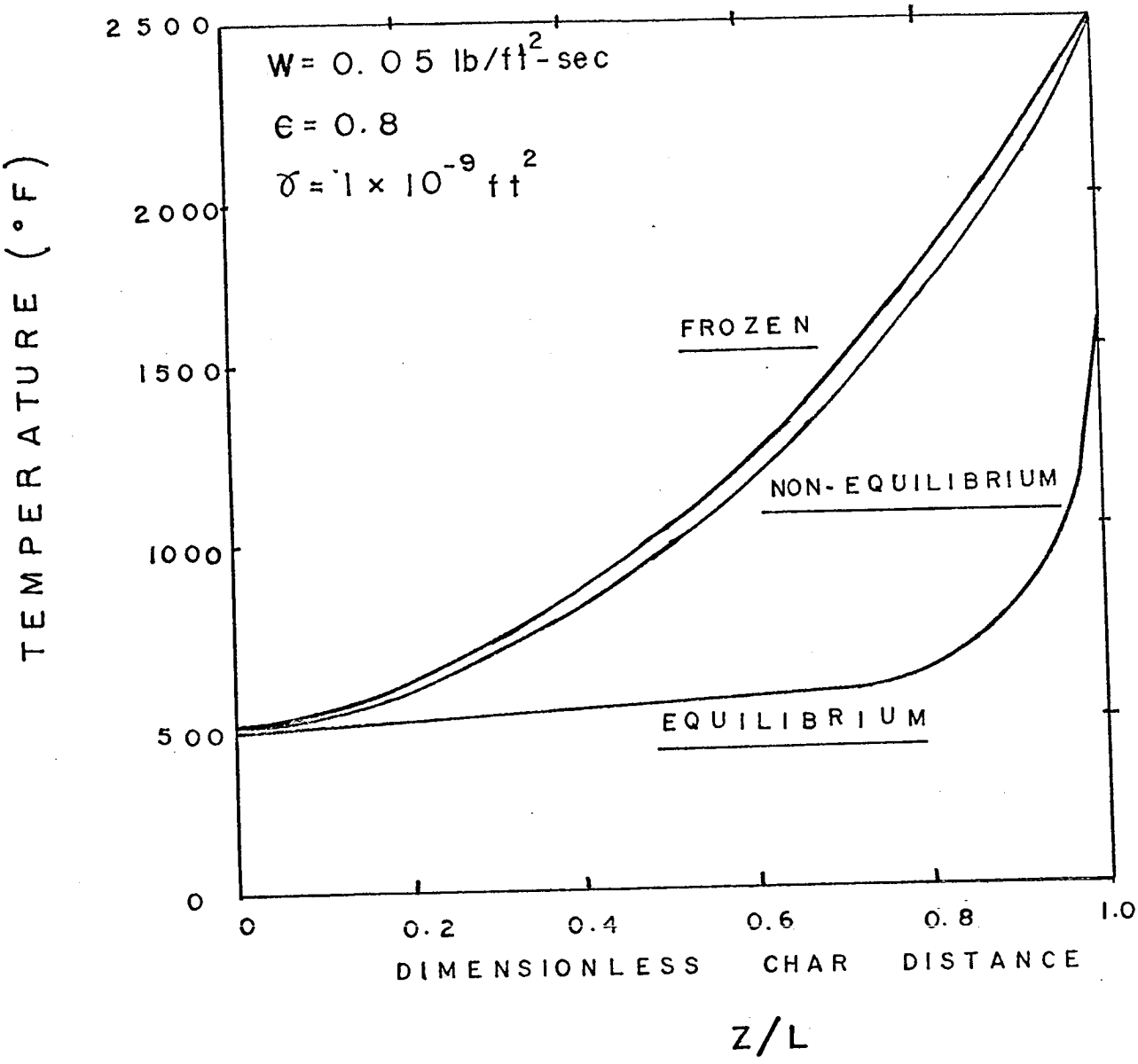


Figure 1. Comparison of the Temperature Distributions for Non-Equilibrium, Equilibrium and Frozen Flow in the Char Zone with a 2500°F Surface Temperature.

of 2500°F. As shown the temperature distribution for non-equilibrium flow is only slightly less than that for frozen flow. However the temperature distribution for equilibrium flow is significantly different than that for frozen and non-equilibrium flow. The effect of small changes in composition due to chemical reactions cause the temperature profile for non-equilibrium flow to only be slightly different than that for frozen flow. However, the temperature profile for equilibrium flow is significantly different than that for non-equilibrium flow, and this is a result of the energy absorbed due to the significant changes in composition determined by thermodynamic equilibrium.

Although the temperature profile is essentially the same there is a significant difference between the heat flux at the high temperature surface for non-equilibrium and frozen flow as seen in Table 2. This is mainly a result of the decomposition of CH_4 by reactions 1, 5 and 6 and the formation of CO by reaction 8. This is seen in Table 2 by the change in degradation product composition from 500°F to 2500°F. The energy absorbed considering the flow in thermodynamic equilibrium is much larger than that for non-equilibrium flow, and the reason is the large changes in composition as shown in Table 2. Thus if some means could be devised to increase the rate of reactions, there is the potential for a sizeable increase in amount of energy that could be absorbed. This would mean a reduction in heat shield weight.

Given in Table 2 are the pressure drop through the char calculated using equation (2) for non-equilibrium, equilibrium and frozen flow. As would be expected the pressure drop predicted by assuming the flow to be in equilibrium is less than that for either frozen or non-equilibrium flow since the viscosity is an increasing function of temperature. As would

Table 2 - Comparison of the High Temperature Surface Heat Flux, Composition of Degradation Products and Pressure Drop for Frozen, Equilibrium, and Non-Equilibrium Flow

Mass Flux - 0.05 lb per ft^2 - sec

Char Characteristics: Porosity - 0.8
Permeability - 1×10^{-9} ft^2

DEGRADATION PRODUCT COMPOSITION (Mole Percent)

Component	Entering the Char At 500° F	Leaving the Front Surface at 2500° F Non-Equilibrium Flow	Equilibrium Flow
CH_4	55.47	54.50	0.10
H_2O	32.48	33.20	0.01
N_2	8.06	8.00	4.21
CO_2	1.52	0.02	Trace
H_2	1.45	1.44	77.03
NH_3	0.02	0.01	Trace
CO	Trace	1.71	18.65

Model	Heat Flux at Surface (BTU/ft^2-sec)	Pressure Drop (lb/ft^2)
Frozen Flow	52.22	12.97
Non-Equilibrium Flow	107.64	12.45
Equilibrium	271.25	9.75

be expected the pressure drop for non-equilibrium and frozen flow is essentially the same.

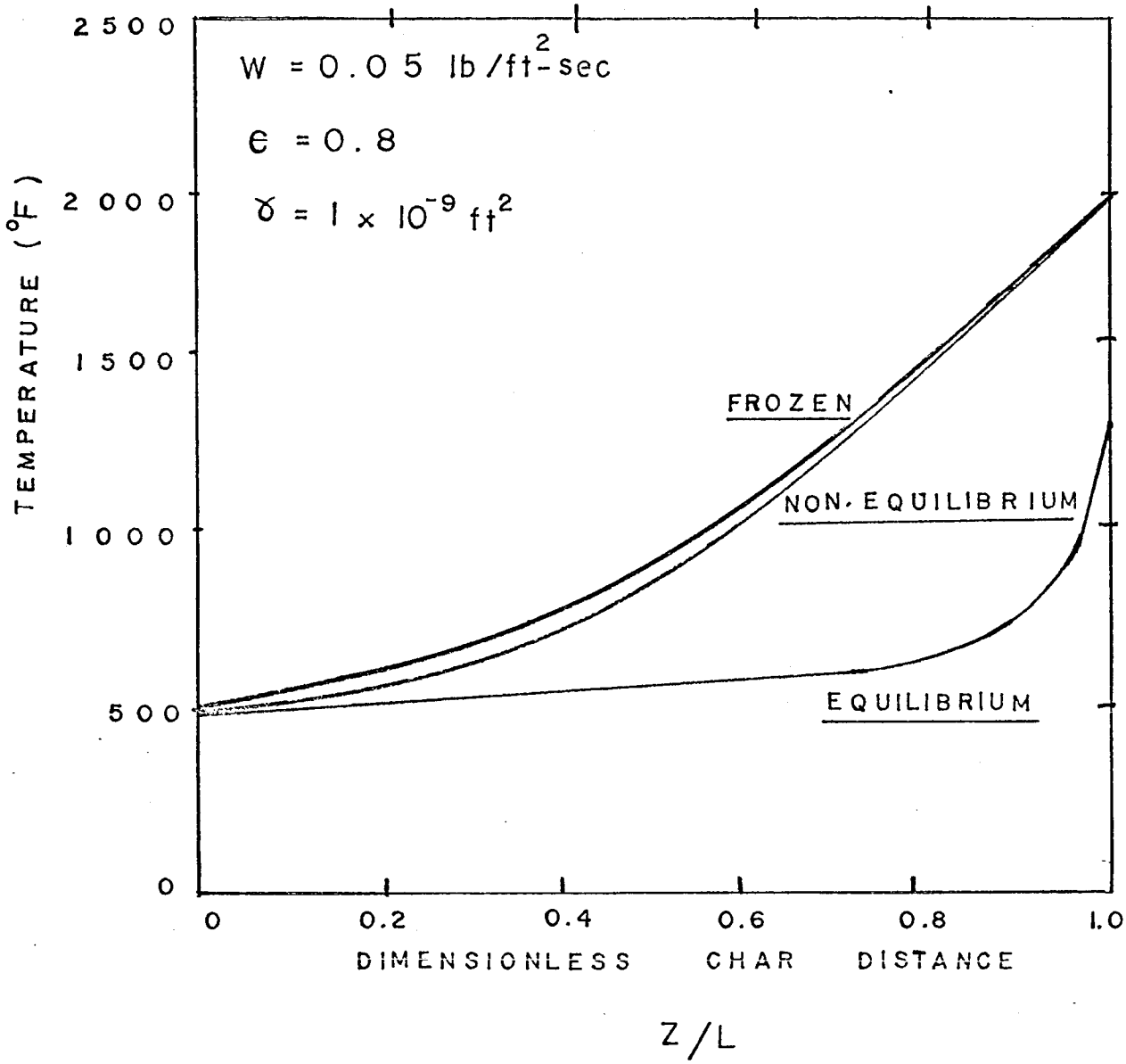
In Figure 2 similar results to that of Figure 1 and Table 2 are shown except for a front surface temperature of 2000°F. As would be expected the temperature profiles are similar to that of Figure 1. However, on comparing the surface heat flux it is seen that there is only a slight difference between that for frozen and non-equilibrium flow. Consequently the major energy absorption occurs in the temperature range from 2000°F to 2500°F. This would be expected since the rate of reaction increases exponentially with temperature. Thus it would also be expected that for cases with higher char temperatures the heat absorbed by chemical reactions would be much more significant. Currently work is underway to extend these analyses to higher surface temperatures.

IV. EXPERIMENTAL SIMULATION OF THE CHAR ZONE DURING ABLATION

A. Char Zone Thermal Environment Simulator

Experiments are being conducted to establish the accuracy of the non-equilibrium flow model with an experimental system that simulates the char zone during ablation. A schematic diagram of the Char Zone Thermal Environment Simulator is shown in Figure 3.

In this simulator actual chars formed in the large arc jets at the Langley Research Center are mounted in a char holder as shown. The holder is constructed of concentric tubes so gases of compositions that are typical of the degredation products can flow through the char as they would have on leaving the decomposition zone. Chars are removed from 3" diameter arc jet samples, and saureisen cement is poured around the sides of the char inside a mold. This mounts the char with front and back surface



MODEL	SURFACE HEAT FLUX BTU/ft²-sec	PRESSURE DROP LB/ft²	MIDPOINT TEMPERATURE °F
FROZEN	44,67	15.3	948.7
NON-EQUILIBRIUM (10 REACTIONS)	45.17	15.1	890.6
EQUILIBRIUM	180.83	9.22	537.6

Figure 2. Comparison of the Solutions of the Energy and Momentum Equations for Non-Equilibrium, Equilibrium and Frozen Flow in the Char Zone with a 2000°F Surface Temperature.

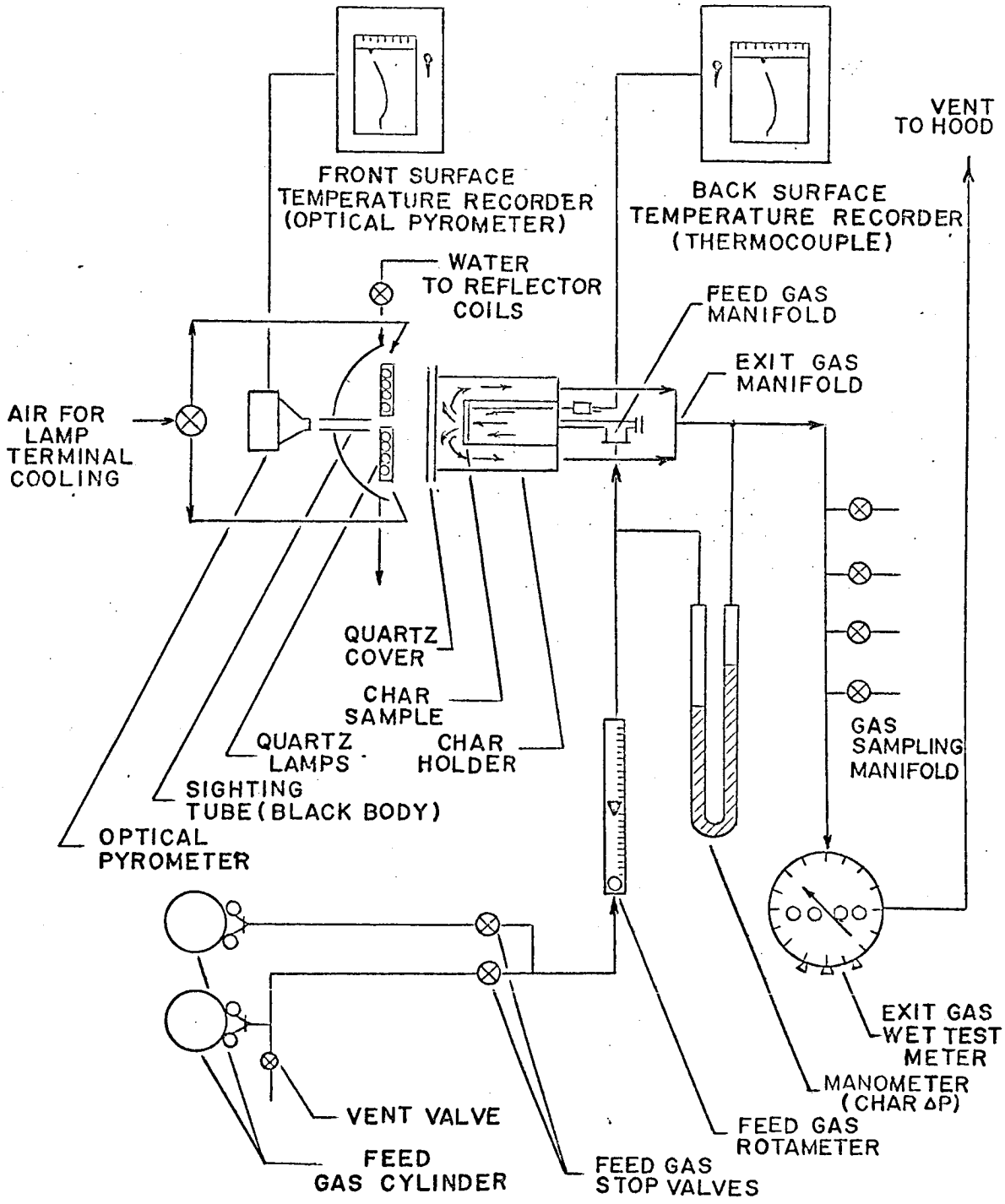


FIGURE 3

CHAR ZONE THERMAL ENVIRONMENT SIMULATOR

exposed in a uniform inert ceramic casing which is mounted in the char holder.

To have a temperature profile comparable to that on re-entry a bank of 15 G. E. 1000 T3 quartz lamps are used to heat the char surface. The bank is located about 1-1/2' from the char surface, is surrounded by a reflector, and has a total output of about 15 KW.

A total radiation pyrometer (Leeds and Northrup, Narrow Angle Rayotube) is focused on the front surface of the char through the bank of lamps to give an accurate measure of the front surface temperature. This is recorded on a strip chart recorder. This accuracy (± 20°F at 2000°F) was established by comparing the temperature measured by the total radiation pyrometer with that of a calibrated optical pyrometer. Also it was established that the pyrometer was not being affected by sighting through the quartz lamps. This was accomplished by operating the lamps without the char holder in place, and with the lamp on the pyrometer did not register an increase in temperature. The usual corrections to the measured temperature due to the reflected radiation from the lamps were made. This correction was less than 25°F at a char surface temperature of 1650°F.

The back surface temperature was measured with a shielded iron-constantan thermocouple and recorded on a strip chart recorder. The thermocouple made firm contact with the char surface to insure an accurate surface temperature measurement. The thermocouple responded very rapidly when the bank of heating lamps was turned on indicating that good contact was being made between the char surface and the thermocouple tip.

A blend of gases simulating the composition of the degradation products was made in a high pressure cylinder. The composition of feed blend number one is reported in Table 3. The gas is passed through a regulator

and is metered by a calibrated rotameter to the char holder. Having passed through the char the gases flow through a sample manifold where periodic samples are taken for gas chromatographic analysis and then through a wet test meter where volume (flow rate)is measured.

The composition of the feed and products are analyzed on a Packard Instrument Corporation gas chromatograph with a thermal conductivity detector. Hydrocarbons and CO_2 are determined on a 12 ft. column filled with Porapak S packing with helium as a carrier gas. Nitrogen, oxygen and carbon monoxide are determined on a 6 ft. column packed with 5A molecular sieve with helium as a carrier gas. Hydrogen is determined on this column using argon as a carrier gas.

The pressure drop across the char is measured with a U-tube manometer using water as the manometer fluid. The taps of the manometer are located on the entrance and exit gas lines. The actual pressure drop across the char is determined by subtracting from the total pressure drop, the pressure drop measured without the char in place. The pressure drop without the char in place for the range of flow rates employed in the test was less than 0.5 inch of water.

The operating procedure consisted of a start-up phase, a steady state phase, and a shut-down phase. In the start-up phase cooling water and air flow rates are adjusted, recorders are started, helium flow through the char is set and then power is applied to the bank of lamps. The temperature of the system rises to a steady-state value, and now in the steady-state phase at these conditions a set of data are collected which represents frozen flow in the char. Then the flow is switched to a feed of a composition typical of the degradation products. When temperature transients have damped (about 3-5 minutes), product samples are taken at 5 minute intervals for a run time of more than 20 minutes. Operating conditions are then changed to obtain another set of

data or the system is shut down.

To shut-down the operation of the system, the flow through the char is changed to helium and then the power to the lamps is turned off. The system is allowed to cool to near room temperature and all of the flows are turned off.

B. Experimental Results

In Table 3 a comparison is given between typical experimental results (0.005 lb per ft^2-sec mass flux, 1650°F front surface temperature, 900°F back surface temperature) and the models for non-equilibrium and equilibrium flow. The inlet composition is the concentration of the stream entering the char at 900°F and the outlet composition is the concentration leaving the front surface of the char at 1650°F. The experimentally measured values are shown in Table 3 along with the values that are computed by the model of non-equilibrium flow and equilibrium flow. As shown the amount of chemical reactions that actually took place was only slight and this is accurately predicted by non-equilibrium flow. The computed values of the composition agree within experimental error with the experimental values. For this temperature range the flow is essentially frozen (no chemical reaction).

For comparison the exit composition computed for equilibrium flow is also given in Table 3. If the gases were actually in thermodynamic equilibrium flowing through the char, there would have been a significant heat absorption due to reaction. In fact nearly all of the methane is decomposed and essentially all of the carbon dioxide is converted. Thus this would be an extremely poor characterization of the flow to consider it to be in thermodynamic equilibrium in this temperature range and unrealistically high surface heat flux values would be computed as shown in Figure 4.

Table 3. Comparison Between a Typical Set of Experimental Results (Experimental Test 9) and Non Equilibrium Flow Computations

Operating Conditions: Mass Flux - 0.005 lb/ft^2 sec

Surface Temperatures: Front - 1650°F

Back - 900°F

Char - Specimen No. 52*, Thickness - 0.25 inch.

Degradation Product Compositions (mole per cent)

Component	Inlet Composition	Outlet Composition: Experimentally Measured	Outlet Composition: Computed Non-Equil. Flow	Outlet Composition: Computed Equil. Flow
CH_4	44.61	44.68	43.40	1.52
H_2	35.81	35.79	35.01	81.91
N_2	11.13	11.12	12.68	7.59
CO_2	4.75	4.70	5.21	0.02
CO	3.71	3.80	3.70	8.65
H_2O	0	0	0	0.31
Total	100.00	100.00	100.00	100.00

Pressure Gradient Across Char

Experimentally Measured - 2.1 psf

Computed by Non-Equilibrium Flow - 2.3 psf

*Low density phenolic-nylon tested in Langley Research Center arc jet using a 4 in. dia. nozzle with a 3% O_2 - 97% stream having a 2000 Btu/# stream enthalpy at a heating rate of 100 Btu/ft^2 sec. and at a test time of 100 sec.

The pressure drop computed by equation (2) is compared with the experimentally measured pressure drop in Table 3. As can be seen there is excellent agreement between the experimental and computed values.

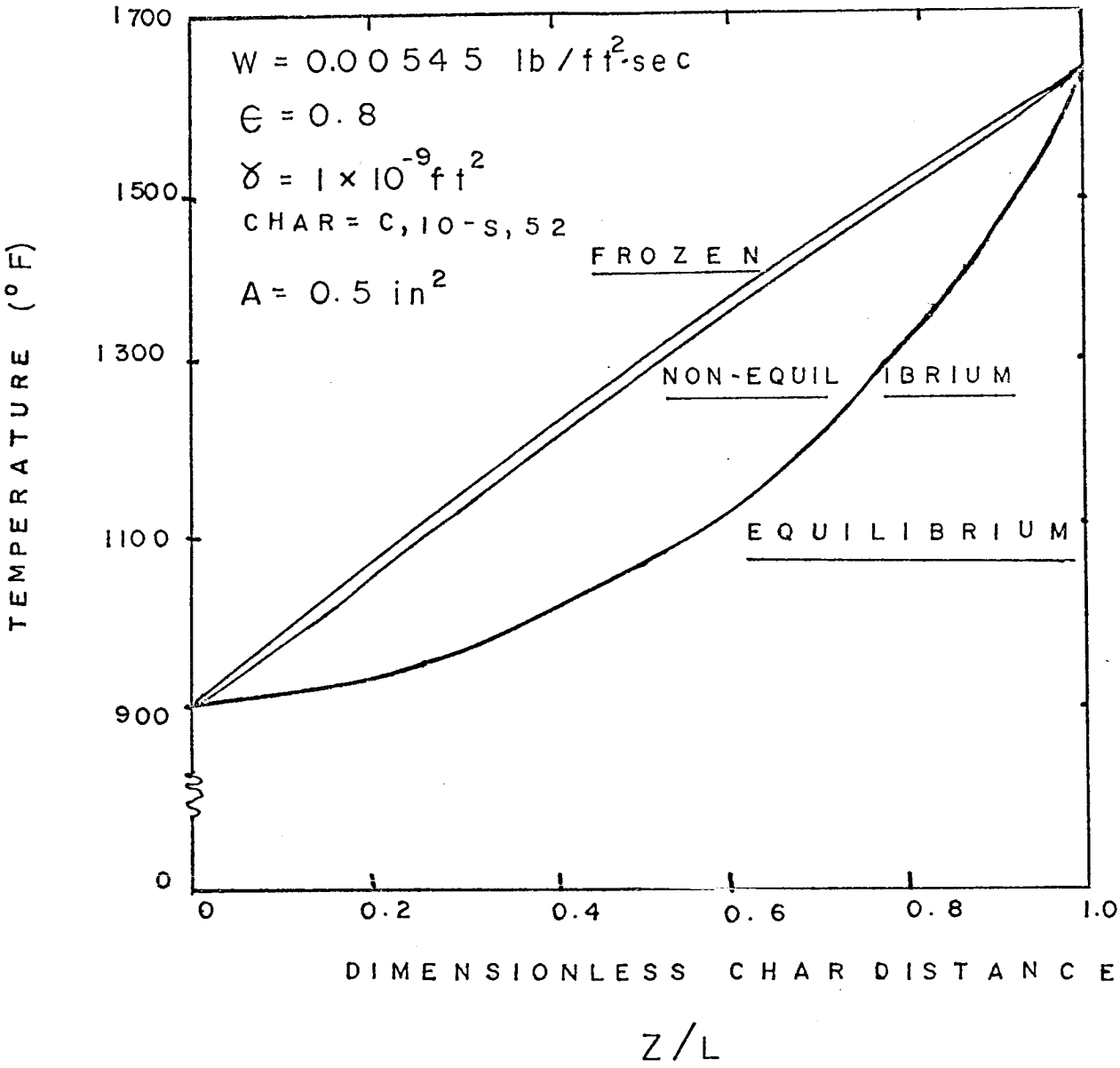
As a means for further comparison the temperature profile for each of the three flow models is presented in Figure 4. The non-equilibrium flow temperature profile lies very near the profile for frozen flow while the equilibrium flow deviates significantly as would be expected. The energy absorbed due to chemical reactions is shown by the increase of 0.85 Btu/ft^2-sec in the surface heat flux over that of frozen flow. However, the heat flux predicted for equilibrium flow is over 6 times that for non-equilibrium flow. This high and notrealistic surface heat flux is due to the large change in composition.

In conclusion it can be stated that in the temperature range of the experiments only a small change in composition occurs due to chemical reactions as the gas flows through the char. This is due to the short residence time of the gas in the char as a result of the high mass flux through the char. The flow is essentially frozen. If the chemical species are assumed to be in thermodynamic equilibrium flowing through the char, there would be over a six fold error in computing the surface heat flux, i.e. the energy absorbed in the char zone.

V. GENERALIZED REACTION KINETICS ANALYSIS

The purpose of this section is to present the equations that permit the calculation of the reaction rates for an arbitrary number of simultaneous chemical reactions involving an arbitrary number of chemical species. This will be illustrated with the reactions given in Table 1.

A chemical reaction can be written in general as:



MODEL	SURFACE HEAT FLUX BTU/FT^2 SEC	PRESSURE DROP LB/FT^2	MIDPOINT TEMPERATURE, °F
FROZEN	2.73	2.27	1276.5
NON-EQUILIBRIUM	3.58	2.25	1274.7
EQUILIBRIUM	23.50	1.76	1049.3

Figure 4. Comparison of Momentum and Energy Transfer Computed For Experimental Test 9.

$$\sum_{j=1}^{K} r_{ij}A_j \underset{k_{ri}}{\overset{k_{fi}}{\rightleftarrows}} \sum_{j=1}^{K} p_{ij}A_j \tag{4}$$

For this i th chemical reaction, the r_{ij} and p_{ij} represent the stochiometric coefficients of the reactants and products respectively for species A_j. The forward and reverse reaction rate constants are k_{fi} and k_{ri}. There are a total of K chemical species.

For the rate of reaction of the jth species, R_j, this is given by the following equation for n chemical reactions:

$$R_j = \sum_{i=1}^{n} (p_{ij} - r_{ij}) \left[k_{fi} \prod_{j=1}^{K} c_j^{r_{ij}} - k_{ri} \prod_{j=1}^{K} c_j^{p_{ij}} \right] \tag{5}$$

where c_j is the concentration of component j in appropriate units.

This equation has the powers on the composition terms the same as the stochiometric coefficients. However, it is not necessary to do this. If this is not the case for some of the reactions being use, it is only necessary to include two additional matrices besides r_{ij} and p_{ij} in the computer implementation.

To illustrate the use of equations (4) and (5) the matrix form of the reactions listed in Table 1 are shown in Table 4. This is equation (4) for 10 reactions and 13 chemical species.

To illustrate the use of equation (5), the rate of reaction of methane (component 2) is given by the following:

$$r_2 = \sum_{i=1}^{10} (p_{i2} - r_{i2}) \left[k_{fi} \prod_{j=1}^{13} c_j^{r_{ij}} - k_{ri} \prod_{j=1}^{13} c_j^{p_{ij}} \right] \tag{6}$$

or expanding

Table 4. Matrix Formulation of the Chemical Reactions Given in Table 1

$$
\begin{bmatrix}
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3/2 & 0
\end{bmatrix}
\begin{bmatrix}
H_2 \\ CH_4 \\ C_2H_6 \\ C_2H_4 \\ C_2H_2 \\ C \\ C_6H_6 \\ CO_2 \\ CO \\ NH_3 \\ N_2 \\ O_2 \\ H_2O
\end{bmatrix}
=
\begin{bmatrix}
1/2 & 0 & 1/2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
3/2 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
2 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\
3/2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/2 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
H_2 \\ CH_4 \\ C_2H_6 \\ C_2H_4 \\ C_2H_2 \\ C \\ C_6H_6 \\ CO_2 \\ CO \\ NH_3 \\ N_2 \\ O_2 \\ H_2O
\end{bmatrix}
$$

$$r_2 = (0 - 1) \left\{ k_{f1}\, c_2 - k_{r1}\, c_1^{\frac{1}{2}}\, c_3^{\frac{1}{2}} \right\} +$$

$$(0 - 1) \left\{ k_{f5}\, c_2 - k_{r5}\, c_1^{3/2}\, c_5 \right\} +$$

$$(0 - 1) \left\{ k_{f6}\, c_2 - k_{r6}\, c_1^{2}\, c_6 \right\} +$$

$$(0 - 1) \left\{ k_{f10}\, c_2 c_{12}^{\frac{1}{2}} - k_{r10}\, c_8\, c_{13} \right\} \qquad (7)$$

The above equation contains six other terms in the expanded form, but these are not included since the coefficients were zero. Of course this equation is not exactly correct since the powers on the compositions are different in some cases for the actual rate expressions. For example, the carbon-carbon dioxide reaction involves the surface area of carbon, and not a "concentration" of carbon. To take the surface area of the char into account the reaction rate constant can be modified, and the exponent on the carbon "concentration" can be set equal to zero.

Equation (5) has been incorporated into the main program which generates the solution to the energy equation using a fourth order Runge-Kutta Method (1). With this it is possible to predict the energy absorbed in the char zone for non-equilibrium flow. Some of these results have been presented in a preceding section along with a comparison of experimental results obtained by flowing typical compositions of degradation products through actual chars. Additional experimental results will be presented in a subsequent report.

VI. CRITERIA FOR REACTION SELECTION

In a previous report (3) the literature was surveyed for the kinetics of chemical reactions that could possibly occur in the char zone during ablation. At that time a number of reactions and species were located,

and since then additional information has become available. These results have been up-dated and will be presented in a forthcoming report. However, it can be shown that not all of these possible reactions are important in the temperature range of interest. To determine the chemical reactions that would occur with a significant conversion in the char, two procedures were used. One procedure consists of computing the conversion for one reaction of an equal molal mixture of reactants flowing isothermally through the char. The other procedure consist of estimating the species and the composition that enter the char zone from thermal-gravimetric analysis and pyrolysis gas chromatographic analysis. These two procedures combined determine the important reactions that occur in the char, and these are discussed in the next sections.

A Isothermal Flow Analysis

There is a sizeable number of possible chemical reactions that can occur in the char zone as was previously discussed. To attempt to include all of these reactions in the solution of the energy equation to predict the energy absorbed in the char zone for non-equilibrium flow would be very difficult. Consequently it was necessary to devise a screening procedure to eliminate from consideration the reactions that are not important in the temperature range of current interest (500°F - 2500 °F). The following reasoning was applied.

The rate of reaction increases with temperature. For a particular reaction, if a significant conversion of reactants to products was obtained with the char at a uniform and high temperature, then it could be assumed that there may be a significant conversion when the char is subjected to a temperature gradient (low temperature at 500°F to a high temperature at 2500°F). Thus these reactions should be considered in any analysis of the char zone.

Conversely if there is essentially no conversion at a high temperature (2500°F) for the char at this uniform temperature, there will be no conversion with an increasing temperature gradient in the char. Thus these reactions can be eliminated from consideration. Correspondingly if there is complete conversion within the char at a low temperature, there will be complete conversion for the case of a temperature gradient. Thus this reaction can be eliminated from consideration and only the products are considered to be present.

To determine the important chemical reactions in the temperature range from 500°F to 2500°F, the conversion of an equal molal mixture of the reactants flowing in the char was determined at mass flux rates of 0.01 and 0.05 lb per ft^2-sec for nearly all of the reactions reported in reference (3) and some additional reactions. These results are tabulated in Appendix B for temperatures from 500°F to 3000°F in 500°F intervals for a mass flux of 0.01 lb per ft^2-sec. The lower mass flux rate gave a longer residence time of the species in the char, and consequently a higher conversion. However, in comparing the conversions in general there was only a relatively small decrease in conversion due to the five-fold increase in the mass flux rate. Consequently only the conversions are reported at a mass flux of 0.01 lb per ft^2-sec in Tables B1 through B4.

In Figure 5 the conversion for two reactions are given as a function of temperature. These are the thermal decomposition of pure ethylene and pure acetylene. It can be concluded by examining this figure that there would be no conversion of ethylene in the char for temperatures less than 1000°F and no conversion of acetylene for temperatures less than 2000°F. However the thermal cracking of ethylene would be important for temperatures above 1000°F and for acetylene above 2000°F.

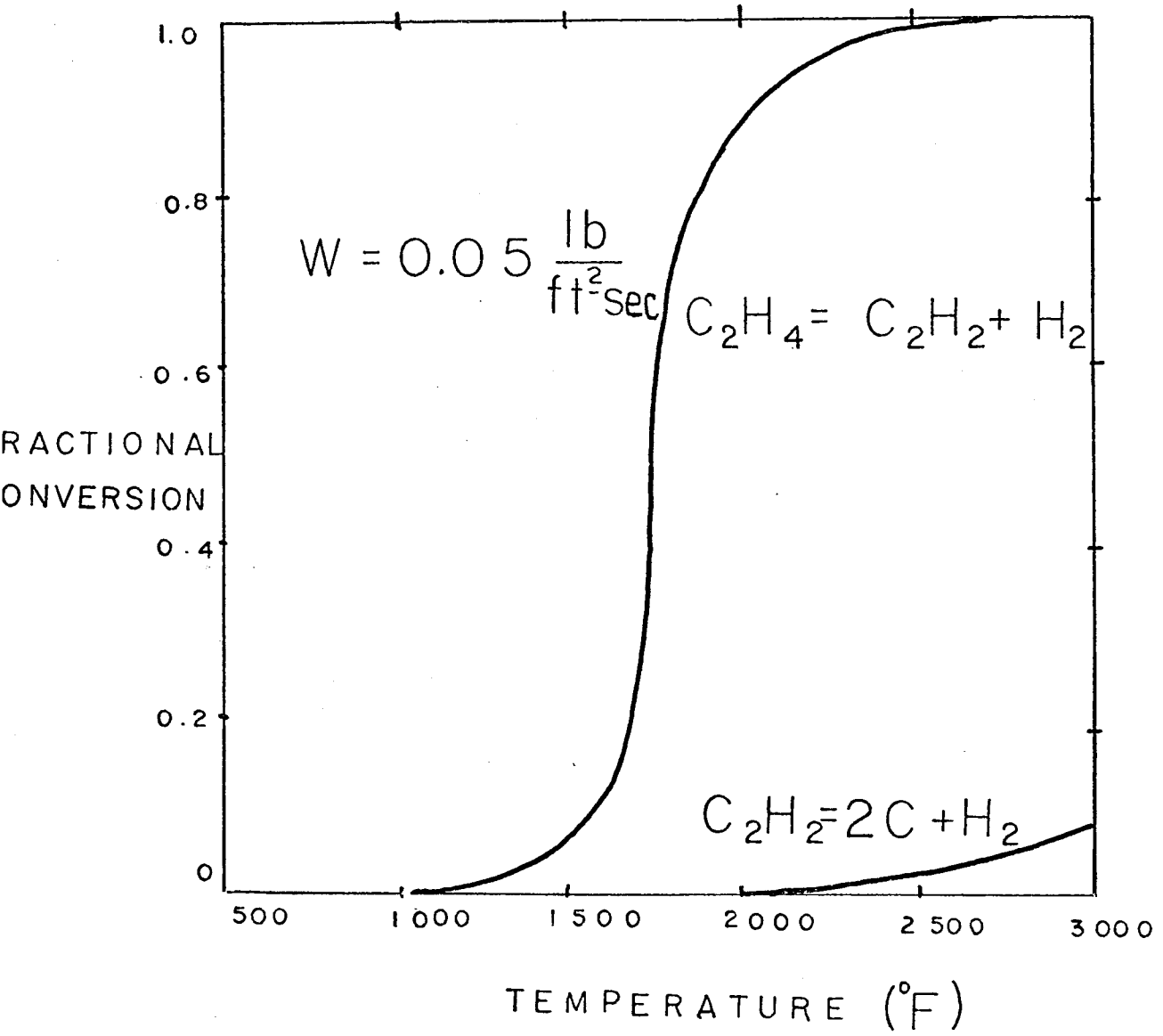


Figure 5. Conversion as a Function of Temperature for the Thermal Decomposition of Pure Ethylene and Pure Acetylene Flowing Isothermally in the Char.

To make the discussion quantative, the conversion of a reactant is defined as the ratio of the amount consumed by reaction to the amount present initially. To determine the conversion of a chemical reaction of the form:

$$aA + bB + cC = nN + oO + pP \tag{8}$$

a material balance is made on component j flowing through a volume section of the char of area A and width Δz as shown in Figure 6. If N_j is the molal flux of component j at z, the material balance on component j for steady flow in the z direction is:

accumulation of component j = input of component j - output of component j

$$0 = N_j M_j A\Big|_z + r_j M_j A \Delta z - N_j M_j A\Big|_{z + \Delta z} \tag{9}$$

where r_j is the rate of formation of species j by chemical reaction. Rearranging the above and taking the limit as Δz approaches zero gives:

$$\frac{dN_j}{dz} = r_j \tag{10}$$

The fractional conversion X_j of component j is defined as:

$$X_j = (N_{jo} - N_j) \,/\, N_{jo} \tag{11}$$

where N_{jo} is the molal flux of component j entering the char zone. Differentiating the above with respect to z gives:

$$N_{jo} \cdot \frac{dX_j}{dz} = - \frac{dN_j}{dz} \tag{12}$$

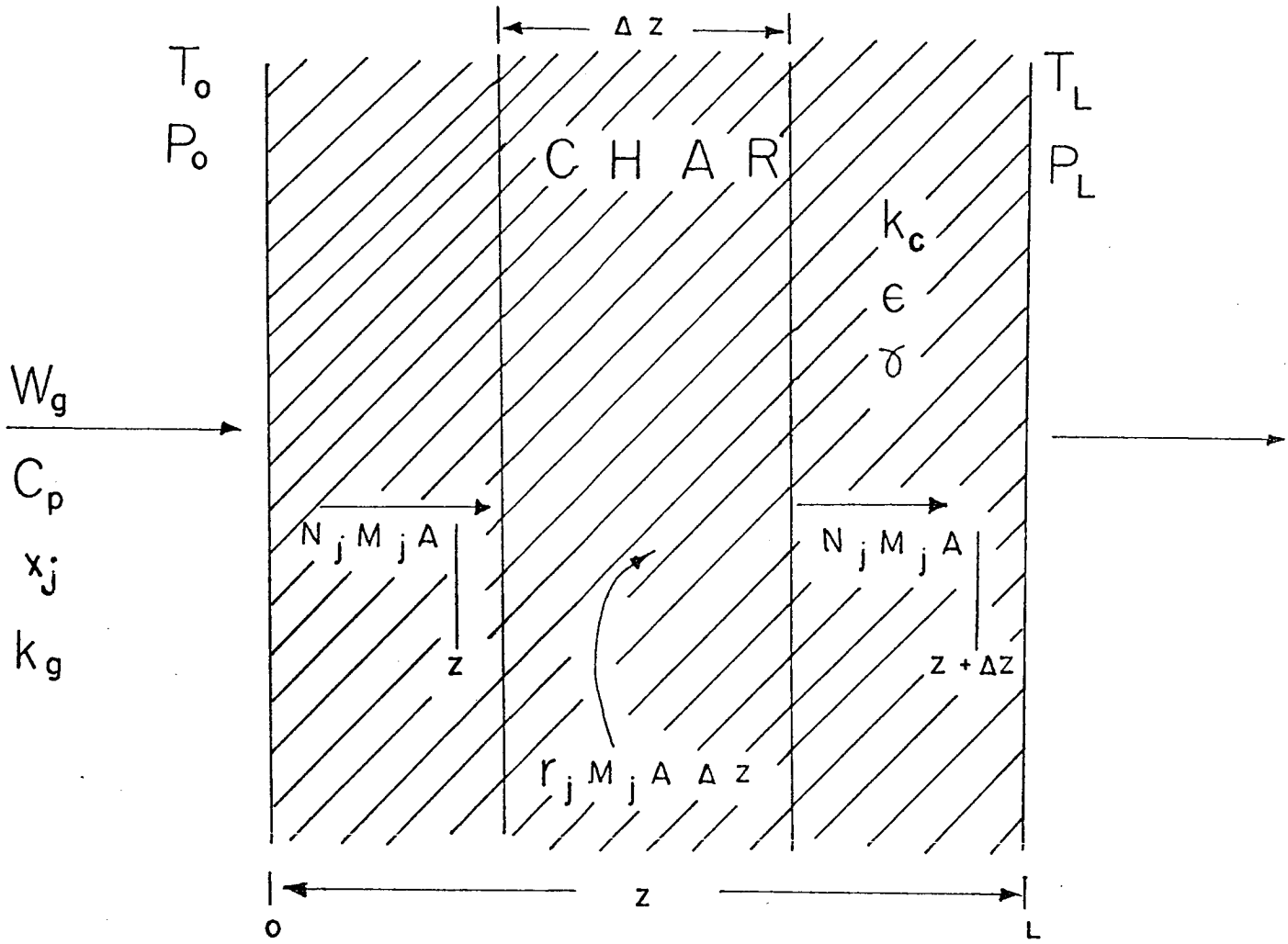


Diagram of the Char Zone

Figure 6 .

The continuity equation in terms of the volumetric flow rate Q of gas entering the char is:

$$Q = (N_{jo}/x_{jo}) \ \bar{M}_o A/\rho \tag{13}$$

Equation (10) using equations (12) and (13) becomes:

$$\frac{\rho x_{jo}}{\bar{M}_o} \cdot \frac{dX_j}{-r_j} = \frac{A}{Q} \, dz \tag{14}$$

This can be integrated from the front surface of the char where X_j and z are zero to the back surface at $z = L$ where $X_j = X_{jL}$ and the result is:

$$\frac{\rho x_{io}}{\bar{M}_o} \int_o^{X_{jL}} \frac{dX_j}{-r_j} = \frac{A \cdot L}{Q} = \frac{V}{Q} = S_t \tag{15}$$

where S_t is the average residence time or space time, i.e., the average time a molecule stays in the char.

The reaction rate r_j for component A of equation (8) has the form:

$$r_A = -k_f \ C_A^a C_B^b C_C^c + k_r C_N^n C_O^o C_P^p \tag{16}$$

and this is needed to integrate equation (15). A trial and error solution of the above integral equation is necessary to determine the final conversion X_{jL} since the average residence time, S_t, is known for a given char depth and decomposition products mass flux.

A computer program was written which obtains the solution for equation (15) using equation (16). The final conversion is varied in the solution technique until the calculated value of S_t corresponds to the known S_t to

with 0.1%. A Simpson's rule integration is employed to evaluate the integral of equation (15). A flow diagram of the program is given in Figure B1 of Appendix B along with a print-out of the program and a set of typical calculations.

The results of the computations using this program are given in Tables B-1 through B-4. This includes the conversion for each reaction as a function of temperature from 500°F to 3000°F in steps of 500°F. As is seen there are a number of reactions which have a significant conversion in this temperature range. All of these reactions could occur in the char zone if the reactants are among the species formed by the phenolic resin-nylon decomposition, or if the reactants are products from other reactions of the degradation species. A further reduction in the number of reactions can be obtained and is discussed below.

B. Estimation of Species Entering the Char Zone

The number of chemical reactions that should be considered for non-equilibrium flow can be reduced further if the composition of the plastic degradation products entering the char from the decomposition zone is known. There are two sources to estimate this initial composition - from thermodynamic equilibrium calculations and from thermal- gravimetric and pyrolysis gas chromatographic analyses. A comparison of the initial compositions from these two methods are shown in Table 5. It can be seen that there is agreement in the order of magnitude of each species present.

The results given for the composition of the degradation products from a 50% (wt) phenolic resin - 50% (wt) nylon mixture was computed by the free energy minimization technique described by del Valle, et.al., (4). Other species were also considered to be present and appdared in concentrations of less than 10^{-20} mole per cent. These were atomic and molecular

Table 5. Composition of Degradation Products from Phenolic Resin, Nylon and a 50% Phenolic Resin - 50% Wt. Nylon Mixture in mole percent

	Equilibrium Composition Calculated for the Phenolic-Nylon Mixture (4)		Thermalgravimetric and Pyrolysis Gas Chromatographic Analyses		
			Phenolic Resin Only (5)		Nylon - 6 Only (6) ≠
Component	at 500°K	at 800°K	at 500°C	100-1000°C	at 400°C
H_2	1.45	43.25	15.1	50.1	0
H_2O	32.47	19.01	34.8	23.4	35.4
N_2	8.06	6.28	0	0	0
NH_3	0.02	0.02	0	0	0
HCN	10^{-11}	10^{-5}	0	0	0
CO	10^{-3}	1.85	4.5	5.5	0
CO_2	1.52	3.42	0.9	1.6	55.8
CH_4	56.48	26.15	7.8	10.0	0
C_2H_2	10^{-20}	10^{-10}	0	0	0
C_2H_4	10^{-10}	10^{-5}	0	0	0.4
C_6H_6	10^{-20}	10^{-13}	0.2	0.2	5.8
C_7H_8	*	*	0.8	0.3	0
C_6H_5OH	*	*	28.1	7.1	0
$(CH_3)_2C_6H_3OH$	*	*	7.8	1.8	0
Others	0	0	0	0	2.6
Total	100.0	100.0	100.0	100.0	100.0

* not considered due to the lack of the necessary free energy data for computations.

≠ liquid products that were obtained during the pyrolysis were not identified, constituted 95% of the total pyrolysis products.

oxygen and atomic hydrogen. The ratio of moles of solid carbon to total moles of gases was 1.55 at 500°K and 1.35 at 800°K.

Results given in Table 5 for the degradation products from phenolic resin by pyrolysis gas chromatographic analysis were reported by Sykes and Nelson (5). The composition is given at 500°C (773°K) and the average from 100°C to 1000°C for comparison. Also for comparison the composition of the degradation products from the pyrolysis of nylon by thermal gravimetric analysis is given in Table 5 from Madorski (6).

Examining these compositions it is seen that the order of magnitude is the same for the composition of the degradation products obtained from thermodynamic equilibrium calculations and a linear blend of the data from the thermal-gravimetric and pyrolysis gas chromatographic analyses. If these are the compounds that enter the char zone in high concentrations and examining the reactions reported in Tables B1 through B4, it can be concluded that the chemical reactions given in Table 1 are the ten important ones in the temperature range from 500°F to 2500°F.

These reactions were included in the non-equilibrium flow analysis to determine the energy transfered in the char zone. The analysis is currently being extended to cover a higher temperature range where a number of other reactions are important.

Nomenclature

A	cross sectional area of the char zone
c	concentration
H_j	enthalpy per unit mass of component j
K	number of species
k_f	forward reaction rate constant
k_r	reverse reaction rate constant
L	width of char zone
$\bar{M}$	average molecular weight of degredation products
M_j	molecular weight of component j
N_j	molal flux of component j
n	number of chemical reactions
p_{ij}	stochiometric coefficients of the products
Q	volumetric flow rate
q	heat flux
R	universal gas constant
R_j	reaction rate of component j in moles per unit time per unit volume
r_{ij}	stochiometric coefficients of the reactants
S_t	average residence time
V	volume of the char
W_g	mass flux of gas in the char pores
X_j	conversion of component j
x_j	mole fraction of component j
z	coordinate axis
γ	permeability

Δ	forward difference operator
ϵ	porosity
ρ	density
μ	viscosity

Subscripts

cz	refers to char zone
i	refers to chemical reactions
j	refers to specie
o	refers to initial value
L	refers to final value

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IX. APPENDIX A: DEVELOPMENT OF EQUATIONS OF CHANGE FOR FLOW IN THE CHAR ZONE

A. Energy Equation

Referring to Figure 6, the energy equation for one dimensional flow of gases through a porous medium accompanied by chemical reactions is obtained by simplifying the general energy equation (7), and this gives:

$$W_g \epsilon \bar{C}_p \frac{dT}{dz} = \epsilon \frac{d}{dz} \left[k_g \frac{dT}{dz} \right] - \epsilon \sum_{i=1}^{K} H_j r_j \qquad \text{(A1)}$$

The energy equation for the solid phase is:

$$0 = (1 - \epsilon) \frac{d}{dz} \left[k_c \frac{dT}{dz} \right] - (1 - \epsilon) H_c r_c \qquad \text{(A2)}$$

Adding equations (A1) and (A2) and defining:

$$k_e = \epsilon k_g + (1 - \epsilon) k_c \qquad \text{(A3)}$$

as the effective thermal conductivity of the char, gives the differential equation that describes the energy transfer in the char zone:

$$W_g \epsilon \bar{C}_p \frac{dT}{dz} = \frac{d}{dz} \left[k_e \frac{dT}{dz} \right] - \sum_{j=1}^{K+1} H_j r_j \qquad \text{(A4)}$$

For frozen flow in the char zone the above equation reduces to equation (A5):

$$W_g \bar{C}_p \epsilon \frac{dT}{dz} = \frac{d}{dz} \left[k_e \frac{dT}{dz} \right] \qquad \text{(A5)}$$

Expanding and rearranging results in a second order, ordinary differential equation which when solved gives the temperature profile in the char.

$$\frac{d^2T}{dz^2} = \frac{dT}{dz}\left[\frac{W_g\bar{C}_p\epsilon}{k_e} - \left(\frac{dk_e}{dT}\right)\left(\frac{dT}{dz}\right)\left(\frac{1}{k_e}\right)\right] \tag{A6}$$

The energy equation for the equilibrium flow model requires the evaluation of the summation term in equation (A4). Equation (10) for the reaction rate, r_j, can be written as:

$$r_j = \left(\frac{dN_j}{dT}\right)\cdot\left(\frac{dT}{dz}\right) \tag{A7}$$

Substituting (A7) into (A4) expanding and rearranging gives the energy equation for flow with chemical reaction:

$$\frac{d^2T}{dz^2} = \frac{dT}{dz}\left[\frac{W_g\epsilon\bar{C}_p}{k_e} - \left(\frac{dk_e}{dT}\right)\left(\frac{dT}{dz}\right)\left(\frac{1}{k_e}\right) + \left(\frac{1}{k_e}\right)\cdot\sum_{j=1}^{K+1}\frac{dN_j}{dT}\cdot M_j\cdot H_j\right] \tag{A8}$$

In equations (A6) and (A8), the surface temperatures are specified defining a two point boundary value problem. Therefore, an iterative procedure to find the correct initial slope that satisfies the boundary conditions was required to define the temperature profile in the char.

B. Momentum Equation

To obtain the pressure distribution within the char zone the momentum equation for flow in a porous media must be solved. Because of the relatively high gas mass flux values ($W_g \cong 0.06$ lb/ft^2-sec) inertial as well as viscous effects must be included. The equation with these terms is given below for one dimensional flow in a porous media:

$$-\frac{dP}{dz} = \epsilon\mu u/\gamma + \beta\rho u^2 \tag{A9}$$

where $\epsilon\mu u/\gamma$ represents the viscous term and $\beta\rho u^2$ the inertial term (11).

To obtain an equation applicable across a finite char thickness, the continuity equation, $W_g = \rho u$; and the ideal gas law, $\rho = \bar{P}\bar{M}/RT$ are combined with equation (A9) to give:

$$-PdP = \frac{RT}{\bar{M}} \cdot (\epsilon\mu\, W_g/\gamma + \beta\, W_g^2)\, dz \qquad \text{(A10)}$$

Integrating this equation from the front surface where the pressure is P_L to any point P into the char at z gives:

$$P = \left\{P_L^2 + 2R\left[\frac{\epsilon}{\gamma}\int_{z=z}^{z=L} \frac{W_g \mu T dz}{\bar{M}} + \beta \int_{z=z}^{z=L} \frac{W_g^2 T dz}{\bar{M}}\right]\right\}^{1/2}$$

(A11)

<u>Evaluation of γ and β from Experimental Data</u>: In order to solve equation (A11) for the pressure profile within the char zone, γ and β, the permeability and inertial coefficient, must be known. Data on γ and β for char materials are very scarce. However some data were recently obtained by Southern Research Institute (12) and these were used in this work. Their data were analyzed using the integrated form of equation (A10) given below:

$$\frac{\bar{M}\,\Delta(P^2)}{2W_g\bar{\mu}\,RTL} = \frac{\epsilon}{\gamma} + \beta\left(\frac{W_g}{\bar{\mu}}\right) \qquad \text{(A12)}$$

A plot of $\left[\frac{\bar{M}\,\Delta(P^2)}{2W_g\bar{\mu}\,RTL}\right]$ vs $\left(\frac{W_g}{\bar{\mu}}\right)$ is a straight line with ϵ/γ as the y-intercept and β, the slope.

A plot of the experimental data from Southern Research Institute (12) is shown in Figure A1.

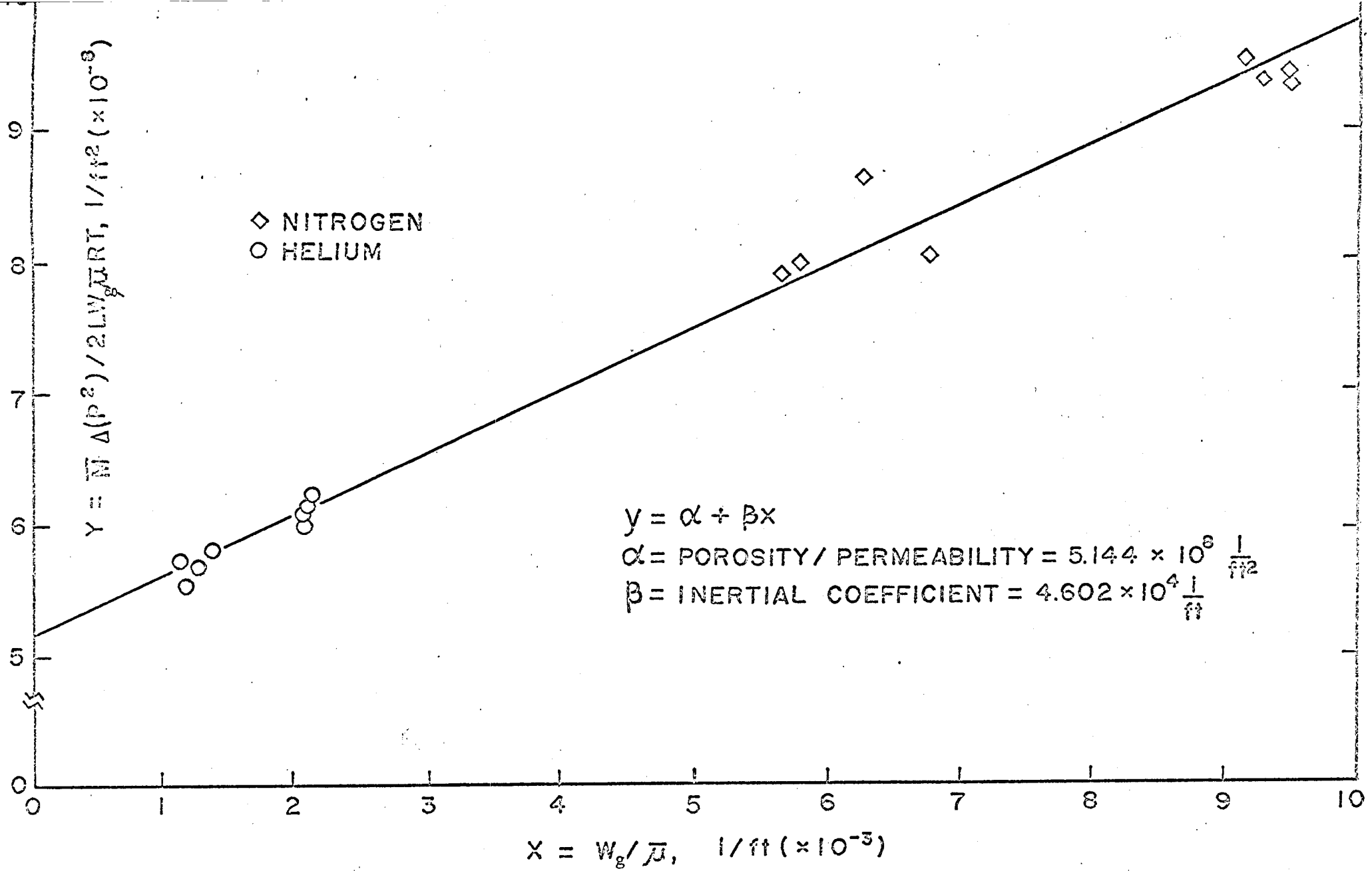


FIGURE A1 CORRELATION OF SOUTHERN RESEARCH INSTITUTE DATA FOR THE PERMEABILTY OF A CHARRED LOW DENSITY PHENOLIC-NYLON RESIN USING A CORNELL-KATZ PLOT

C. Heat Flux at the Char Surfaces

The heat fluxes at the char surfaces are the heat transfer by conduction to and from the surface and are given by:

$$q_L = k_e \left.\frac{dT}{dz}\right|_{z=L} \tag{A13}$$

$$q_o = k_e \left.\frac{dT}{dz}\right|_{z=0} \tag{A14}$$

Frozen Flow: Integrating equation (A5) for frozen flow gives:

$$q_{cz} = (q_L - q_o) = k_e \left.\frac{dT}{dz}\right|_{z=L} - k_e \left.\frac{dT}{dz}\right|_{z=o} = \epsilon \int_{T_o}^{T_L} W_g \bar{C}_p dT \tag{A15}$$

where the difference, $q_{cz} = q_L - q_o$, is the heat absorbed in the char zone.

Flow with Chemical Reaction: Integrating equation (A4) for flow with chemical reactions gives:

$$q_{cz} = \epsilon \sum_{i=j}^{K} \int_{T_o}^{T_L} W_g (C_{p_j}) x_j dT + \sum_{i=1}^{K+1} \int_{T_o}^{T_L} \frac{dN_j}{dT} M_j H_j dT \tag{A16}$$

where q_{cz} is the heat absorbed by a reacting gas mixture of K components.

D. Physical Properties

In order to solve equations (1) and (2) the values of the physical properties as functions of temperature are needed. For the heat capacity of each component the usual polynomial form is employed as shown below where the values of the coefficients are obtained from Hougen et.al. (8)

and McBride (9).

$$C_{p_i} = a + bT + cT^2 + dT^3 + eT^4 \tag{A17}$$

The mean heat capacity of the gas mixture is calculated using a molal weighted average as shown below:

$$\overline{C}_p = \sum_{i=1}^{K} (C_{p_i})\, y_i \tag{A18}$$

The overall thermal conductivity as a function of the gas conductivity, the char conductivity and the porosity is given by equation (A3).

$$k_e = (\overline{k}_g)\,(\epsilon) + (k_c)\,(1 - \epsilon)$$

In this study, experimental data reported for the char conductivity (10) were taken to be equal to the overall thermal conductivity. The reason is that the thermal conductivity measurements were made for char materials containing an inert gas in the pores (10). The equation for the char conductivity was obtained by a least square fit of the data reported for an inert gas within the pores of the char (10).

XI. APPENDIX B - ISOTHERMAL FLOW ANALYSIS

In this appendix the results of the computations of the conversion as a function of temperature are given for a number of chemical reactions. This is part of the information that was required to select the important reactions that occurred in the char zone in the temperature range from 500°F to 2500°F.

In Table B-1 the conversion of a number of hydrocarbon pyrolysis reactions are given in 500°F intervals from 500°F to 3000°F for a mass flux of 0.01 lb per ft^2sec. Similar results are given in Table B-2 for a number of oxygen and hydrogen reactions, in Table B-3 for nitrogen and ammonia reactions, and in Table B-4 for carbon, hydrocarbon and oxygen reactions. In Figure B-1 as flow diagram of the program is given that outlines the method of computing the conversion as discussed in the previous section of this report. Following the flow diagram a print-out of the computer program is given in Table B-5 along with a print-out of typical results.

The kinetic constants employed in the calculations were mainly obtained from a literature survey (3). In the comment column of Tables B-1, B-2, B-3, and B-4 the reference is given for the source of the kinetic data. The information given in these four tables should not be considered to be complete as additional data is being found almost every day. A future report will up-date this information and give a comparison of all of the kinetic data found in the literature.

Table B-1 Conversion of Pyrolysis Reactions in Percent for a Mass Flux of 0.01 lb per ft^2-sec

Equation	Temperature 500°f	1000°F	1500°F	2000°F	2500°F	3000°F	Comment
$CH_4 \rightarrow 1/2\ C_2H_6 + 1/2\ H_2$	0	0	0	0	20.3	100	(3)
$CH_4 \rightarrow C + 2\ H_2$	0	0	0	2.6	6.6	12.4	(13)
$CH_4 \rightarrow 1/2\ C_2H_2 + 1/2\ H_2$	0	0	0	0	4.2	7.4	(3)
$C_2H_6 \rightarrow (H_2,\ CH_4,\ C_2H_4,\ C)$	0	0	15.8	100	100	100	(3)
$C_2H_4 \rightarrow (C_2H_2,\ C_2H_6,\ CH_4,\ H_2)$	0	0	8.9	87.9	100	100	(3)
$C_2H_2 \rightarrow (C_1H_2,\ TrC_4H_2 > 900°k)$	0	0	0	0	1.8	6.7	(3), (14)
$C_3H_8 \rightarrow (C_3H_6,\ C_3H_4,\ CH_4,\ H_2)$	0	0	31.1	100	100	100	(3)
$C_3H_6 \rightarrow (H_2,\ CH_4,\ C_2H_4$,others)	0	0	2.7	100	100	100	(3)
$C_3H_6+H_2 \rightarrow CH_4 + C_2H_4\ (trC_3H_8,\ C_2H_8)$	0	0	0	1.0	15.2	60.9	(3)
Cyclobutane $\rightarrow 2C_2\ H_4$	0	1.2	100	100	100	100	(3)
Methylcyclobutane $\rightarrow C_2H_4+C_3H_8$	0	1.1	100	100	100	100	(3)
t-butanol $\rightarrow$ isobutene + H_2O	0	0	29.0	100	100	100	(3)
Cyclopentene $\rightarrow$ cyclopentadiene + H_2	0	0	70.1	100	100	100	(3)
$n\text{-}C_4H_{10} \rightarrow CH_4 + C_3H_6$	0	1.6	100	100	100	100	(3)
Isobutene $\rightarrow$ products	0	0	1.4	97.3	100	100	(3)
$C_6H_6 \rightarrow 3\ C_2H_2$	0	0	0	35.7	99.3	100	(3)
$C_6H_6 \rightarrow 1/2\ C_{12}H_{10} + 1/2\ H_2$	0	0	54.2	97.0	99.5	99.8	(3)
$CH_3CHO \rightarrow CH_4 + CO$	0	0	0	0	7.4	90.5	(3)

Table B-1 Continued

Equation	500°F	1000°F	1500°F	2000°F	2500°F	3000°F	Comment
$CH_2O \rightarrow H_2 + CO$	0	0	0	8.1	59.3	98.6	(3)
$CH_4 + H \rightarrow H_2 + CH_3$	100	100	100	100	100	100	(3)
$CH_2N_2 \rightarrow CH_2 + N_2$	0	100	100	100	100	100	(3)
$C_2H_6 + H \rightarrow C_2H_5 + H_2$	100	100	100	100	100	100	(3)
$C_2H_4 + H_2 \rightarrow C_2H_6$	0	0	0	1.2	11.6	44.7	(3)

Table B-2 Conversion of Hydrogen, Oxygen and Hydrogen - Oxygen Reactions in Percent for a Mass Flux of 0.01 lb per ft^2 sec.

Equation	500°F	1000°F	1500°F	2000°F	2500°F	3000°F	Comment
$H_2 + M \rightleftarrows 2H + M$	0	0	0	---	---	---	(3)
$O_2 + M \rightleftarrows 2O + M$	0	0	0	0	---	---	(3)
$2O_2 \rightleftarrows O_3 + O$	0	0	0	0	0	3.5	(3)
$O_3 + M \rightleftarrows O + O_2 + M$	0	0	0	0	100	100	(3)
$O + M \rightleftarrows O^+ + e^- + M$	0	0	0	0	0	0	(3)
$H + O_2 \rightleftarrows OH + O$	0	0	0	0	0	0	(3)
$O + H_2 \rightleftarrows OH + H$	0	0	0	0	0	0	(3)
$O + H_2O \rightleftarrows 2OH$	100	100	100	100	100	100	(3)
$H_2O + M \rightleftarrows OH + H + M$	0	0	0	---	---	---	(3)
$H_2O + H \rightleftarrows H_2 + OH$	100	100	100	100	100	100	(3)
$H_2 + O_2 \rightarrow 2OH$	0	0	0	0	0	4.7	(3)
$OH + M \rightleftarrows O + H + M$	0	0	0	---	---	---	(3)
$H_2 + O \rightleftarrows H_2O$	100	100	100	100	100	100	(3)
$H + O_2 + M \rightleftarrows HO_2 + M$	100	100	100	100	100	100	(3)

Table B - 3 Conversion of Nitrogen, and Ammonia Reaction in Percent for a Mass Flux of 0.01 lb per ft^2 sec.

Equation	500°F	1000°F	1500°F	2000°F	2500°F	3000°F	Comment
$N_2 + M \rightleftarrows 2N + M$	0	0	0	0	0	0	(3)
$2NO \rightleftarrows NO_2 + N$	0	0	0	0	0	1.3	(3)
$2NO \rightleftarrows N_2 + O_2$	0	0	0	0	0	1.1	(3)
$NO + M \rightleftarrows N + O + M$	0	0	0	---	---	---	(3)
$NO_2 + M \rightleftarrows NO + O + M$	0	0	0	0	100	100	(3)
$N_2O \rightleftarrows N_2 + 1/2\ O_2$	0	0	0	47.0	100	100	(3)
$N_2O + M \rightleftarrows N_2 + O + M$	0	0	0	0	0	3.5	(3)
$N_2O + O \rightleftarrows N_2 + O_2$	3.4	62.0	90.0	95.7	97.4	98.1	(3)
$N_2O + O \rightleftarrows 2NO$	0	71.5	99.1	100	100	100	(3)
$NO + O \rightleftarrows O_2 + N$	0	0	0	0	0	0	(3)
$NO + N \rightleftarrows N_2 + O$	100	100	100	100	100	100	(3)
$NO + O_2 \rightleftarrows NO_2 + O$	0	0	0	0.7	7.4	30.3	(3)
$NO + N_2 \rightleftarrows N_2O + N$	0	0	0	0	0	0	(3)
$NO + N_2O \rightleftarrows NO_2 + N_2$	0	0	0.6	27.8	85.6	95.0	(3)
$NO_2 + O_2 \rightleftarrows N_2 + O_2 + O$	0	0	0	0	0	0	(3)
$NO_2 + O_2 \rightleftarrows NO + O_3$	0	0	0.9	54.1	100	100	(3)
$NO_3 + M \rightleftarrows NO_2 + O + M$	0	0	0	0	0	0	(3)

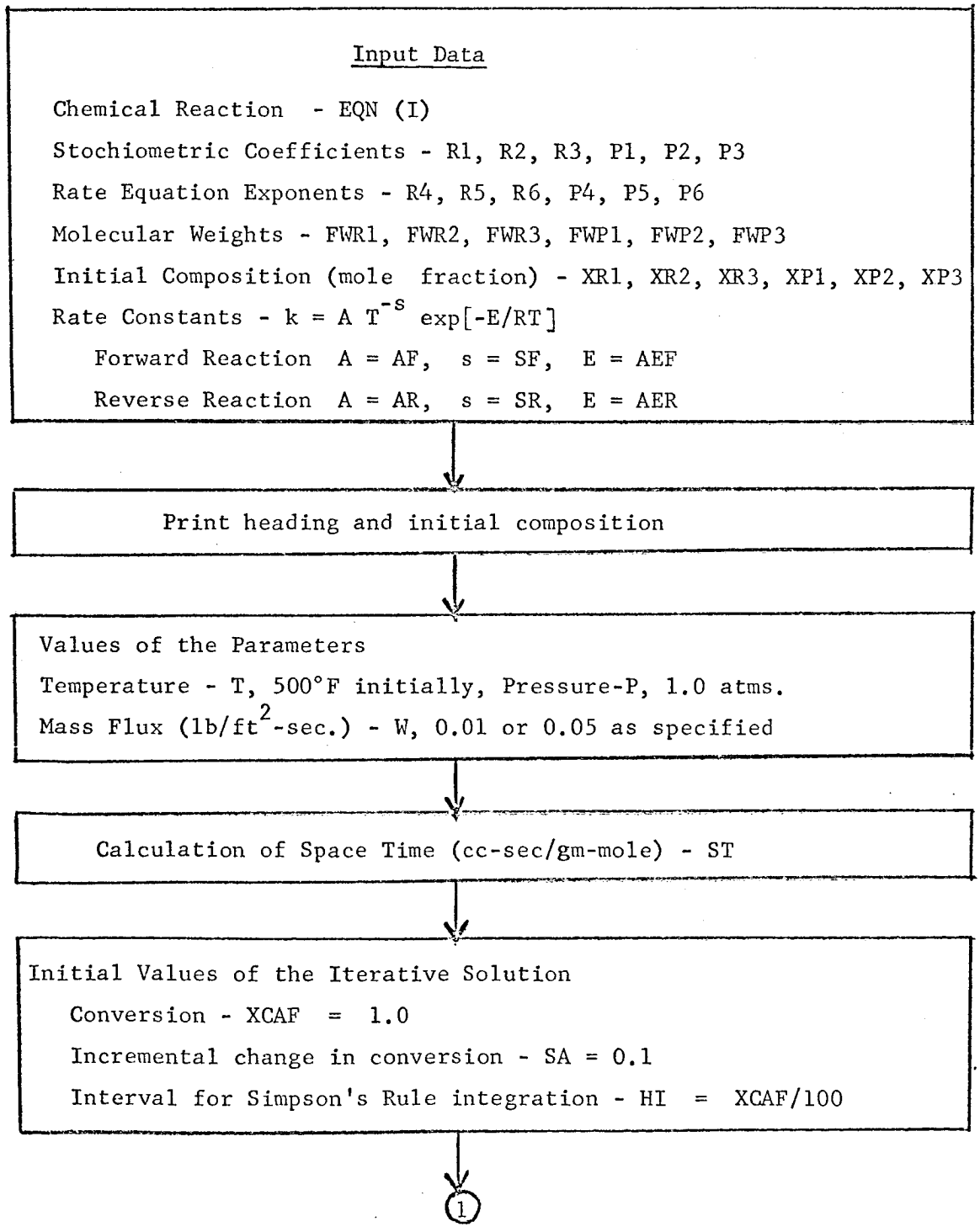
Table B-3 Continued

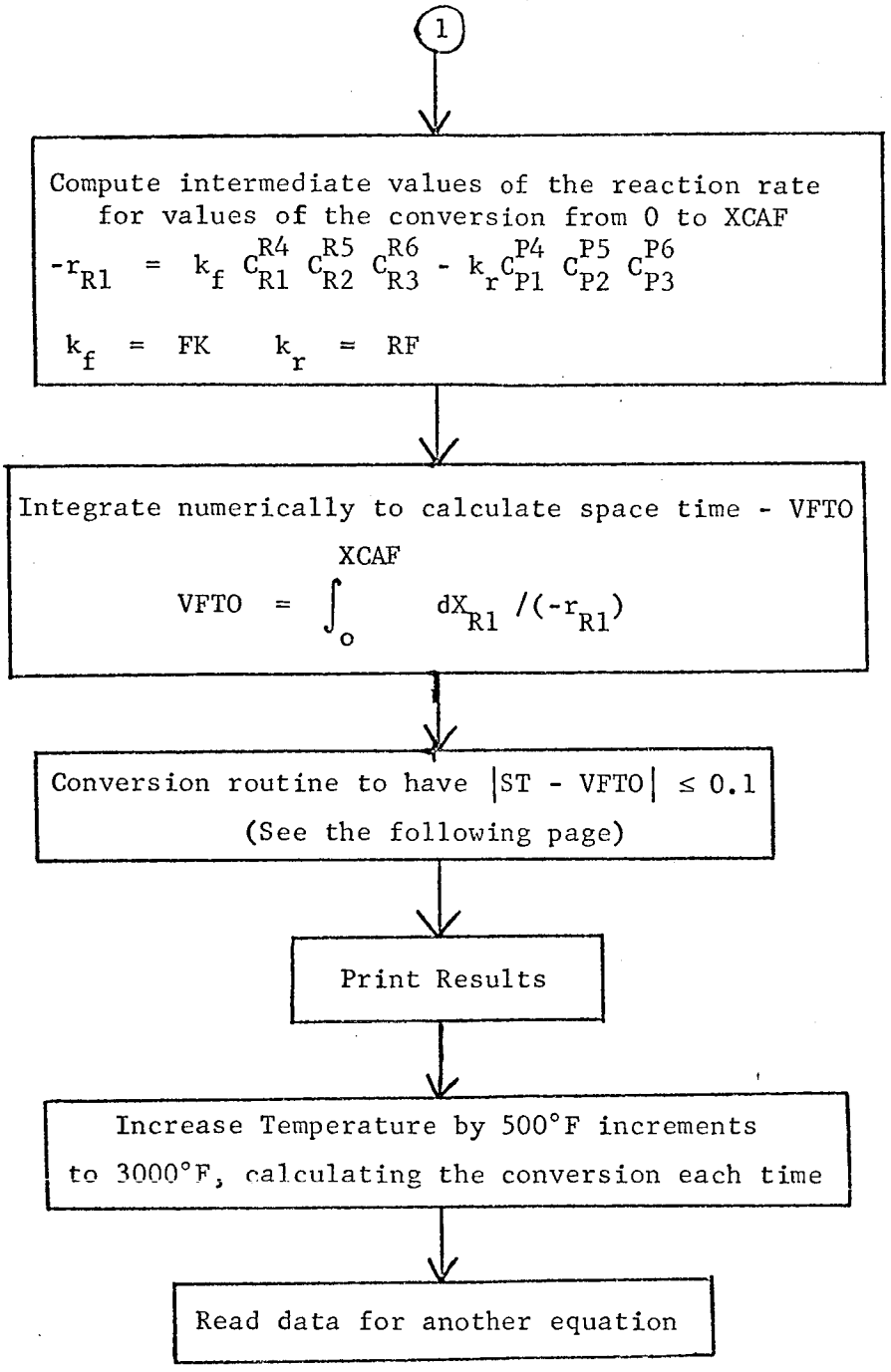
Equation	500°F	1000°F	1500°F	2000°F	2500°F	3000°F	Comment
$H + N_2O \rightleftarrows N_2 + OH$	98.4	100	100	100	100	100	(3)
$NH_3(g) + C_{(s)} \rightleftarrows HCN(s) + H_2(g)$	0	0	0	0	0	0	(3)
$NH_3 \rightleftarrows 1/2\ N_2 + 3/2\ H_2$	0	0	0	0	0	0.6	(3)
$NH_3 + 5/2\ O \rightleftarrows 3/2\ H_2O + NO$	100	100	100	100	100	100	(3)
$N + M \rightleftarrows N^+ + e^- + M$	0	0	0	0	0	0	(3)
$N + NO \rightleftarrows N_2 + O^+ + e^-$	0	0	0	0	0	0	(3)
$N_2^+ + e^- \rightleftarrows 2N$	100	100	100	100	100	100	(3)
$N_2^+ + N \rightleftarrows N_2 + N^+$	0	0	0	0	0.	0	(3)
$O_2^+ + e^- \rightleftarrows 2O$	100	100	100	100	100	100	(3)

Table B-4 Conversion of Carbon, Hydrocarbon, and Oxygen Reaction in Percent for a Mass Flux of 0.01 lb per ft^2 sec

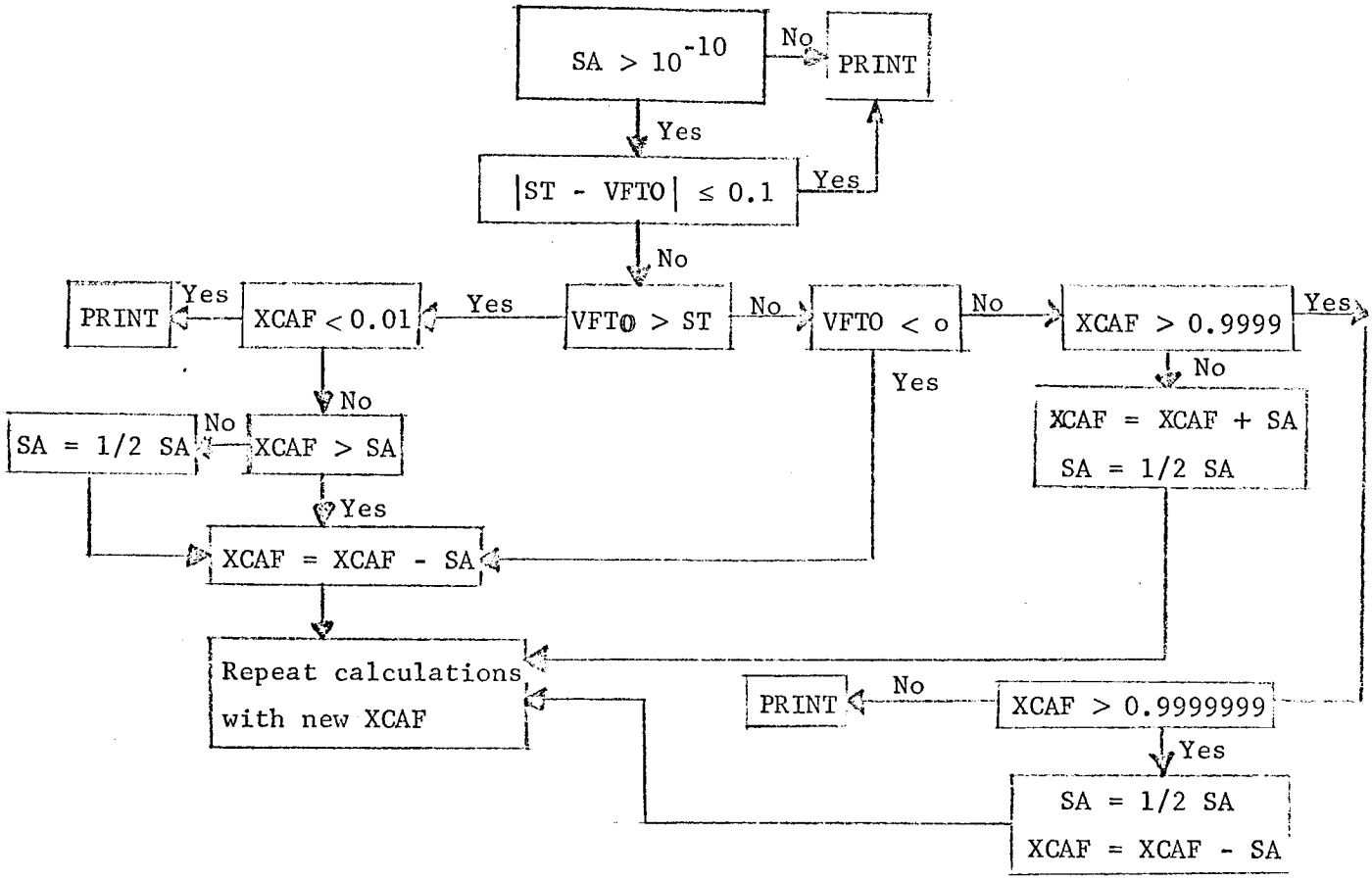
Equation	500°F	1000°F	1500°F	2000°F	2500°F	3000°F	Comment
$C(s) + CO_2(g) \rightleftarrows 2CO$	0	0	0	55.6	100	100	(3)
$CO_2 + M \rightleftarrows CO + O + M$	0	0	0	0	4.9	100	(3)
$CH_4 + O_2 \rightarrow (CO, CO_2, H_2O, CH_2O, \ldots)$	0	0	20.2	59.3	78.0	---	(3)
$CH_4 + O_2 \rightarrow (CO, CO_2, H_2O, CH_2O, \ldots)$	1.0	57.6	86.5	93.2	95.5	---	(3)
$CH_4 + O + M \rightarrow CO, CO_2, H_2O, CH_2O \ldots$	0	0	0	0	0	0	(3)
$C_3O_2 \rightarrow C(s) + 2CO$	0	7.0	100	100	100	100	(3)
$CO + OH \rightleftarrows H + CO_2$	100	100	100	100	100	100	(3)
$CH_4 + OH \rightleftarrows CH_3 + H_2O$	100	100	100	100	100	100	(3)

Figure B-1. Flow Diagram of the Computer Program to Compute the Conversion of a Chemical Reaction Occurring in the Char Zone Isothermally




1
Compute intermediate values of the reaction rate for values of the conversion from 0 to XCAF
$-r_{R1} = k_f C_{R1}^{R4} C_{R2}^{R5} C_{R3}^{R6} - k_r C_{P1}^{P4} C_{P2}^{P5} C_{P3}^{P6}$
k_f = FK k_r = RF
Integrate numerically to calculate space time - VFTO
$VFTO = \int_0^{XCAF} dX_{R1} / (-r_{R1})$
Conversion routine to have $|ST - VFTO| \leq 0.1$
(See the following page)
Print Results
Increase Temperature by 500°F increments to 3000°F, calculating the conversion each time
Read data for another equation

Conversion Routine



```
$IBFTC MAIN
C       NASA PROJECT NO. 135-30-8621
C       CALCULATION OF THE CONVERSION FOR CHEMICAL REACTIONS
C       THAT POSSIBLY OCCUR IN THE DECOMPOSITION ZONE OF
C       CHARRING ABLATORS. THE RESULTS COMPUTED ARE FOR THE
C       ISOTHERMAL FLOW IN THE CHAR ZONE AT TEMPERATURES
C       FROM 500.0-OF TO 3000.0-OF
C       NASA GRANT NGR-19-001-016
C       EVALUATION OF THE ENERGY TRANSFER IN THE CHAR ZONE DURING ABLATION
C       PROJECT NUMBER 1303 53067
C
        DIMENSION Y(150), EQN(150)
C
C       READ THE EQUATION R1+R2+R3=P1+P2+P3
 1111   READ729,(EQN(I),I=1,12)
 729    FORMAT(12A6)
C
C       READ THE STOCHIOMETRIC COEFFICIENTS OF THE RATE EQUATION
        READ730,R1,R2,R3,P1,P2,P3
C
C       READ EXPONENTS ON THE COMPOSITIONS OF THE RATE EQUATION
        READ 730,R4,R5,R6,P4,P5,P6
 730    FORMAT(6F4.0)
C
C       READ THE MOL WGT OF THE COMPONENTS
        READ731,FWR1,FWR2,FWR3,FWP1,FWP2,FWP3
 731    FORMAT(6F5.0)
C
C       READ THE INITIAL COMPOSITION OF THE REACTANTS IN MOLE FRACTION
        READ5,XR1,XR2,XR3,XP1,XP2,XP3
 5      FORMAT(6E10.0)
C
C       READ THE COEFFICIENTS OF THE FORWARD REACTION RATE CONSTANT
C       UNITS OF AF ARE IN CUBIC-CM,GM-MOLES AND SEC
C       UNITS OF AEF ARE IN KCAL PER GM-MOLE
        READ733,AF,SF,AEF
 733    FORMAT(E8.0,2F6.0)
C
C       READ THE COEFFICIENTS OF THE REVERSE REACTION RATE CONSTANT
C       UNITS OF AR ARE IN CUBIC-CM,GM-MOLES AND SEC
C       UNITS OF AER ARE IN KCAL PER GM-MOLE
        READ733,AR,SR,AER
C
 828    PRINT829,(EQN(I),I=1,12)
 829    FORMAT(1H1,12A6)
        PRINT 830
 830    FORMAT( 1X,35HINITIAL COMPOSITION (MOLE FRACTION))
        PRINT 833,XR1,XR2,XR3,XP1,XP2,XP3
```

```
C
      PRINT 831
 831  FORMAT(1HC,105HFINAL COMPOSITION (MOLE FRACTION)
     1 TEMP  FRACTIONAL  SP.TIME(CC-SEC/MOL) REACTION RATE  )
      PRINT 8311
 8311 FORMAT(1H ,105H    R1        R2        R3        P1        P2        P3
     1 (OF)  CONVERSION  COMPUTED  SPECIFIED (MOL/CC-SEC)   )
C
C     MASS FLUX OF DECOMPOSITION PRODUCTS, W, IN LB/FT2-SEC
      W=0.01
C
C     INITIAL VALUE OF TEMPERATURE,T,IS 500-OF
      T=500.
C     INITIAL VALUE OF THE PRESSURE ,P, IS 1.0 ATMS
      P=1.0
C     GAS CONSTANT,R,IN CALORIES/GMMOLE-OK
      R=1.987
C
C     CALCULATION OF THE AVERAGE MOL WGT OF THE GAS,FWA
C     ENTERING THE CHAR ZONE
      FWAR=FWR1*XR1+FWR2*XR2+FWR3*XR3
      FWAP=FWP1*XP1+FWP2*XP2+FWP3*XP3
      FWA=FWAR+FWAP
C
C     CALCULATION OF THE MOLAL FLOW RATE OF THE GAS,FTO
C     FTO HAS UNITS OF GMMOLES PER FT-FT SEC
      FTO=(454.0*W)/FWA
C
C     CALCULATION OF MOLAL FLUX OF THE INDIVIDUAL COMPONENTS
C     MOLAL FLUX UNITS ARE GMMOLES PER FT-FT SEC
      FR10=XR1*FTO
      FR20=XR2*FTO
      FR30=XR3*FTO
      FP10=XP1*FTO
      FP20=XP2*FTO
      FP30=XP3*FTO
C
C     CALCULATION OF THE SPACE TIME,ST,IN CUBIC-CM SEC/GMMOLES
      ST=(0.25*144.0)/(FTO*0.06103)
C
C     CONVERSION OF 100 PERCENT IS ASSUMED INITIALLY
C     XCAF IS THE CONVERSION OF COMPONENT A, INITIALLY 1.0
      XCAF=1.0
C     NO CONVERSION OF PRODUCTS INITIALLY
      XCA=0.0
C     INITIAL INCREMENTAL CHANGE,SA,OF THE CONVERSION XCAF
      SA=0.1
C
C     CALCULATION OF SPACE TIME FOR AN ASSUMED CONVERSION,XCAF.
C     REPEAT CALCULATIONS UNTIL CALCULATED SPACE TIME IS EQUAL
C     TO THE KNOWN VALUE. THIS DETERMINES THE CORRECT VALUE
C     OF THE FINAL CONVERSION
C
C     FIRST
C     DETERMINE CONCENTRATION OF COMPONENTS FOR VARIOUS
C     INTERMEDIATE CONVERSIONS,XCA.CONCENTRATION ARE
C     IN GM-MOLES/CUBIC-CM
C     INCREMENTAL CHANGE IN XCA IS HI
 2222 HI=XCAF/100.0
```

```
      XCA=C.0
C
      CC1 I=1,101
C
C     F/S ARE MCLAL FLUXES CORRESPONDING TO CONVERSION XCA
C     MOLAL FLUXES HAVF UNITS OF GMMCLES/FT-FT SEC
C
      FR1=(1.0-XCA)*FR1O
      FR2=FR2C-(FR1O*XCA*R2)/R1
      FR3=FR3O-(FR1O*XCA*R3)/R1
      FP1=FP1O+(FR1O*XCA*P1)/R1
      FP2=FP2C+(FR1O*XCA*P2)/R1
      FP3=FP3C+(FR1O*XCA*P3)/R1
C
C     THE TOTAL MOLAL FLUX CORRESPONDING TO CONVERSION XCA IS FT
C     FT HAS UNITS OF CM-MOLES/FT-FT-SEC
      FT=FTC+(FR1O*XCA)*(P1+P2+P3-R1-R2-R3)/R1
C
C     CALCULATICN OF THE COMPOSITION OF THE REACTING MIXTURE
C     C/S ARE CCNCENTRATIONS IN GMMOLES/CUBIC-CM
      RR=82.054
      TCK=(T+460.0)/1.8
      H=P/(RR*TCK*FT)
      CR1=FR1*H
      CR2=FR2*H
      CR3=FR3*H
      CP1=FP1*H
      CP2=FP2*H
      CP3=FP3*H
C
C     CALCULATICN OF RATE CONSTANTS FOR FORWARD AND REVERSE REACTIONS
C     RATE CONSTANT UNITS ARE IN CUBIC CM,GMMOLES AND SEC
C
C     FCRWARD REACTICN RATE CONSTANT, FK
      FK=AF*TOK**(-SF)*EXP((-AEF*1C00.0)/(R*TOK))
C
C     REVERSE REACTICN RATE CONSTANT, RK
      RK=AR*TOK**(-SR)*EXP((-AER*1C00.0)/(R*TOK))
C
C     CALCULATICN OF REACTION RATE,RA,OF COMPONENT A
C     RA HAS UNITS OF GMMOLES/CUBIC-CM SEC
      RA=FK*(CR1**R4)*(CR2**R5)*(CR3**R6)-RK*(CP1**P4)*(CP2**P5)*
     1(CP3**P6)
C
C     CALCULATICN OF FUNCTION UNDER INTEGRAL-1/RA=Y(I)
      Y(I)=1.0/RA
C
C
 1    XCA=XCA+HI
C     STEP XCA TO GENERATE 101 VALUES OF Y(I)
C     CALCULATICN OF FINAL COMPOSITION (MOLE FRACTION)
      YR1=FR1/FT
      YR2=FR2/FT
      YR3=FR3/FT
      YP1=FP1/FT
      YP2=FP2/FT
      YP3=FP3/FT
C
C     CALCULATICN OF SPACE TIME FOR THE SPECIFIED CONVERSION,XCAF
```

```
C       INTEGRATICN IS PERFORMED USING SIMPSONS RULE
        SUM1=0.0
        SUM2=0.0
        DO2 I=2,100
 2      SUM1=2.0*Y(I)+SUM1
        DO3 I=2,100,2
 3      SUM2=2.0*Y(I)+SUM2
C       INTEGRAL VALUE IS VINT-UNITS ARE CUBIC-CM SEC/GMMOLES OF A
        VINT=(HI/3.0)*(Y(1)+SUM1+SUM2+Y(101))
C       SPACE TIME CALCULATED IS VFTO-UNITS ARE CUBIC-CM SEC/GMMOLES
        VFTO=XR1*VINT
C
C
C       COMPUTATICN STOPS IF SA IS LESS THAN 1.0E-10
        IF(SA.GT.1.0E-10)GO TO 777
        GO TO 123
 777    CONTINUE
C       DETERMINE IF THE DIFFERENCE BETWEEN THE SPECIFIED AND
C       CALCULATED SPACE TIME IS WITHIN 0.1. IF YES INCREASE THE
C       TEMPERATURE BY 500-OF
        CALL SSWTCH(1,JOB)
        GO TO (1111,778),JOB
 778    IF(ABS(ST-VFTO).LT.0.1) GO TO 123
C
C       DETERMINE IF VFTO IS GREATER THAN ST
        IF(VFTO.GT.ST)GOTO1234
C
C       VFTO IS LESS THAN ST
C
C       IS VFTO NEGATIVE
C       YES-REDUCE XCAF
C       NO-CONTINUE
        IF(VFTO.LT.0.0) GO TO 1321
C
C       THE CALCULATICN STOPS IF THE CONVERSION IS GREATER THAN 99.99  PERCENT
        IF(XCAF.GT.0.9999)GO TO 321
C
C       THE PREVIOUS VALUE OF VFTO IS RECALCULATED BY INCREASING
C       XCAF BY THE AMOUNT OF SA
C       THEN CHANGE SA TO 0.5*SA
        XCAF=XCAF+SA
        SA=0.5*SA
        GOTO 2222
C
C       CHECK TO INSURE XCAF IS LESS THAN 1.0
  321   IF(XCAF.GT.0.9999999)GO TO 112
        GOTO123
  112   SA=0.5*SA
        XCAF = XCAF - SA
        GO TO 2222
C
C       VFTO IS GREATER THAN ST
C
C       THE CALCULATION STOPS IF THE CONVERSION IS LESS THAN 0.05 PERCENT
 1234   IF(XCAF.LE.0.01)GOTO123
C
C
C       A CHECK TO PREVENT XCAF - SA = 0
 1321   IF(XCAF.GT.SA) GO TO 4321
```

```
      SA = 0.5*SA
C
C     THE VALUE OF XCAF IS REDUCED BY THE VALUE OF SA
 4321 XCAF=XCAF-SA
C
C     THEN THE CALCULATICN IS REPEATED TO DETERMINE A
C     NEW SPACE TIME FOR COMPARISON
C
      GO TC  2222
C
C     VFTC IS ESSENTIALLY EQUAL TO ST (WITHIN 0.1)
C                          OR
C     CONVERSICN, XCAF, IS LESS THAN 0.5 PERCENT
C                          OR
C     CONVERSION, XCAF, IS GREATER THAN 99.99  PERCENT
C     PRINT THE RESULTS
  123 PRINT 833,YR1,YR2,YR3,YP1,YP2,YP3,T,XCAF,VFTO,ST,RA
  833 FORMAT(1HC,6F8.4,F9.1,F8.4,3E12.5)
C
C     READ NEW DATA IF THE CONVERSION IS 100 PERCENT
C     CONVERSICN WILL BE 100 PERCENT FOR ALL HIGHER TEMPERATURES
      IF(XCAF.GT.0.99) GO TO 2208
C
C     THEN REPEAT THE CALCULATIONS AT THE NEW TEMPERATURE
C
C     INCREASE THE TEMPERATURE BY 500-OF
      T=T+500.
C
C     RESET XCAF AND SA
      SA = 0.1
      XCAF=1.0
C
C     IF THE TEMPERATURE IS LESS THAN OR EQUAL TO 7000-OF
C     CONTINUE THE CALCULATION
      IF(T.LE.7000.0)GOTO 2222
C
C
C     PRINT DATA
 2208 PRINT 2209,W
 2209 FORMAT(1H-,25H MASS FLUX(LB/FT2-SEC) = , F8.4)
      PRINT2210,AF,SF,AEF
 2210 FORMAT(1HC,3HAF=,E9.2,5H  SF=,F6.2,6H  AEF=,F6.1)
      PRINT2211,AR,SR,AER
 2211 FORMAT(1HO,3HAR=,E9.2,5H  SR=,F6.2,6H  AER=,F6.1)
      PRINT2212
 2212 FORMAT(1HO,29HFWR1 FWR2 FWR3 FWP1 FWP2 FWP3)
      PRINT2213,FWR1,FWR2,FWR3,FWP1,FWP2,FWP3
 2213 FORMAT(1HO,6F6.1)
      PRINT 2218
 2218 FORMAT(1HO,28H  STOCHIOMETRIC COEFFICIENTS)
      PRINT2214
 2214 FORMAT(1HC,24H  R1  R2  R3  P1  P2  P3)
      PRINT2215,R1,R2,R3,P1,P2,P3
 2215 FORMAT(1HO,6F4.1)
      PRINT 2219
 2219 FORMAT(1HO,45H  EXPONENTS ON THE COMP. OF THE RATE EQUATICN)
      PRINT 2216
 2216 FORMAT(1HO,24H  R4  R5  R6  P4  P5  P6)
      PRINT 2217,R4,R5,P4,P5,P6
```

```
 2217 FORMAT(1HC,6F4.1/1H1)
C     READ IN NEW DATA FOR CALCULATIONS OF NEXT EQUATION
      GOTO1111
   24 STOP
      END
$ENTRY
```

C + CO2 = 2CO

INITIAL COMPOSITION (MOLE FRACTION)

0.5000	0.5000	0.0000	0.0000	0.0000	0.0000

FINAL COMPOSITION (MOLE FRACTION)

R1	R2	R3	P1	P2	P3	TEMP (OF)	FRACTIONAL CONVERSION	SP.TIME(CC-SEC/MOL) COMPUTED	SP.TIME(CC-SEC/MOL) SPECIFIED	REACTION RATE (MOL/CC-SEC)
0.4969	0.4969	0.0000	0.0062	0.0000	0.0000	500.0	0.0062	0.14224E 23	0.36380E 04	0.21970E-24
0.4969	0.4969	0.0000	0.0062	0.0000	0.0000	1000.0	0.0062	0.16729E 11	0.36380E 04	0.18680E-12
0.4969	0.4969	0.0000	0.0062	0.0000	0.0000	1500.0	0.0062	0.24013E 05	0.36380E 04	0.13014E-06
0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	2000.0	1.0000	0.13083E 04	0.36380E 04	0.38215E-03

MASS FLUX(LB/FT2-SEC) = 0.0100

AF= 0.15E 11 SF= 0.00 AEF= 85.0

AR= 0.10E-29 SR= 0.00 AER= 0.0

FWR1 FWR2 FWR3 FWP1 FWP2 FWP3

12.0 44.0 0.0 28.0 0.0 0.0

STOCHIOMETRIC COEFFICIENTS

R1 R2 R3 P1 P2 P3

1.0 1.0 0.0 2.0 0.0 0.0

EXPONENTS ON THE COMP. OF THE RATE EQUATION

R4 R5 R6 P4 P5 P6

0.0 0.0 0.0 0.0 0.0

APPENDIX C

TEMPRE - PROGRAM FOR THE SOLUTION OF THE FROZEN FLOW, EQUILIBRIUM AND NON-EQUILIBRIA FLOW MODELS

The program for the solution of the frozen flow, equilibrium and non-equilibrium flow cases is composed of several individually tested programs written in Fortran IV for the IBM 7040 computer. These are labeled TEMPRE, PROPT, OMEGA, CHAR, MOLFRA, MATINV AND KINET, represented in Figures C1-C5 . The specific function of each will be discussed in detail in the following section.

TEMPRE

This program forms the core of the entire system. All common input information required by the system is channeled through TEMPRE to the specific subprograms. The main function of TEMPRE is to calculate the temperature distribution using a fourth order Runge-Kutta analysis which includes the convergence sequence used in determining the initial slope needed to produce a valid profile.

A second portion of TEMPRE is used to calculate the pressure distribution and heat flux within the char zone. Simpson's Rule is used to evaluate integrals in the pressure distribution and heat flux equations. Subprogram OMEGA is used as an interpolation program to first calculate the viscosity of the gas mixture from the collision integral table and secondly to interpolate from the temperature distribution (previously generated in TEMPRE) for values corresponding to a specific char depth.

PROPT

This is the first major subprogram which calculates the physical property data for the gases as functions of temperature (heat capacity, thermal conductivity, change in thermal conductivity with temperature). Information is retrieved from PROPT at each temperature interval generated in the Runge-Kutta analysis in TEMPRE. Subprogram PROPT depends on OMEGA for the value of the collision integral necessary in calculating the gas physical properties and CHAR for the value of the char thermal conductivity.

OMEGA

This is the first minor subprogram which calculates the collision integral for a pure gas at a specified temperature level. An $n^{\underline{th}}$ order Lagrangian interpolation procedure is used to select the value from a table containing the collision integral as a function of temperature and the pure gas in question.

CHAR

This minor subprogram fits a curve to available char thermal conductivity data for use in calculating an effective conductivity value. Any curve fitting method which best describes the given data can be used.

The above programs comprise the system for the frozen flow model. Extension to include the equilibrium flow model is accomplished by the addition of MOLFRA AND MATINV, while the non-equilibrium flow model requires the addition of KINET to the frozen flow programs.

MOLFRA

This is the second major subprogram which is used to determine the

equilibrium gas composition (in term of mole fractions), average molecular weight, net change in the total molar flux, and reaction rate expression as functions of temperature. The procedure involves the minimization of the free energy at various tabulated temperature levels. Transfer of data from MOLFRA to TEMPRE is accomplished using OMEGA as an interpolation method.

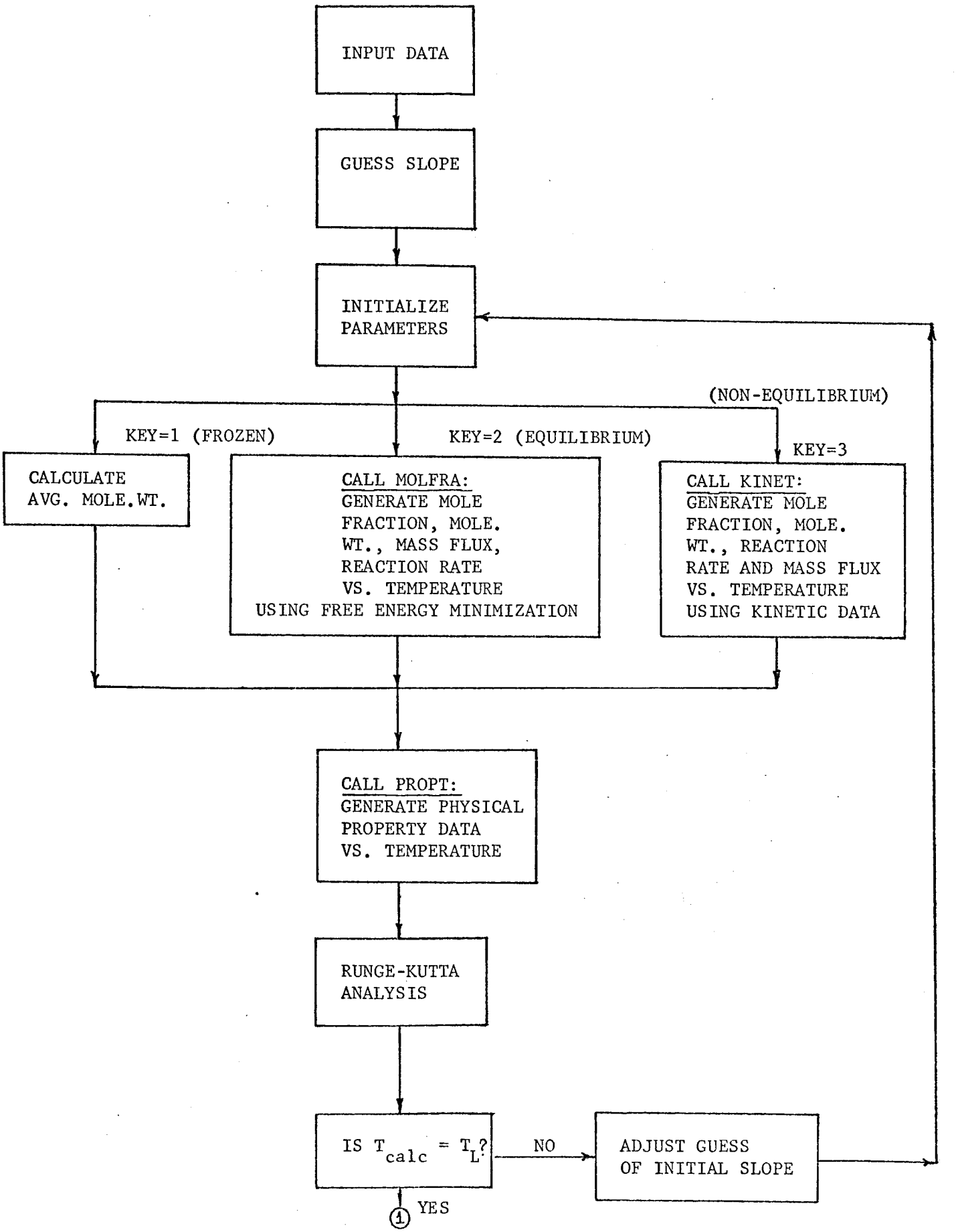
MATINV

This minor subprogram is used to find the inverse of a non-singular N x N matrix. The inversion is performed iteratively by reducing the original matrix to an identity matrix by a sequence of row operations followed by applying the same operation to the identity matrix to generate the inverse.

KINET

This is the third major subprogram which estimates the composition (in terms of mole fractions), average mole weight, mass flux and reaction rate as a function of temperature supplied from TEMPRE. The procedure utilizes the kinetic data of pertinent chemical reactions that occur in the char zone. Transfer of data for the temperature profile is accomplished in the argument of the call statement. After calculation of the correct temperature profile pertinent data is retreived from KINET using OMEGA, the interpolation subprogram.

FIGURE C 1
TEMPRE-PROGRAM FOR THE CALCULATION OF THE TEMPERATURE-PRESSURE PROFILES AND THE HEAT FLUX AT THE SURFACE IN THE CHAR ZONE OF A CHARRING ABLATOR



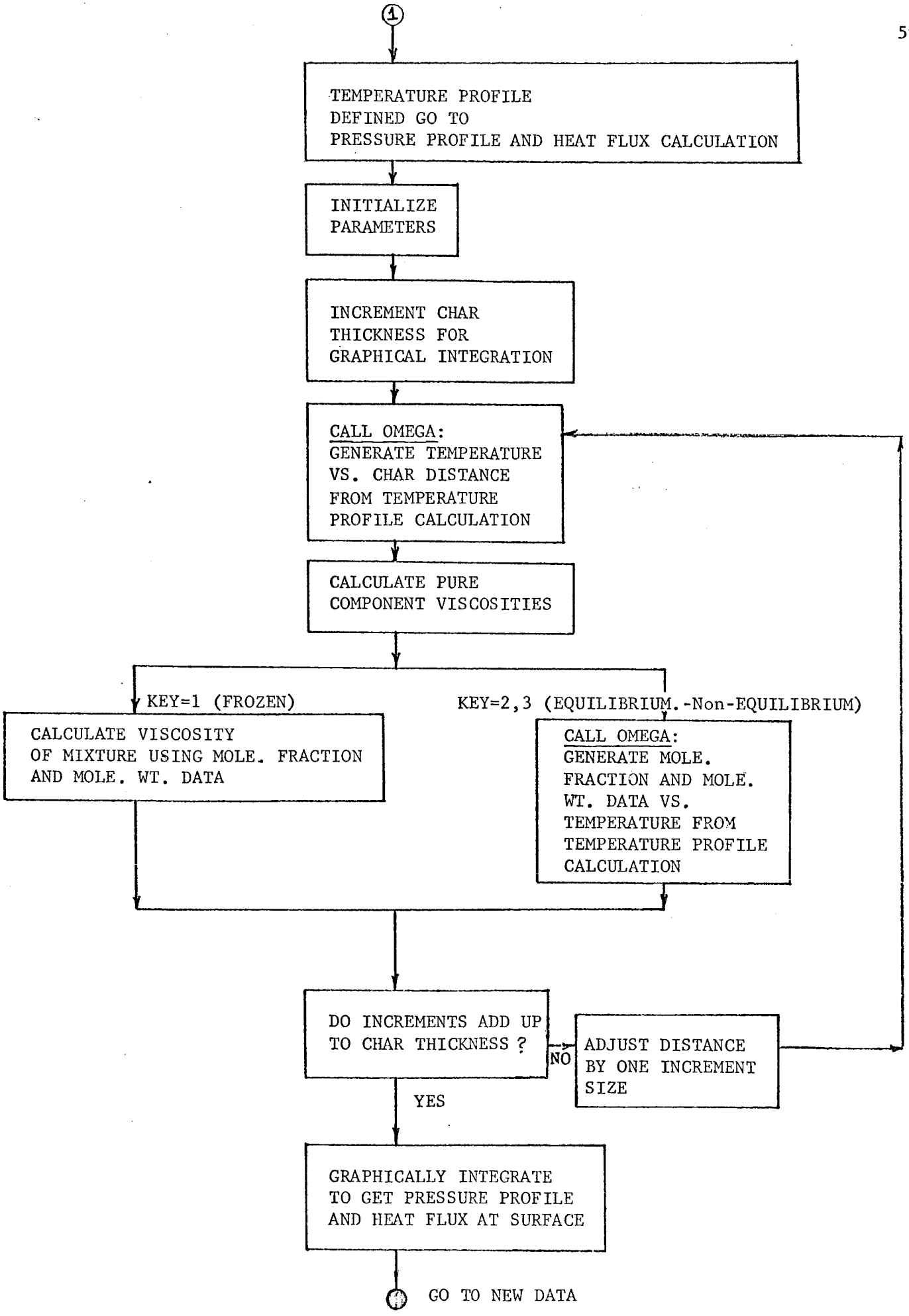

1
TEMPERATURE PROFILE DEFINED GO TO PRESSURE PROFILE AND HEAT FLUX CALCULATION
INITIALIZE PARAMETERS
INCREMENT CHAR THICKNESS FOR GRAPHICAL INTEGRATION
CALL OMEGA: GENERATE TEMPERATURE VS. CHAR DISTANCE FROM TEMPERATURE PROFILE CALCULATION
CALCULATE PURE COMPONENT VISCOSITIES
KEY=1 (FROZEN)
KEY=2,3 (EQUILIBRIUM.-Non-EQUILIBRIUM)
CALCULATE VISCOSITY OF MIXTURE USING MOLE. FRACTION AND MOLE. WT. DATA
CALL OMEGA: GENERATE MOLE. FRACTION AND MOLE. WT. DATA VS. TEMPERATURE FROM TEMPERATURE PROFILE CALCULATION
DO INCREMENTS ADD UP TO CHAR THICKNESS ?
NO
ADJUST DISTANCE BY ONE INCREMENT SIZE
YES
GRAPHICALLY INTEGRATE TO GET PRESSURE PROFILE AND HEAT FLUX AT SURFACE
1
GO TO NEW DATA

Figure C 2
PROPT - SUBPROGRAM FOR CALCULATING
PHYSICAL PROPERTY DATA

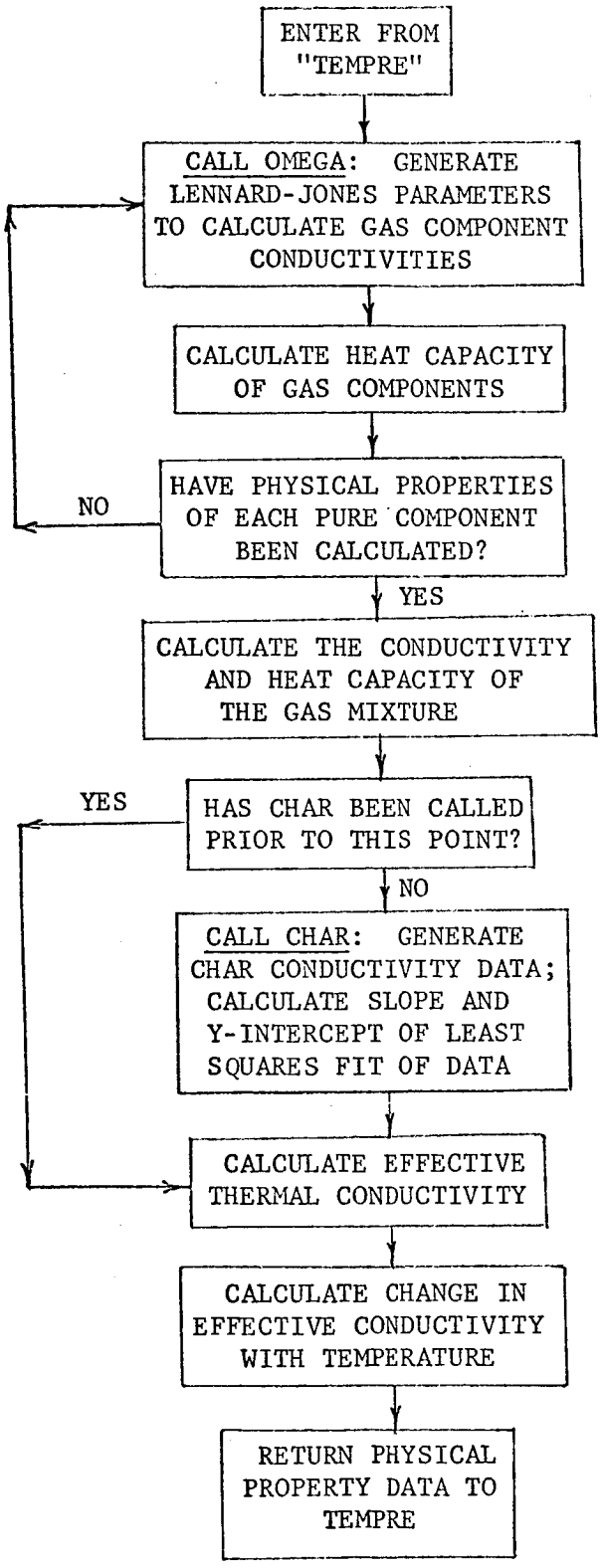
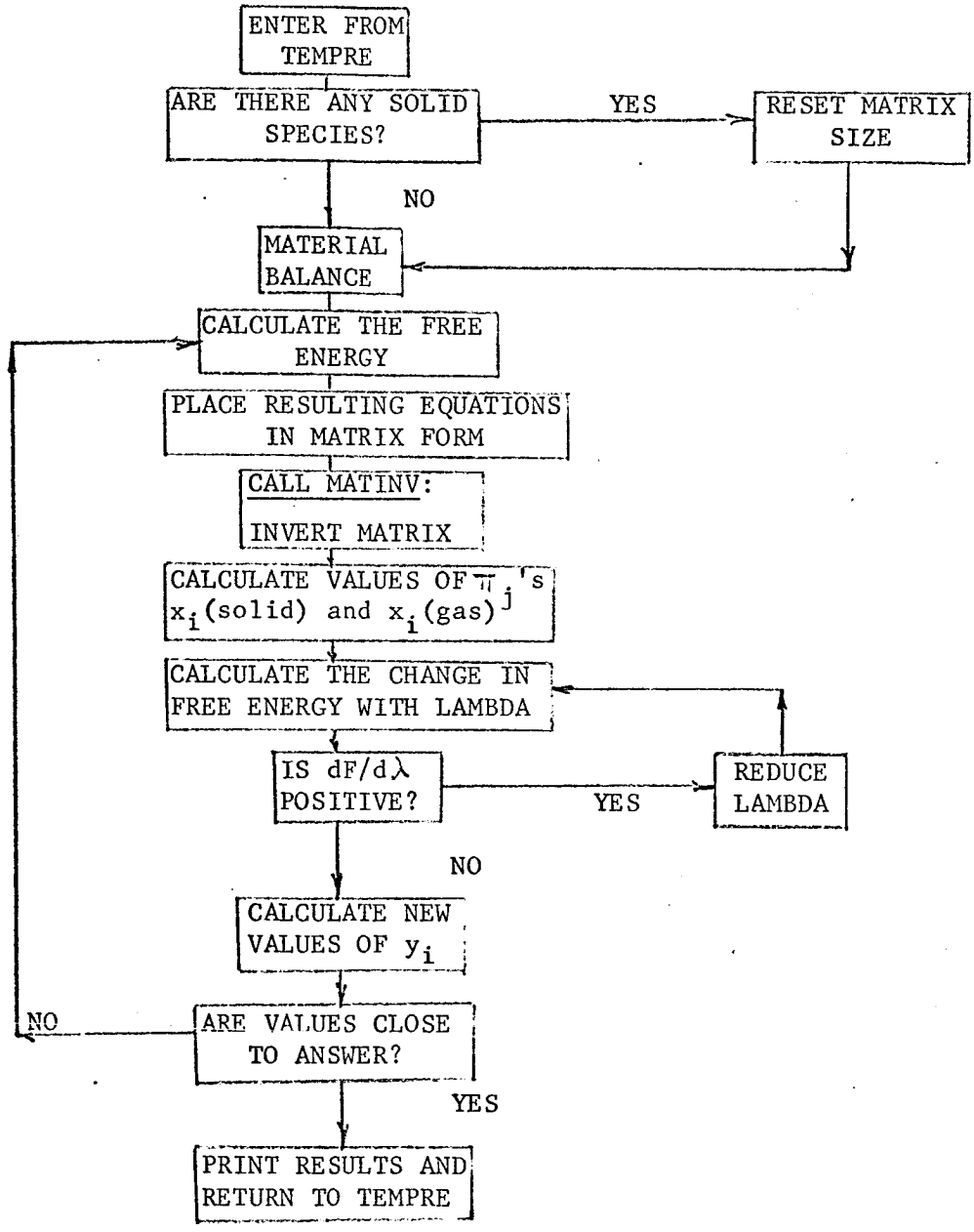


Figure C 4

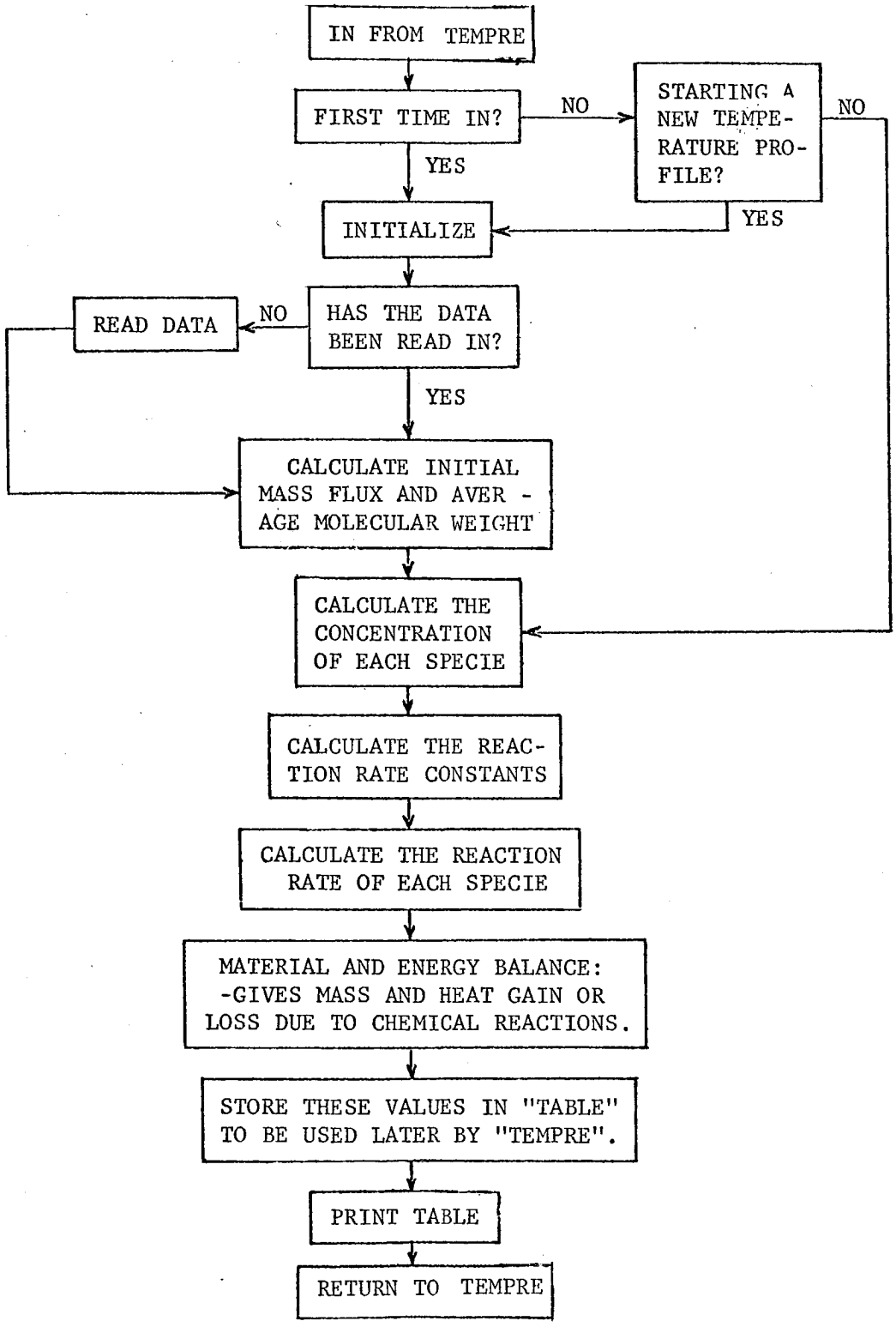
MOLFRA - SUBPROGRAM FOR THE CALCULATION OF MOLE FRACTIONS, AVERAGE MOLECULAR WEIGHT, MASS FLUX, AND HEAT OF REACTION VALUES VS. TEMPERATURE BY A FREE ENERGY MINIMIZATION METHOD



MATINV - SUBPROGRAM TO INVERT THE MATRIX FORMED IN MOLFRA

(STANDARD MATRIX INVERSION COMPUTER PROGRAM)

Figure C 5
"KINET"-- SUBROUTINE FOR THE CALCULATION OF THE RATE OF REACTION, MASS FLUX, AVERAGE MOLECULAR WEIGHT AND HEAT GENERATED DUE TO CHEMICAL REACTIONS



FORTRAN SOURCE LIST

```
 SOURCE STATEMENT

10 [illegible]
   DIMENSION [illegible](20),ALPA(20),AA(20,6),
 1  S1(4),S2(4),S3(4),S4(4),S5(4),A11(4),A22(4) A33(4),A44(4),A55(4)
   DIMENSION AI(20),BI(20),CI(20),DI(20),EI(20),FI(20),GI(20),
 1  AII(20),BII(20),CII(20),DII(20),EII(20),FII(20),GII(20),FW(20),
 2  YI(20),[illegible](20),SIG(20),Y(20)
   DIMENSION [illegible],FT(300),XTKE(100),ZOMGA(100),XM(300),FN(300),
 1  [illegible],TP(300),CP(20),COND(20),CV(20),VIS(20),XAXIS(300),
 2  YAXIS(300),GT(300),ODT(300),Z(300),PROD(300),CAPAC(300),
 3  PROD[illegible](300),PRODLP(300),ZX(300),P(300),ZY(300),TABLE(30,30)
   COMMON NC,NS,[illegible],WI,PL,RR,TZERO,DELTK,ICODE,ALPA,AA,S1,S2,S3,
 1  S4,S5,A11,A22,A33,A44,A55
   COMMON AI,BI,CI,DI,EI,FI,GI,AII,BII,CII,DII,EII,FII,GII,FW,YI
   COMMON [illegible]IG,[illegible]S,Y
   NC=NO. OF GAS COMPONENTS
   NS=NO. OF CONDENSED PLUS GAS COMPONENTS
   MA=NO. OF ELEMENTS
12 READ[illegible],NC,NS,MA
   [illegible] GAS MASS FLUX VALUE AT Z=0 (LB/FT2-SEC)
   [illegible] AT Z=L (LB/FT2)
   RR=GAS CONSTANT (1.987 BTU/LB-MOLE/OR)
   [illegible] REFERENCE TEMPERATURE (298.2 OK)
   [illegible] TEMPERATURE INCREMENT USED TO CALCULATE DKC/DT (OK)
   READ12,[illegible],TZERO,DELTK
   [illegible] WEIGHT
   YI=[illegible] MOLE FRACTION OF GASES AT Z=0
   [illegible] (GAS),   =1 (SOLID)
   [illegible] IDENTIFICATION
   [illegible](I),YI(I),ALPA(I),ICODE(I),I=1,NS)
   [illegible]
   S1 THRU S5=EMPIRICAL CONSTANTS FOR HEAT CAPACITY OF ELEMENTS
                                         (UP TO 1000 OK)
   READ1[illegible],S1(J),S2(J),S3(J),S4(J),S5(J)
   A11 THRU A55=EMPIRICAL CONSTANTS FOR HEAT CAPACITY OF ELEMENTS
                                          (ABOVE 1000 OK)
   READ1[illegible],A11(J),A22(J),A33(J),A44(J),A55(J)
15 CONTINUE
   DO16 I=1,NS
   AA=[illegible] NUMBER
   READ13,(AA(I,J),J=1,MA)
   AI THRU GI=EMPIRICAL CONSTANTS FOR HEAT CAPACITY (ABOVE 1000 OK)
   READ14,AI(I),BI(I),CI(I),DI(I),EI(I),FI(I),GI(I)
   AII THRU GII=EMPIRICAL CONSTANTS FOR HEAT CAPACITY (UP TO 1000 OK)
   READ14,AII(I),BII(I),CII(I),DII(I),EII(I),FII(I),GII(I)
16 CONTINUE
   EP=POTENTIAL PARAMETER/BOLTZMAN CONSTANT
   SIG=COLLISION DIAMETERS (A)
   READ1[illegible],([illegible](I),SIG(I),ALPA(I),I=1,NC)
   [illegible] POROSITY
   [illegible]
1[illegible] [illegible]
1[illegible] [illegible]
1[illegible] [illegible](A6,I[illegible])
14 [illegible]
17 [illegible]
```

PROGRAM SOURCE LIST TEMPRE

```
SOURCE STATEMENT

10 DIMENSION(9,13,3)
   COMMON/ACCESS COEFFICIENT IN DARCY EQUATION (1/FT)
   BETA/INITIAL COEFFICIENT IN FORCHEIMER EQUATION (1/FT2)
   GAMMA,ALPHA,BETA
   NDATA=20, NO. OF XTKE VS. ZETA DATA POINTS
   NDIM1=20, NO. OF DIMENSIONED LOCATIONS FOR EQUILIBRIUM PROGRAM CALCULATIONS
                                IN SUBPROGRAM OMEGA
   NDIM2=20, NO. OF DIMENSIONED LOCATIONS FOR TEMPERATURE-DISTANCE CALCULATIONS
                                IN SUBPROGRAM OMEGA
   NDIM3=20, NO. OF DIMENSIONED LOCATIONS FOR PHYSICAL PROPERTY CALCULATIONS
                                IN SUBPROGRAM OMEGA
   KEY= 1 (PROPANE FLOW),  = 2 (EQUILIBRIUM FLOW)  = 3 (NON-EQUILIBRIUM FLOW)
   READ(5,1,DATA,NDIM1,NDIM2,NDIM3,KEY
   XTKE=PRODUCT OF TEMPERATURE AND 1/EK VALUE
   ZETA=COLLISION INTEGRAL FACTOR VS XTKE
   READ(4,(XTKE(I),ZETA(I),I=1,NDATA)
22 FORMAT(2F15.5)
23 FORMAT(5I6)
24 FORMAT(2F15.5)
   JCOUNT=1
   I=1
30 Z(I)=0.0
   TL=TEMPERATURE AT Z=L (DEG)
   T(1)=TEMPERATURE AT Z=0 (DEG)
   GT(1)=TEMPERATURE GRADIENT AT Z=0 (DEG/FT)
   ZL=CHANNEL LENGTH (FT)
   DZ=DELTA INCREMENT SIZE (FT)
   HS(1)=SURFACE RULE INCREMENT SIZE (FT)
27 WRITE(6,1)TL,T(1),ZL,DZ,HS(1),NS
31 FORMAT(/,7F15.4)
   DO 125 I=1,NC
125 SUM=SUM+Z(I)
   DO 127 I=1,NC
127 Y1(I)=Z(I)/SUM
   Y1(NC)=Z(NC)/SUM
   CALL OMEGA(-3)
   NC=1
                    NC4=NC+4
                    KOUNT=1
                                    TP1=T(1)
                                    K7=1
40 K=1
   TRST=500.0
   DO 1
   DO 41 I=1,NC
   Y(I)=Z(I)
41 CONTINUE
   P=1
                                    KO=1
   YOMIS(1)=0.0
   YOMIS(1)=0.0
50 ZETA=0.0
55 DO(K-1)55,55,101
56 T(K+1)=MAX(T(1),T(K))
```

FORTRAN SOURCE LIST TEMPRE

```
      SOURCE STATEMENT

   62 GROUP=(W*EPS*GASCP/CDO)-(DCDO*DTC/CDO)
      GO TO 65
   63                 GROUP=(W*EPS*GASCP/CDO)-(DCDO*DTC/CDO)+(REACT/CDO)
   65 DA=ARK*GROUP
      TPREV=TC
  105 GO TO (110,120,130,135),MX
  110 A1=ARK
      DA1=DA
      TC=THETA+0.5*A1
      DTC=DTHETA+0.5*DA1
      MX=2
      IF(TC)133,133,103
  120 A2=ARK
      DA2=DA
      TC=THETA+0.5*A2
      DTC=DTHETA+0.5*DA2
      MX=3
      IF(TC)133,133,103
  130 A3=ARK
      DA3=DA
      TC=THETA+A3
      DTC=DTHETA+DA3
      MX=4
      IF(TC)133,133,103
  133 PRINT 2222,TC
 2222 FORMAT(1H0,3HTC=,1X,F15.6,8X,8HNEGATIVE)
      DT(1)=DT(1)*0.5
      GO TO 40
  135 A4=ARK
      DA4=DA
      T(N+1)=T(N)+(1.0/6.0)*(A1+2.0*A2+2.0*A3+A4)
      DT(N+1)=DT(N)+(1.0/6.0)*(DA1+2.0*DA2+2.0*DA3+DA4)
      TLIMIT=TL+500.0
      IF(T(N+1)-TLIMIT)5000,5000,6000
 6000 IF(T(N+1))136,136,138
  136 PRINT 137, T(N+1)
  137 FORMAT(1H0,7HT(N+1)=,1X,F15.6,8X,8HNEGATIVE)
      DT(1)=DT(1)*0.5
      GO TO 40
 5000 PRINT 8000,T(N+1),TLIMIT
      PRINT 8001,DT(N+1),N
 8000 FORMAT(1H0,7HT(N+1)=,1X,F15.6,4X,8HEXCEEDED,1X,15HTLIMIT VALUE OF
     1,1X,F15.6)
 8001 FORMAT(1H0,8HDT(N+1)=,1X,F20.5,8X,2HN=,1X,I6)
      TRATIO=(TL-T(N+1))/TL
      DT(1)=DT(1)*(1.0+0.5*TRATIO)
      TCHECK=T(N+1)
      IF(DT(N+1))300,300,40
  38  Z(N+1)=Z(N)+H
      XAXIS(N+1)=Z(N+1)/ZL
      YAXIS(N+1)=(T(N+1)-T(1))/(TL-T(1))
      IF(ABS(TL-T(N+1))-.0001)150,150,145
  45  N=N+1
      GO TO 101
  50  DT(N)=T(N+1)
```

FORTRAN SOURCE LIST TEMPRE

```
      SOURCE STATEMENT

      QDT(NO)=DT(1)
      CAPAC(N+1)=CAPAC(N)
      DIFF=ABS(TL-T(N+1))
 1117 PRINT1111,T(1),DT(1)
 1111 FORMAT(1H0,5HT(1)=,1X,F15.6,4X,6HDT(1)=,1X,F15.6)
      STEP=(10.0*(ZL/HS)+5.0)/10.0
      LSTEP=STEP
      LCHAR=LSTEP + 1
      PRINT180
 180  FORMAT(1H0,3X,4HT(L),8X,5HDT(L),9X,8HXAXIS(L),7X,8HYAXIS(L),
     1    5X,8HCAPAC(L),4X,1HL)
      DO200 L=1,LCHAR
      PRINT190,T(L),DT(L),XAXIS(L),YAXIS(L),CAPAC(L),L
 190  FORMAT(1X,5F13.5,I5)
 200  CONTINUE
      IF(DIFF-1.0)155,155,153
 152  TRATIO=(TL-T(N+1))/TL
      DT(1)=DT(1)*(1.0+0.9*TRATIO)
      TCHECK=T(N+1)
      NO=NO+1
      GO TO 40
 153  IF(NO-1)152,152,154
 154  RATIO=(TL-QT(NO))/(QT(NO-1)-QT(NO))
      RDASH=RATIO*(QDT(NO-1)-QDT(NO))
      DT(1)=DT(1)+RDASH
      NO=NO+1
      GO TO 40
 155  PRINT 3333
 3333 FORMAT(1H0,11HTEMPERATURE,1X,7HPROFILE,1X,7HDEFINED)
      CALCULATION OF PRESSURE PROFILE
      DELTT=(TL-T(1))
      SIMP1=0.0
      SIMP2=0.0
      SIMP3=0.0
      SIMP4=0.0
      ZS=ZL/HS
      JS=(10.0*ZS+5.0)/10.0
      LS=JS+1
      ZX(LS)=ZL
      TP(LS)=TL
      P(LS)=PL
      DO 260 N=1,JS
      NBAR=N-1
      HN=NBAR
      LO=LS-NBAR
      ZX(LO)=ZX(LS)-HN*HS
      ZSIMP=HS/HSIMPI
      MS=(10.0*ZSIMP+5.0)/10.0
      MP=MS+1
      ZY(MP)=ZX(LO)
      DO 240 N=1,MP
      MBAR=N-1
      HM=MBAR
      MO=MP-MBAR
      ZY(MO)=ZY(MP)-HM*HSIMPI
```

FORTRAN SOURCE LIST TEMPRE

```
      SOURCE STATEMENT

      ZVAR=ZY(MO)
      ITEMP=LCHAR
      CALL OMEGA(ZVAR,Z,T,ITEMP,NDIM2,TVIS)
 205  TK=(TVIS+460.0)/1.8
 209  DO 216 I=1,NC
      TKE=(1.0/EK(I))*TK
      IMAX=MDATA
 211  CALL OMEGA(TKE,KTKE,ZOMGA,IMAX,NDIM3,OMGA)
      VIS(I)=2.6693*10.**(-3.)*(FW(I)*TK)**0.5/(SIG(I)**2.0)*OMGA
 216  CONTINUE
      IF(NC-1)238,238,220
 220  GO TO(222,221,221),KEY
 221                  TVAR=TK
                      DO217 KL=2,NN4
                      CALL OMEGA(TVAR,TABLE(1,1),TABLE(1,KL),KMAX,NDIM1,
     1                          VARY)
                      IF(KL.GT.2)GO TO 214
                      REACT=VARY
                      GO TO 217
 214                  IF(KL.GT.3)GO TO 215
                      AVGFW=VARY
                      GO TO 217
 215                  IF(KL.GT.4)GO TO 219
                      W=VARY
                      GO TO 217
 219                  Y(KL-4)=VARY
                      IF(Y(KL-4))218,218,217
 218                  Y(KL-4)=1.0E-10
 217                  CONTINUE
 222  VMIX=0.0
      DO 237 J=1,NC
      TERM=1.0
 223  DO 230 L=1,NC
      IF(L-J)226,225,226
 225  GO TO 230
 226  TOPV=(1.0+(VIS(J)/VIS(L))**0.5*(FW(L)/FW(J))**0.25)**2.0
 227  BOTV=2.0*SQRT(2.0)*(1.+FW(J)/FW(L))**0.5
 228  PHIV=TOPV/BOTV
      TERM=TERM+PHIV*(Y(L)/Y(J))
 230  CONTINUE
      VMIX=VMIX+(VIS(J)/TERM)
 237  CONTINUE
      GO TO 2380
 238  VISCOS=VIS(I)*2.42/3600.0
      GO TO 239
 2380 VISCOS=VMIX*2.42/3600.0
 239  TT(MO)=(TVIS/AVGFW)*W**2
      PROD(MO)=TVIS*VISCOS*W/AVGFW
      CALL OMEGA(TVIS,T,CAPAC,ITEMP,NDIM2,CPBAR)
      PRODCP(MO)=CPBAR*W
      GO TO(240,2401,2401),KEY
 2401                 PRODR(MO)=REACT
 240  CONTINUE
      ZX(LO-1)=ZX(LO)-HS
      TP(LO-1)=TT(1)*AVGFW/W**2
```

FORTRAN SOURCE LIST TEMPRE

```
      SOURCE STATEMENT

      DELTP=TP(LO)-TP(LO-1)
      SUM1=0.0
      SUM2=0.0
      SUM3=0.0
      SUM4=0.0
      SUM5=0.0
      SUM6=0.0
      SUM7=0.0
      SUM8=0.0
      MEVEN=MP-1
      DO255 KP=2,MEVEN,2
      SUM1=SUM1+4.0*PROD(KP)
      SUM3=SUM3+4.0*TT(KP)
254   SUM5=SUM5+4.0*PRODCP(KP)
      GO TO(255,2540,2540),KEY
2540                  SUM7=SUM7+4.0*PRODR(KP)
255   CONTINUE
      MODD=MP-2
      DO256 KP=3,MODD,2
      SUM2=SUM2+2.0*PROD(KP)
      SUM4=SUM4+2.0*TT(KP)
257   SUM6=SUM6+2.0*PRODCP(KP)
      GO TO(256,2570,2570),KEY
2570                  SUM8=SUM8+2.0*PRODR(KP)
256   CONTINUE
      SIMP1=(HSIMPI/3.0)*(PROD(1)+PROD(MP)+SUM1+SUM2)+SIMP1
      SIMP2=(HSIMPI/3.0)*(TT(1)+TT(MP)+SUM3+SUM4)+SIMP2
      P(LO-1)=SQRT(PL**2+(2.*RR)*(778.16/32.2)*(ALPHA*SIMP1+BETA*SIMP2))
      SIMP3=DELTP*HSIMPI/(HS*3.0)*(PRODCP(1)+PRODCP(MP)+SUM5+SUM6)+SIMP3
      GO TO(258,258,258),KEY
258                   SIMP4=DELTP*HSIMPI/(HS*3.0)*(PRODR(1)+PRODR(MP)+
     1                      SUM7+SUM8)+SIMP4
260   CONTINUE
      GO TO(2600,2601,2601),KEY
2600  QL=EPS*SIMP3
      GO TO 261
2601                  QL=EPS*(SIMP3+SIMP4)
261   PRINT 262
262   FORMAT(1H0,5H(I),3X,5HZX(I),10X,5HTP(I),11X,4HP(I))
265   DO268 I=1,LS
      PRINT266,I,ZX(I),TP(I),P(I)
266   FORMAT(1H0,I5,3F15.6)
268   CONTINUE
      PRINT2680
2680  FORMAT(1H0,38HTEMPERATURE-PRESSURE PROFILES DEFINED.,10X,21HHEAT F
     1LUX CALCULATED.)
      DELP=(P(1)-PL)
      GO TO(270,2701,2703),KEY
270   PRINT2700
2700  FORMAT(1H0,20X,13HFROZEN FLOW RESULTS)
      GO TO 271
2701                  PRINT2702
2702                  FORMAT(1H0,20X,24HEQUILIBRIUM FLOW RESULTS)
                      GO TO 271
2703                              PRINT2704
```

FORTRAN SOURCE LIST TEMPRE

```
      SOURCE STATEMENT

      CT(N+1)=CT(N)
      GO TO 138
 101  TC=T(N)
                                        TPREV=T(N-1)
      TLSTV=T(N)
 102  DTC=DT(N)
      CT=CTL=CT(N)
      KX=1
      IF(CT(1))1109,1109,103
1109  DT(1)=DT(1)/((1.+0.5*((TL-TCHECK)/TL))*2.0)
      GO TO 46
103   APA = P*DTC
998                                     TNOW=TC
      BALSI=TC*460.0
      TVAR=RANK(N)/1.8
                                        DEL=TNOW-TPREV
                                        DELZ=DEL/DTC
      GO TO (58,60,61),KEY
 58   AVGFX=0.0
      DO 59 I=1,NC
      AVGFX=AVGFX+Y(I)*FX(I)
 59   CONTINUE
      GO TO 164
 63                 IF(KOUNT.EQ.2)GO TO 710
                    CALL KOLFRA(KOUNT,KPT3,TABLE,K6)
                    KMIN=2
                    KMAX=KPT3
 710                DO 737 KL=2,KM4
                    CALL CRSSO(TVAR,TABLE(1,1),TABLE(1,KL),KMAX,ND(KL),
     1                         VARY)
                    IF(KL.GT.2)GO TO 704
                    REACT=VARY
                    GO TO 737
 704                IF(KL.GT.3)GO TO 705
                    AVGFX=VARY
                    GO TO 737
 705                IF(KL.GT.4)GO TO 708
                    W=VARY
                    GO TO 737
 708                Y(KL-4)=VARY
                    IF(Y(KL-4))706,706,707
 706                Y(KL-4)=1.0E-10
 707                CONTINUE
 61                                     CALL KLEFT(TP1,TVAR,DELZ,KN,K7,
     1                                          DTC,REACT,W,KPT3,TABLE,AVGFX)
                                        KN=2
                                        KMAX=KPT3
                                        K7=2
 164  CALL PROPT(TVAR,JCHAR,NDATA,XTKE,ZDMGA,NDIM3,CPMX,CDD,DCDD)
      RLMAX=2
      DATCP=(CPMX/AVGFX)*RR
      IF(ABS(Z(N)-DC)-1.0E-5)156,106,107
106   DATCP=DATCP
      Z=DC/DTC
107   GO TO(62,63,63),KEY
```

FORTRAN SOURCE LIST PRCPT

SOURCE STATEMENT

```
50  CDCN=CDO
    DELTF=DELTK*1.8
    DCDC=(CDCP-CDCN)/(DELTF*2.0)
    TC=T
    GO TO 500
60  RETURN
    END
```

FORTRAN SOURCE LIST TEMPRE

SOURCE STATEMENT

```
2704                                FORMAT(1H0,25X,28HNON-EQUILIBRIUM FLOW R
    1ESULTS)
 271 PRINT 272
 272 FORMAT(1H0,3X,5HDELTT,6X,4HDELP,7X,2HQL)
     PRINT273,DELTT,DELP,QL
 273 FORMAT(1H0,3F10.4)
    SWITCH NO. 1 = OFF, SWITCH NO. 2 = OFF --- GO TO NEW CASE
    SWITCH NO. 1 = OFF, SWITCH NO. 2 = ON --- FROZEN TO NON-EQUILIBRIUM
    SWITCH NO. 1 = ON, SWITCH NO. 2 (NOT NEEDED) --- JOBS IN SEQUENCE
     CALL SSWTCH(1,JOB)
     GO TO(274,275),JOB
 274 KEY=KEY+1
     IF(KEY-3)2740,2740,278
2740 GO TO 30
 275 IF(KEY-1)276,276,278
 276 CALL SSWTCH(2,JIB)
     GO TO(277,278),JIB
 277 KEY=KEY+2
     IF(KEY-3)2770,2770,278
2770 GO TO 30
 278 GO TO 10
 300 STOP
     END
```

FORTRAN SOURCE LIST

SOURCE STATEMENT

```
$IBFTC PROPT
C     SUBROUTINE PROPT  (HEAT CAPACITY AND CONDUCTIVITY VS. TEMPERATURE)
      SUBROUTINE PROPT(TVAR,JCHAR,NDATA,XTKE,ZOMGA,NDIM3,CPMX,CDO,DCDO)
      DIMENSION ICODE(20),ALPA(20),AA(20,6),
     1  S1(4),S2(4),S3(4),S4(4),S5(4),A11(4),A22(4),A33(4),A44(4),A55(4)
      DIMENSION AI(20),BI(20),CI(20),DI(20),EI(20),FI(20),GI(20),
     1  AII(20),BII(20),CII(20),DII(20),EII(20),FII(20),GII(20),FW(20),
     2   YI(20),EK(20),SIG(20),Y(20)
      DIMENSION CP(20),CV(20),COND(20),XTKE(100),ZOMGA(100)
      COMMON NC,NS,MM,WI,PL,RR,TZERO,DELTK,ICODE,ALPA,AA,S1,S2,S3,
     1   S4,S5,A11,A22,A33,A44,A55
      COMMON AI,BI,CI,DI,EI,FI,GI,AII,BII,CII,DII,EII,FII,GII,FW,YI
      COMMON EK,SIG,EPS,Y
      RANKIN=1.8*TVAR
      FAREN=RANKIN-460.0
      T=TVAR
      TC=T+DELTK
500   DO516 I=1,NC
      TKE=(1.0/EK(I))*TC
      IMAX=NDATA
      CALL OMEGA(TKE,XTKE,ZOMGA,IMAX,NDIM3,OMGA)
      IF(TC-1000.0)505,505,506
505   CP(I)=AII(I)+BII(I)*TC+CII(I)*TC**2+DII(I)*TC**3+EII(I)*TC**4
      GO TO 507
506   CP(I)=AI(I)+BI(I)*TC+CI(I)*TC**2+DI(I)*TC**3+EI(I)*TC**4
507   CV(I)=(CP(I)-RR)
          TOP=2.6693*10.0**(-5.0)*(TC/FW(I))**0.5*(CV(I)+4.47)
          BOT=(SIG(I)**2.0*OMGA)
          COND(I)=TOP/BOT
516   CONTINUE
          CPMX=0.0
          CDMX=0.0
      DO537 J=1,NC
          SUMCP=CP(J)*Y(J)
          CPMX=CPMX+SUMCP
          SUMCD=COND(J)*Y(J)
          CDMX=CDMX+SUMCD
537   CONTINUE
      GO TO (538,539),JCHAR
538   CALL CHAR(SLOPE,YINTCP,KODE)
539   SCHAR=SLOPE
      YCHAR=YINTCP
      CDCHAR=(SCHAR*TC)+YCHAR
      CHARK=(CDCHAR*30.48)/(252.0*1.8)
      GASK=(CDMX*30.48)/(252.0*1.8)
      GO TO(5400,5401),KODE
5400  CDO=CHARK
      GO TO 5402
5401  CDO=GASK*EPS + CHARK*(1.0-EPS)
5402  IF(ABS(T-TC)-.00001)560,560,540
540   IF(T-TC)541,550,550
541   CDOP=CDO
      TC=T-DELTK
      JCHAR=2
      GO TO 500
```

FORTRAN SOURCE LIST

SOURCE STATEMENT

```
IBFTC OMEGA
      SUBROUTINE OMEGA (VAR,X,F,IMAX,NAME,SOM)
      DIMENSION X(NAME),F(NAME),XN(300),FN(300)
      NPTS=3
607   XUP=1.E30
      DO611 I=1,IMAX
      T=VAR-X(I)
      IF(T)608,609,609
608   T=-T
609   IF(T-XUP)610,611,611
610   IP=I
      XUP=T
611   CONTINUE
      IN=1
      NPP=NPTS+1
      DO613I=1,NPP
      FN(I)=F(IP)
      XN(I)=X(IP)
      IF(IN)612,612,613
612   IQ=IP-I
      GO TO 615
613   IQ=IP+I
      IF(IMAX-IQ)614,615,615
614   IP=IP-1
      GO TO 618
615   IF(IQ)616,616,617
616   IP=IP+1
      GO TO 618
617   IP=IQ
      IN=-IN
618   CONTINUE
      SOM=0.0
      FACT=1.0
      DO620 J=1,NPTS
      SOM=SOM+FACT*FN(1)
      DO619 I=J,NPTS
      IQ=I-J+1
619   FN(IQ)=(FN(IQ+1)-FN(IQ))/(XN(I+1)-XN(IQ))
620   FACT=FACT*(VAR-XN(J))
      RETURN
      END
```

FORTRAN SOURCE LIST

SOURCE STATEMENT

```
BFTC CHAR
     SUBROUTINE CHAR (CHAR CONDUCTIVITY VS. TEMPERATURE----SLOPE AND INTERCEPT)
     SUBROUTINE CHAR(SLOPE,YINTCP,KODE)
     DIMENSION XCOND(100),YCOND(100)
     MDATA=NO. OF XCOND VS. YCOND DATA POINTS
     KODE= 1 (DATA WITH INERTS IN PORES)  = 2 (DATA WITH EVACUATED PORES)
     READ700,MDATA,KODE
     XCOND=TEMPERATURE (OK)
     YCOND=CHAR CONDUCTIVITY TABULATED  VS TEMPERATURE (CAL/CM-SEC-OK)
     READ701,(XCOND(I),YCOND(I),I=1,MDATA)
700  FORMAT(2I6)
701  FORMAT(F15.0,E15.5)
          SUMX=0.0
          SUMY=0.0
          SUMXY=0.0
          SUMX2=0.0
          SUMY2=0.0
     TN=MDATA
     DO710 J=1,MDATA
          SUMX=SUMX+XCOND(J)
          SUMY=SUMY+YCOND(J)
          SUMXY=SUMXY+XCOND(J)*YCOND(J)
          SUMX2=SUMX2+XCOND(J)**2.0
          SUMY2=SUMY2+YCOND(J)**2.0
10   CONTINUE
20        SLOPE=(SUMXY-(SUMX*SUMY/TN))/(SUMX2-(SUMX**2.0/TN))
30       YINTCP=(SUMY-(SLOPE*SUMX))/TN
     RETURN
     END
```

FORTRAN SOURCE LIST

SOURCE STATEMENT

```
IBFTC MOLFRA
      SUBROUTINE MOLFRA(KOUNT,KPT3,TABLE,K6)
      EDUARDO C. DEL VALLE-NASA PROJECT-135-30-8621-LSU PROJECT NO-04-1303-40068

      CHEMICAL EQUILIBRIUM IN COMPLEX MIXTURE-METHOD OF WHITE-JOHNSON-DANTZIG

      RAND METHOD(STEEPEST DESCENT),JOURNAL-CHEMICAL PHYSICS-VOL-28-NO5-1958
      DIMENSION ICODE(20),ALPA(20),AA(20,6),
     1  S1(4),S2(4),S3(4),S4(4),S5(4),A11(4),A22(4),A33(4),A44(4),A55(4)
      DIMENSION AI(20),BI(20),CI(20),DI(20),EI(20),FI(20),GI(20),
     1  AII(20),BII(20),CII(20),DII(20),EII(20),FII(20),GII(20),FW(20),
     2   YI(20),EK(20),SIG(20),Y(20)
      DIMENSION YAVG(20),XMW(20),YAVG1(20),X(20),FY(20),C(20),FORT(20),
     1  F(31,31),B(31,1),PI(31),IPIVOT(30),BB(20),INDEX(31,2),BBP(31),
     2  FSUM(20),YSUM(20),YY(20),XY(20),XMASS(20),YX(20),PERC(20),
     3  DELTA(20),APART(20),BPART(20),ENT(20),DOTA(25,25),DOTA1(25,25),
     4  CPOT(20),CPOT1(20),TABLE(30,30)
      DIMENSION HO(4),DELH(5),FOHO(5)
      COMMON NC,NS,MM,WI,PL,RR,TZERO,DELTK,ICODE,ALPA,AA,S1,S2,S3,
     1   S4,S5,A11,A22,A33,A44,A55
      COMMON AI,BI,CI,DI,EI,FI,GI,AII,BII,CII,DII,EII,FII,GII,FW,YI
      COMMON EK,SIG,EPS,Y
      IF(K6.GT.1)GOTO3174
      XT=INITIAL TEMPERATURE AT WHICH EQUILIBRIUM PROGRAM IS STARTED
      TMAX=FINAL TEMPERATURE AT WHICH EQUILIBRIUM PROGRAM IS ENDED
      TINC=TEMPERATURE INTERVAL IN EQUILIBRIUM PROGRAM CALCULATIONS
      CRIT=CRITERION FOR CONVERGENCE IN EQUILIBRIUM PROGRAM
      READ7,XT,TMAX,TINC,CRIT
      NMAX=MAXIMUM SIZE OF THE SQUARE MATRIX
      NFREQ=NO. AFTER WHICH TRACE COMPONENTS ARE CHECKED
      READ2,NMAX,NFREQ
    7 FORMAT(4E10.4)
    2 FORMAT(2I6)
 3174 K6=2
      CALL FPTRAP(-3)
      DO 3 I=1,NS
      Y(I)=YI(I)
      XMW(I)=FW(I)
    3 CONTINUE
      W=WI
      NN=NC
      NQ=NS
      MA=1
      NA=MM+1+NQ-NN
      P=PL/2160.0
      KPT=0
      KPT1=0
      MAXNT=100
      KCODE=0
      KREAD=0
      T=XT
      KOS=NN+4
      LL=NN+1
      M=MA
      N=NA
```

FORTRAN SOURCE LIST MOLFRA

```
SOURCE STATEMENT

      KX=0
      XBETA=CRIT
500   PRINT4
    4 FORMAT(///6X,1H1,19X,5HFO/RT,13X,12HINITIAL Y(I)//)
      DO 433 I=1,NQ
      IF(ICODE(I).EQ.0)GOTO433
      KCODE=1
433   CONTINUE
   45 NTEST=NFREQ
      NT=1

      DELH(3) AND DELH(6) ARE THE HEATS OF FORMATION OF ETHANE AND BENZENE
      AT 0K. RESPECTIVELY.

      DELH(6)=2.4000E4
      DELH(3)=-1.6517E4

      HO IS THE CHEMICAL POTENTIAL OF  THE ELEMENTS,THAT IS,THE SENSIBLE
      ENTHALPY CHANGE FROM 298.16 DEGREES KELVIN TO 0K.,DIVIDED BY RR*T.
      HO(1) AND HO(2) ARE THE SUBSCRIPT FOR CARBON AND HYDROGEN RESPEC-
      TIVELY.

      HO(1)=-251.2/(RR*T)
      HO(2)=-2023.8/(RR*T)

      IF(T.GT.1000.)GOTO6205
      DO 41  I=1,NQ
      APART(I)=AII(I)*(1.-ALOG(T))-BII(I)*T/2.-CII(I)*(T**2)/6.
      BPART(I)=-DII(I)*(T**3)/12.-EII(I)*(T**4)/20.+FII(I)/T-GII(I)
      FORT(I)=APART(I)+BPART(I)
      PRINT14,ALPA(I),FORT(I),Y(I)
   41 CONTINUE
4     FORMAT(1X,A6,2F20.8)
      GOTO1020
205   DO 6206 I=1,NQ
      APART(I)=AI(I)*(1.-ALOG(T))-BI(I)*T/2.0-CI(I)*(T**2)/6.0
      BPART(I)=-DI(I)*(T**3)/12.0-EI(I)*(T**4)/20.0+FI(I)/T-GI(I)
      FORT(I)=APART(I)+BPART(I)
      PRINT14,ALPA(I),FORT(I),Y(I)
206   CONTINUE
020   IF(T.GT.1500.)GOTO9131

      FOHC(3) AND FOHO(6) REPRESENTS THE TERM F-H/(R*T),WHICH IS CALCU-
      LATED USING THE DATA BY DUFF.(LOS ALAMOS SCIENTIFIC LABORATORY
      REPORT NUMBER 2556,SEPT 18,1961),AND IT IS FOR ETHANE AND BENZENE
      RESPECTIVELY

      FORT(3)=FORT(3)+DELH(3)/(RR*T)+AA(3,1)*HO(1)+(AA(3,2)/2.)*HO(2)
      FORT(6)=FORT(6)+DELH(6)/(RR*T)+AA(6,1)*HO(1)+(AA(6,2)/2.)*HO(2)
      GO TO 1000
131   FORT(3)=FORT(3)+DELH(3)/(RR*T)+AA(3,1)*HO(1)+(AA(3,2)/2.)*HO(2)
      FORT(6)=FORT(6)+DELH(6)/(RR*T)+AA(6,1)*HO(1)+(AA(6,2)/2.)*HO(2)
000   DO320J=1,MM
      BB(J)=0.0
```

FORTRAN SOURCE LIST MOLFRA

SOURCE STATEMENT

```
      DO 320 I=1,NQ
      BB(J)=BB(J)+AA(I,J)*Y(I)
320   CONTINUE
300   YBAR=0.0
      DO50I=1,NN
 50   YBAR=YBAR+Y(I)
      DO10I=1,NN
      C(I)=FORT(I)+ALOG(P)
      FAC=Y(I)/YBAR
      IF(FAC.LT.1.E-38)FAC=1.E-38
      FY(I)=Y(I)*(C(I)+ALOG(FAC))
 10   CONTINUE
      IF(KCODE.EQ.0)GOTO111
      DO 11 I=LL,NQ
      FY(I)=Y(I)*FORT(I)
 11   CONTINUE
111   DO30J=1,MM
      DO30K=1,MM
      ASUM=0.0
      DO20I=1,NN
      WAY=AA(I,J)*AA(I,K)*Y(I)
 20   ASUM=ASUM+WAY
      R(J,K)=ASUM
 30   CONTINUE
      DO70K=1,MA
      DO70J=1,MM
      SUM=0.
      DO130I=1,NN
130   SUM=SUM+AA(I,J)*FY(I)
      BSUM=SUM+BB(J)
      B(J,K)=BSUM
 70   CONTINUE
      CSUM=0.0
      DO80I=1,NN
 80   CSUM=CSUM+FY(I)
      JJ=MM+1
      DO91J=1,M
 91   B(JJ,J)=CSUM
      DO 103 K=1,MM
      DSUM=0.0
      DO 101 I=1,NN
101   DSUM=DSUM+AA(I,K)*Y(I)
      BBP(K)=DSUM
103   CONTINUE
      DO90J=1,MM
 90   R(J,JJ)=BBP(J)
      DO94K=1,MM
 94   R(JJ,K)=R(K,JJ)
      KK=MM+1
      KL=JJ
      IF(KCODE.EQ.0)GOTO1050
      DO 29 I=LL,NQ
      KK=KK+1
      DO 29 J=1,MM
      R(J,KK)=AA(I,J)
```

FORTRAN SOURCE LIST MOLFRA

```
    SOURCE STATEMENT

 29 CONTINUE
    KL=NQ-NN+JJ
    KK=MM+2
    DO 95 K=KK,KL
    DO97 J=1,MM
 97 R(K,J)=R(J,K)
 95 CONTINUE
    KM=MM+1
    DO 1052 J=1,MA
    DO 1053 I=LL,NQ
    KM=KM+1
1053 B(KM,J)=FORT(I)
1052 CONTINUE
1050 CONTINUE
    DO 1044 J=JJ,KL
    DO 1045 K=JJ,KL
1045 R(J,K)=0.0
1044 CONTINUE
 24 FORMAT(E16.8)
    CALL MATINV(R,N,B,M,DETERM,IPIVOT,INDEX,NMAX,ISCALE)
    DO100I=1,JJ
 100 PI(I)=B(I,M)
    U=PI(JJ)
    XBAR=U*YBAR
    IF(KCODE.EQ.0)GOTO59
    KK=MM+2
    LW=LL
    DO 1002 J=KK,KL
    X(LW)=B(J,M)
1002 LW=LW+1
 59 DO60I=1,NN
 60 FSUM(I)=-FY(I)+(Y(I)/YBAR)*XBAR
    DO110I=1,NN
    PSUM=0.
    DO120J=1,MM
 120 PSUM=PSUM+PI(J)*AA(I,J)
    YSUM(I)=PSUM*Y(I)
 110 X(I)=FSUM(I)+YSUM(I)
    XLAMBD=1.
 310 DO 86 I=1,NQ
    DELTA(I)=X(I)-Y(I)
 86 CONTINUE
    DEBAR=0.
    DO87I=1,NN
87  DEBAR=DEBAR+DELTA(I)
 93 DFDL=0.
    DO88I=1,NQ
    IF(ICODE(I).EQ.1)GOTO83
 96 FAC=(Y(I)+XLAMBD*DELTA(I))/(YBAR+XLAMBD*DEBAR)
 98 IF(FAC.GT.0.)GOTO82
391 XLAMBD=.9*XLAMBD
    IF(XLAMBD.GT.1.0E-20)GOTO96
 82 DFDL=DFDL+DELTA(I)*(C(I)+ALOG(FAC))
    GOTO88
 83 DFDL=DFDL+DELTA(I)*FORT(I)
```

FORTRAN SOURCE LIST MOLFRA

SOURCE STATEMENT

```
 88 CONTINUE
    IF(CFDL.LT.0.)GOTO89
    XLAMBD=.9*XLAMBD
    IF(XLAMBD.GT.1.0E- 9)GOTO93
 89 DO76I=1,NQ
    Y(I)=Y(I)+XLAMBD*DELTA(I)
 76 CONTINUE
    SUMY=0.
    DO370I=1,NN
370 SUMY=SUMY+Y(I)
    DO340I=1,NQ
340 PERC(I)=(Y(I)/SUMY)*100.
350 BETA=0.
    DO85I=1,NQ
 85 BETA=BETA+ABS(DELTA(I))
    IF(BETA.LT.XBETA)GOTO800
    IF(KX.GT.0)GOTO560
560 IF(NT.GE.MAXNT)GOTO600
    NT=NT+1
    IF(KX.GT.0)GOTO300
    GOTO1000
600 XBETA=XBETA+.000001
    MAXNT=MAXNT+100
    NT=NT+1
    GOTO300
300 NN=NC
    KX=KX+1
    IF(KX.LT.2)GOTO300
801 PRINT16,NT
 16 FORMAT(//1X,30HNT = NO. ITERATIONS REQUIRED = I5//)
    PRINT201,XBETA
201 FORMAT(//1X,7HBETA = E12.4//)
    PRINT204,P,T
    PRINT32
204 FORMAT(/////1X, 9HPRESSURE=E13.5,5X,6HTEMP =E13.5//)
 32 FORMAT(//6X,1HI,21X,4HY(I),14X,7HPERCENT)
    XSUMY=0.
    DO580I=1,NN
    XSUMY=XSUMY+Y(I)
580 CONTINUE
    XMWGAS=0.0
    DO81I=1,NN
    XMWGAS=XMWGAS+XMW(I)*Y(I)
 81 CONTINUE
    DO 191I=1,NQ
    XMASS(I)=Y(I)*XMW(I)/XMWGAS
191 CONTINUE
    DO44I=1,NQ
 44 PRINT19,I,ALPA(I),Y(I),PERC(I),XMASS(I)
 19 FORMAT(1X,I6,3X,A6,3E20.8)
    ENTGAS=0.
    PRINT12
 12 FORMAT(///1X,11HENTHALPY(I)//)
    DO 78I=1,NQ
    ENT(I)=(AII(I)+BII(I)*TZERO/2.+CII(I)*(TZERO**2)/3.+DII(I)*(TZERO*
```

FORTRAN SOURCE LIST MOLFRA

SOURCE STATEMENT

```
  1*3)/4.+EII(I)*(TZERO**4)/5.+FII(I)/TZERO)*RR*TZERO
   ENT(3)=-20.236E3
   ENT(6)=19.820E3
   IF(T.LT.1000.0)GOTO6207
   CPDT(I)=(AI(I)*(T-TZERO)+BI(I)*(T**2-TZERO**2)/2.+CI(I)*(T**3-TZER
  1O**3)/3.+DI(I)*(T**4-TZERO**4)/4.+EI(I)*(T**5-TZERO**5)/5.)*RR
   DO 296J=2,MM
   CPDT1(J)=(S1(J)*(T-TZERO)+S2(J)*(T**2-TZERO**2)/2.+S3(J)*(T**3-TZE
  1RO**3)/3.+S4(J)*(T**4-TZERO**4)/4.+S5(J)*(T**5-TZERO**5)/5.)*RR*.5
296 CONTINUE
   CPDT1(1)=(S1(1)*(T-TZERO)+S2(1)*(T**2-TZERO**2)/2.+S3(1)*(T**3-TZE
  1RO**3)/3.+S4(1)*(T**4-TZERO**4)/4.+S5(1)*(T**5-TZERO**5)/5.)*RR
   PRINT6021,CPDT(I),ENT(I),T
   GOTO6291
207 CPDT(I)=(AII(I)*(T-TZERO)+BII(I)*(T**2-TZERO**2)/2.+CII(I)*(T**3-
  1TZERO**3)/3.+DII(I)*(T**4-TZERO**4)/4.+EII(I)*(T**5-TZERO**5)/5.)*
  2RR
   DO297J=2,MM
   CPDT1(J)=(A11(J)*(T-TZERO)+A22(J)*(T**2-TZERO**2)/2.+A33(J)*(T**3-
  1TZERO**3)/3.+A44(J)*(T**4-TZERO**4)/4.+A55(J)*(T**5-TZERO**5)/5.)*
  2RR*.5
297 CONTINUE
   CPDT1(1)=(A11(1)*(T-TZERO)+A22(1)*(T**2-TZERO**2)/2.+A33(1)*(T**3-
  1TZERO**3)/3.+A44(1)*(T**4-TZERO**4)/4.+A55(1)*(T**5-TZERO**5)/5.)*
  2RR
291 RSUM=0.
   DO 398 J=1,MM
398 RSUM=RSUM+AA(I,J)*CPDT1(J)
   PRINT6021,CPDT(I),ENT(I),T
021 FORMAT(1H0,3E15.5)
   ENT(I)=ENT(I)+CPDT(I)-RSUM
   ENT(1)=0.
   ENT(7)=0.
   ENT(9)=0.
   ENT(13)=0.
   PRINT6022,ENT(I),T
022 FORMAT(1H0,2E15.5)
 78 CONTINUE
   ENTGAS=0.0
   DO 781 I=1,NN
781 ENTGAS=ENTGAS+ENT(I)*Y(I)
   DO79I=1,NQ
 79 PRINT 24,ENT(I)
   PRINT18,ENTGAS
 18 FORMAT(//1X,21HENTHALPY OF GAS MIX = E16.8)
   XMWGAS=XMWGAS/XSUMY
   PRINT17,XMWGAS
 17 FORMAT(//1X,28HMOLECULAR WEIGHT OF GAS MIX=E16.8//)
   XBETA=CRIT
   KPT=KPT+1
   PRINT1112,W,T
112 FORMAT(1X,2E20.8)
   IF(T.LT.998.)GOTO171
   IF(KPT1.GT.0)GOTO171
   KPT1=KPT
```

FORTRAN SOURCE LIST MOLFRA

```
      SOURCE STATEMENT

171   TABLE(1,KPT)=T
      TABLE(3,KPT)=XMWGAS

      REDEFINE MOLE BASIS

      IF(T.NE.XT)GOTO823
      SUM1=0.
      DO 822 I=1,NN
      Y(I)=(W/XMWGAS)*PERC(I)/100.
822   SUM1=SUM1+Y(I)
      Y(NQ)=PERC(NQ)*SUM1/100.
      RIN=PERC(NQ)/100.*XMW(NQ)/XMWGAS
      ROUT=RIN
      GOTO1711
823   WG=W
      ROUT=PERC(NQ)/100.*XMW(NQ)/XMWGAS
      RATIO=(1.+RIN)/(1.+ROUT)
      W=WG*RATIO
      RIN=ROUT
1711  TABLE(4,KPT)=W

      CALCULATION OF INDIVIDUAL MASS FLUXES

      DO 1712 I=1,NN
      FLUX=W/XMWGAS*PERC(I)/100.*XMW(I)
1712  DOTA(I,KPT)=FLUX
      FLUX=W*ROUT
      DOTA(NQ,KPT)=FLUX
      DO 444 I=5,KOS
      TABLE(I,KPT)=PERC(I-4)/100.
444   CONTINUE
      IF(T.GE.TMAX)GOTO333
      T=T+TINC
      KX=0
      GOTO500
333   TPT1=KPT1
      KPT3=KPT-3
      KCUNT=2
      DO 338 J=5,KOS
      SUMY1=0.
      DO 337 I=1,KPT1
337   SUMY1=SUMY1+TABLE(J,I)
      YAVG(J-4)=SUMY1/TPT1
338   CONTINUE
      KPT2=KPT3-KPT1+1
      TPT2=KPT2
      DO 3338 J=5,KOS
      SUMY1=0.
      DO 3337 I=KPT1,KPT3
3337  SUMY1=SUMY1+TABLE(J,I)
      YAVG1(J-4)=SUMY1/TPT2
3338  CONTINUE
      DO 8000 J=1,KPT3
      IF(J.GT.1)GOTO 732
      DO 8001 I=1,NQ
```

FORTRAN SOURCE LIST MOLFRA

SOURCE STATEMENT

```
      YPRIME=(1./(60.*TINC))*(-137.*DOTA(I,J)+300.*DOTA(I,J+1)-300.*DOTA
     1(I,J+2)+200.*DOTA(I,J+3)-75.*DOTA(I,J+4)+12.*DOTA(I,J+5))
      DOTA1(I,J)=YPRIME
 8001 CONTINUE
      GOTO 8004
  732 IF(J.GT.2)GOTO733
      DO 8002 I=1,NQ
      YPRIME=(1./(60.*TINC))*(-12.*DOTA(I,J-1)-65.*DOTA(I,J)+120.*DOTA(I
     1,J+1)-60.*DOTA(I,J+2)+20.*DOTA(I,J+3)-3.*DOTA(I,J+4))
      DOTA1(I,J)=YPRIME
 8002 CONTINUE
      GOTO 8004
  733 DO 8071 I=1,NQ
      YPRIME=(1./(60.*TINC))*(3.*DOTA(I,J-2)-30.*DOTA(I,J-1)-20.*DOTA(I,
     1J)+60.*DOTA(I,J+1)-15.*DOTA(I,J+2)+2.*DOTA(I,J+3))
      DOTA1(I,J)=YPRIME
 8071 CONTINUE
 8004 CONTINUE
 8000 CONTINUE
      SUM2=0.
      DO 8007 J=1,KPT3
      DO 8006 I=1,NQ
 8006 SUM2=SUM2+DOTA1(I,J)*ENT(I)/XMW(I)
      TABLE(2,J)=SUM2
 8007 CONTINUE
      SUM=0.
      DO 200 J=1,KPT3
  200 SUM=SUM+TABLE(3,J)
      YFLOAT=KPT3
      YMWAVG=SUM/YFLOAT
      DO1I=1,30
      DO1J=1,I
      XXX=TABLE(I,J)
      TABLE(I,J)=TABLE(J,I)
      TABLE(J,I)=XXX
1     CONTINUE
      RETURN
      END
```

FORTRAN SOURCE LIST

```
SOURCE STATEMENT

IBFTC MATINV
      MATRIX INVERSION WITH ACCOMPANYING SOLUTION OF LINEAR EQUATIONS
      SUBROUTINE MATINV(A,N,B,M,DETERM,IPIVOT,INDEX,NMAX,ISCALE)

      DIMENSION IPIVOT(N),A(NMAX,N),B(NMAX,M),INDEX(NMAX,2)
      EQUIVALENCE (IROW,JROW), (ICOLUM,JCOLUM), (AMAX,T,SWAP)

      INITIALIZATION

    5 ISCALE=0
    6 R1=10.0**18
    7 R2=1.0/R1
   10 DETERM=1.0
   15  DO 20 J=1,N
   20 IPIVOT(J)=0
   30 DO 550 I=1,N

      SEARCH FOR PIVOT ELEMENT

   40 AMAX=0.0
   45 DO 105 J=1,N
   50 IF (IPIVOT(J)-1)60,105,60
   60 DO 100 K=1,N
   70 IF (IPIVOT(K)-1)80,100,740
   80 IF (ABS(AMAX)-ABS(A(J,K)))85,100,100
   85 IROW=J
   90 ICOLUM=K
   95 AMAX=A(J,K)
  100 CONTINUE
  105 CONTINUE
      IF (AMAX)110,106,110
  106 DETERM=0.0
      ISCALE=0
      GO TO 740
  110 IPIVOT(ICOLUM)=IPIVOT(ICOLUM)+1

      INTERCHANGE ROWS TO PUT PIVOT ELEMENT ON DIAGONAL

  130 IF (IROW-ICOLUM)140,260,140
  140 DETERM=-DETERM
  150 DO 200 L=1,N
  160 SWAP=A(IROW,L)
  170 A(IROW,L)=A(ICOLUM,L)
  200 A(ICOLUM,L)=SWAP
  205 IF(M)260,260,210
  210 DO 250 L=1,M
  220 SWAP=B(IROW,L)
  230 B(IROW,L)=B(ICOLUM,L)
  250 B(ICOLUM,L)=SWAP
  260 INDEX(I,1)=IROW
  270 INDEX(I,2)=ICOLUM
  310 PIVOT=A(ICOLUM,ICOLUM)

      SCALE THE DETERMINANT
```

FORTRAN SOURCE LIST MATINV

SOURCE STATEMENT

```
 1000 PIVOTI=PIVOT
 1005 IF(ABS(DETERM)-R1)1030,1010,1010
 1010 DETERM=DETERM/R1
      ISCALE=ISCALE+1
      IF(ABS(DETERM)-R1)1060,1020,1020
 1020 DETERM=DETERM/R1
      ISCALE=ISCALE+1
      GO TO 1060
 1030 IF(ABS(DETERM)-R2)1040,1040,1060
 1040 DETERM=DETERM*R1
      ISCALE=ISCALE-1
      IF(ABS(DETERM)-R2)1050,1050,1060
 1050 DETERM=DETERM*R1
      ISCALE=ISCALE-1
 1060 IF(ABS(PIVOTI)-R1)1090,1070,1070
 1070 PIVOTI=PIVOTI/R1
      ISCALE=ISCALE+1
      IF(ABS(PIVOTI)-R1)320,1080,1080
 1080 PIVOTI=PIVOTI/R1
      ISCALE=ISCALE+1
      GO TO 320
 1090 IF(ABS(PIVOTI)-R2)2000,2000,320
 2000 PIVOTI=PIVOTI*R1
      ISCALE=ISCALE-1
      IF(ABS(PIVOTI)-R2)2010,2010,320
 2010 PIVOTI=PIVOTI*R1
      ISCALE=ISCALE-1
  320 DETERM=DETERM*PIVOTI
C
C     DIVIDE PIVOT ROW BY PIVOT ELEMENT
C
  330 A(ICOLUM,ICOLUM)=1.0
  340 DO 350 L=1,N
  350 A(ICOLUM,L)=A(ICOLUM,L)/PIVOT
  355 IF(M) 380,380,360
  360 DO 370 L=1,M
  370 B(ICOLUM,L)=B(ICOLUM,L)/PIVOT
C
C     REDUCE NON-PIVOT ROWS
C
  380 DO 550 L1=1,N
  390 IF(L1-ICOLUM)400,550,400
  400 T=A(L1,ICOLUM)
  420 A(L1,ICOLUM)=0.0
  430 DO 450 L=1,N
  450 A(L1,L)=A(L1,L)-A(ICOLUM,L)*T
  455 IF(M) 550,550,460
  460 DO 500 L=1,M
  500 B(L1,L)=B(L1,L)-B(ICOLUM,L)*T
  550 CONTINUE
C
C     INTERCHANGE COLUMNS
C
  600 DO 710 I=1,N
  610 L=N+1-I
```

FORTRAN SOURCE LIST MATINV

SOURCE STATEMENT

```
620 IF(INDEX(L,1)-INDEX(L,2))630,710,630
630 JROW=INDEX(L,1)
640 JCOLUM=INDEX(L,2)
650 DO 705 K=1,N
660 SWAP=A(K,JROW)
670 A(K,JROW)=A(K,JCOLUM)
700 A(K,JCOLUM)=SWAP
705 CONTINUE
710 CONTINUE
740 RETURN
    END
```

FORTRAN SOURCE LIST

SOURCE STATEMENT

```
$FTC KINET
      SUBROUTINE KINET(TP1,TVAR,DELZ,KN,K7,DTC,HEAT,WNEW,KPT3,TABLE,
     1  AVGFW)
      DIMENSION ICODE(20),ALPA(20),AA(20,6),
     1  S1(4),S2(4),S3(4),S4(4),S5(4),A11(4),A22(4),A33(4),A44(4),A55(4)
      DIMENSION AI(20),BI(20),CI(20),DI(20),EI(20),FI(20),GI(20),
     1  AII(20),BII(20),CII(20),DII(20),EII(20),FII(20),GII(20),FW(20),
     2   YI(20),EK(20),SIG(20),Y(20)
      DIMENSION RSC(20,20),PSC(20,20),REX(20,20),PEX(20,20),AF(20),
     1SF(20),AEF(20),AR(20),SR(20),AER(20),EQN(20),XFW(20),PERCE(20),
     2FLUXMO(20),FLUXMA(20),C(20),FK(20),RK(20),RATE(20),Y1(20)
      DIMENSION TABLE(30,30),YTEMP(20),ENT(20),CPDT(20),CPDT1(20)
      COMMON NC,NS,MM,WI,PL,RR,TZERO,DELTK,ICODE,ALPA,AA,S1,S2,S3,
     1   S4,S5,A11,A22,A33,A44,A55
      COMMON AI,BI,CI,DI,EI,FI,GI,AII,BII,CII,DII,EII,FII,GII,FW,YI
      COMMON EK,SIG,EPS,Y
      CALL FPTRAP(-3)
      DO300 I=1,NS
      XFW(I)=FW(I)
300   CONTINUE
      KSP1=NS
      KSP=NC
      IF(KN.EQ.1)K1=0
      IF(K1.EQ.0)K2=0
      IF(K1.EQ.0)W=WI
      IF(K1.EQ.0)T1=533.33
      IF(K1.EQ.0)DIF=10.
      IF(K7.EQ.1)GOTO88
      IF(K1.NE.0)GOTO74
      DO128 I=1,KSP1
128   Y1(I)=YTEMP(I)
      W=WI
      IF(K7.GT.1)GOTO74
 88   DO 97 I=1,20
      DO 97 J=1,20
      TABLE(I,J)=0.
 97   CONTINUE
      DO 82 I=1,15
      DO 83 J=1,15
      RSC(I,J)=0.
      PSC(I,J)=0.
      REX(I,J)=0.
      PEX(I,J)=0.
 83   CONTINUE
 82   CONTINUE
      READ EQN 1 CH4 = H2 + 0.5C2H6
      READ21,(EQN(I),I=1,12)
      READ THE STOCHIOMETRIC COEFICIENTS OF THE EQUATION
      READ 22,RSC(1,2),DUM1,DUM2,PSC(1,1),PSC(1,3),DUM3
      READ THE EXPONENTS OF THE RATE EQUATION
      READ 22,REX(1,2),DUM4,DUM5,PEX(1,1),PEX(1,3),DUM6
      READ THE COEFECIENTS OF THE FORWARD AND REVERSE REACTION RATE CONS
      UNITS OF AF AND AR ARE IN GM-MOLES,CUBIC-CM,AND SECONDS
      UNITS OF AEF AND AER ARE IN KCAL PER GM-MOLE
      READ23,AF(1),SF(1),AEF(1)
```

FORTRAN SOURCE LIST KINET

SOURCE STATEMENT

```
      READ23,AR(1),SR(1),AER(1)
C     READ EQN 2 C2H6 = H2 + C2H4
      READ21,(EQN(I),I=1,12)
      READ22,RSC(2,3),DUM7,DUM8,PSC(2,1),PSC(2,4),DUM9
      READ22,REX(2,3),DU10,DU11,PEX(2,1),PEX(2,4),DU12
      READ23,AF(2),SF(2),AEF(2)
      READ23,AR(2),SR(2),AER(2)
 23   FORMAT(E8.0,1X,2F6.0)
 22   FORMAT(6F4.0)
 21   FORMAT(12A6)
C     READ EQN 3 C2H4 = H2 + C2H2
      READ21,(EQN(I),I=1,12)
      READ22,RSC(3,4),DU13,DU14,PSC(3,1),PSC(3,5),DU15
      READ22,REX(3,4),DU16,DU17,PEX(3,1),PEX(3,5),DU18
      READ23,AF(3),SF(3),AEF(3)
      READ23,AR(3),SR(3),AER(3)
C     READ EQN 4 C2H2 = 2C + H2
      READ21,(EQN(I),I=1,12)
      READ 22,RSC(4,5),DU19,DU20,PSC(4,13),PSC(4,1),DU21
      READ22,REX(4,5),DU22,DU23,PEX(4,13),PEX(4,1),DU24
      READ23,AF(4),SF(4),AEF(4)
      READ23,AR(4),SR(4),AER(4)
C     READ EQN 5 C6H6 = 3C2H2
      READ21,(EQN(I),I=1,12)
      READ22,RSC(5,6),DU25,DU26,PSC(5,5),DU27,DU28
      READ22,REX(5,6),DU29,DU30,PEX(5,5),DU31,DU32
      READ23,AF(5),SF(5),AEF(5)
      READ23,AR(5),SR(5),AER(5)
C     READ EQN 6 NH3 = 0.5N2 +1.5H2
      READ 21,(EQN(I),I=1,12)
      READ22,RSC(6,8),DU33,DU34,PSC(6,7),PSC(6,1),DU35
      READ22,REX(6,8),DU36,DU37,PEX(6,7),PEX(6,1),DU38
      READ23,AF(6),SF(6),AEF(6)
      READ23,AR(6),SR(6),AER(6)
C     READ EQN 7 CH4 + 2O2 = CO2 + 2H2O
      READ 21,(EQN(I),I=1,12)
      READ22,RSC(7,2),RSC(7,9),DU39,PSC(7,10),PSC(7,12),DU41
      READ22,REX(7,2),REX(7,9),DU42,PEX(7,10),PEX(7,12),DU43
      READ23,AF(7),SF(7),AEF(7)
      READ23,AR(7),SR(7),AER(7)
C     READ EQUATION 8 C + H2O = CO + H2
      READ 21,(EQN(I),I=1,12)
      READ 22,RSC( 8,13),RSC( 8,12),PSC( 8,11),PSC( 8,1)
      READ 22,REX( 8,13),REX( 8,12),PEX( 8,11),PEX( 8,1)
      READ23,AF(8),SF(8),AEF(8)
      READ23,AR(8),SR(8),AER(8)
C     READ EQN 9   CH4= 0.5C2H2 + 1.5H2
      READ 21,(EQN(I),I=1,12)
      READ 22,RSC(9,2),PSC(9,5),PSC(9,1)
      READ 22,REX(9,2),PEX(9,5),PEX(9,1)
      READ23,AF(9),SF(9),AEF(9)
      READ23,AR(9),SR(9),AER(9)
C     READ EQN 10 CH4 = C + 2H2
      READ 21,(EQN(I),I=1,12)
      READ 22,RSC(10,2),PSC(10,13),PSC(10,1)
```

FORTRAN SOURCE LIST KINET

SOURCE STATEMENT

```
      READ 22,PEX(10,2),PEX(10,13),PEX(10,1)
      READ 23,AF(10),SF(10),AEF(10)
      READ 23,AR(10),SR(10),AER(10)
C     READ THE NUMBER OF SPECIES-KSP AND THE NUMBER OF EQUATIONS-NEQ
C     READ THE MOLECULAR WEIGHTS OF THE SPECIES
      READ24,NEQ
   24 FORMAT(I6)
C     CONVERT TO KINET UNITS
       DO 127 I=1,KSP1
      Y1(I)=YI(I)
  127 YTEMP(I)=Y1(I)
   74 K1=K1+1
      P=PL/2160.
      R=82.06
      RR=1.987
      DELZ=DELZ*30.48
   75 FORMAT(1X,I6)
      IF(K1.GT.1)GOTO3
C
C     INITIAL AVERAGE MOLECULAR WEIGHT
C
      PRINT 2137
 2137 FORMAT(//20X,40HINITIAL MOLE FRACTION   MOLECULAR WEIGHT//)
      SUM=0.
      DO1J=1,KSP
      SUM=SUM+XFW(J)*Y1(J)
      PRINT 250,Y1(I),XFW(I)
  250 FORMAT(22X,1E17.8,5X,1E16.8)
    1 CONTINUE
      PRINT 250,Y1(KSP1),XFW(KSP1)
      AVGFW=SUM
C
C     INITIAL MOLAL FLUX OF SPECIE J(GM-MOLES/CM2-SEC)
C
      DO2J=1,KSP1
      FLUXMO(J)=(W/AVGFW)*(454./923.03)*Y1(J)
C
C     INITIAL MASS FLUX OF SPECIE J(GRAMS/CM2-SEC)
C
 2    FLUXMA(J)=FLUXMO(J)*XFW(J)
C
C     CALCULATION OF C(J)
C
      IF(K1.GT.1)GOTO3
      TZERO=298.16
      T=(TP1 +460.)/1.8
      GOTO4
 3    T=TVAR
 4    SUM1=0.
      IF(T.LT.T1)GOTO73
      K2=K2+1
      KOS=KSP+4
      DO17 I=5,KOS
      TABLE(K2,I)=Y1(I-4)
   17 CONTINUE
```

FORTRAN SOURCE LIST KINET

SOURCE STATEMENT

```
   73 DO5J=1,KSP
 5    SUM1=SUM1+FLUXMO(J)*R*T/P
      SUM=0.
      DO6J=1,KSP
      C(J)=FLUXMO(J)/SUM1
    6 SUM=SUM+C(J)
      C(KSP1)=SUM*Y1(KSP1)
C
C     CALCULATE REACTION RATE CONSTANT
C
      DO7I=1,NEQ
      FK(I)=AF(I)*T**(-SF(I))*EXP(-AEF(I)*1000./(RR*T))
 7    RK(I)=AR(I)*T**(-SR(I))*EXP(-AER(I)*1000./(RR*T))
C
C     CALCULATION OF REACTION RATE OF SPECIE(J)
C
      DO12J=1,KSP1
      SUM2=0.
      DO11I=1,NEQ
      XMULTR=1.0
      XMULTP=1.0
      DO10K=1,KSP1
      IF(C(K).LT.1.E-37)C(K)=1.E-37
      XMULTR=XMULTR*(C(K)**REX(I,K))
      XMULTP=XMULTP*(C(K)**PEX(I,K))
   10 CONTINUE
      SUM2=SUM2+(PSC(I,J)-RSC(I,J))*(FK(I)*XMULTR-RK(I)*XMULTP)
   11 CONTINUE
      RATE(J)=SUM2
   12 CONTINUE
  733 WNEW=0.
      SUM3=0.
      DO13J=1,KSP1
      FLUXMA(J)=FLUXMA(J)+RATE(J)*DELZ*XFW(J)
      IF(FLUXMA(J).LE.1.E-37)FLUXMA(J)=1.E-37
      FLUXMO(J)=FLUXMA(J)/XFW(J)
      IF(J.EQ.KSP1)GOTO13
      WNEW=WNEW+FLUXMA(J)*923.03/454.
      SUM3=SUM3+FLUXMO(J)
 13   CONTINUE
      DO14J=1,KSP
      Y1(J)=FLUXMO(J)/SUM3
   14 PERCE(J)=Y1(J)*100.
C
C     CALCUALTION OF THE RATIO OF THE MOLES OF THE
C     SOLID SPECIE TO THE MOLES OF GASES.
      Y1(KSP1)=FLUXMO(KSP1)/SUM3
C
C     SUM7 IS THE ENTHALPY OF THE GAS MIXTURE WITH RESPECT TO
C     THE ELEMENTS AT THEIR STANDARD STATE OF(P=1ATM T=298 OK)
C
      SUM7=0.
      SUM=0.
      DO 78I=1,KSP1
      ENT(I)=(AII(I)+BII(I)*TZERO/2.+CII(I)*(TZERO**2)/3.+DII(I)*(TZERO*
```

FORTRAN SOURCE LIST KINET

SOURCE STATEMENT

```
     1*3)/4.+EII(I)*(TZERO**4)/5.+FII(I)/TZERO)*RR*TZERO
      ENT(3)=-20.236E3
      ENT(6)=19.820E3
      IF(T.LT.1000.0)GOTO6207
      CPDT(I)=(AI(I)*(T-TZERO)+BI(I)*(T**2-TZERO**2)/2.+CI(I)*(T**3-TZER
     1O**3)/3.+DI(I)*(T**4-TZERO**4)/4.+EI(I)*(T**5-TZERO**5)/5.)*RR
      DO 296J=2,MM
      CPDT1(J)=(S1(J)*(T-TZERO)+S2(J)*(T**2-TZERO**2)/2.+S3(J)*(T**3-TZE
     1RO**3)/3.+S4(J)*(T**4-TZERO**4)/4.+S5(J)*(T**5-TZERO**5)/5.)*RR*.5
  296 CONTINUE
      CPDT1(1)=(S1(1)*(T-TZERO)+S2(1)*(T**2-TZERO**2)/2.+S3(1)*(T**3-TZE
     1RO**3)/3.+S4(1)*(T**4-TZERO**4)/4.+S5(1)*(T**5-TZERO**5)/5.)*RR
      GOTO6291
 6207 CPDT(I)=(AII(I)*(T-TZERO)+BII(I)*(T**2-TZERO**2)/2.+CII(I)*(T**3-
     1TZERO**3)/3.+DII(I)*(T**4-TZERO**4)/4.+EII(I)*(T**5-TZERO**5)/5.)*
     2RR
      DO297J=2,MM
      CPDT1(J)=(A11(J)*(T-TZERO)+A22(J)*(T**2-TZERO**2)/2.+A33(J)*(T**3-
     1TZERO**3)/3.+A44(J)*(T**4-TZERO**4)/4.+A55(J)*(T**5-TZERO**5)/5.)*
     2RR*.5
  297 CONTINUE
      CPDT1(1)=(A11(1)*(T-TZERO)+A22(1)*(T**2-TZERO**2)/2.+A33(1)*(T**3-
     1TZERO**3)/3.+A44(1)*(T**4-TZERO**4)/4.+A55(1)*(T**5-TZERO**5)/5.)*
     2RR
 6291 RSUM=0.
      DO 398 J=1,MM
C
C     RSUM IS THE ENTHALPY OF THE ELEMENTS OF THE ITH SPECIE AT TEMPERA-
C     TURE T(OK) WITH RESPECT TO THEIR STANDARD STATE(P=1ATM. T=298 OK).
C
  398 RSUM=RSUM+AA(I,J)*CPDT1(J)
      ENT(I)=ENT(I)+CPDT(I)-RSUM
      ENT(1)=0.
      ENT(7)=0.
      ENT(9)=0.
      ENT(13)=0.
      SUM=SUM+RATE(I)*ENT(I)
      IF(I.EQ.KSP1)GOTO78
      SUM7=SUM7+Y1(I)*(ENT(I)+RSUM)
   78 CONTINUE
      HEAT=(SUM/252.)*(30.48**3)/DTC
      KPT3=K2
      IF(T.LT.T1)GOTO37
      T1=T1+55.55555
      PRINT 889
  889 FORMAT(//7X,8HENTHALPY,5X,13HMOLE FRACTION,5X,7HRATE(I),8X,9HFLUXM
     1A(I)//)
      DO 777 I=1,KSP1
      PRINT 808,ENT(I),Y1(I),RATE(I),FLUXMA(I)
  808 FORMAT(1X,4E16.8)
  777 CONTINUE
      TABLE(K2,1)=T
      TABLE(K2,2)=HEAT
      TABLE(K2,3)=AVGFW
      TABLE(K2,4)=WNEW
```

FORTRAN SOURCE LIST KINET

SOURCE STATEMENT

```
      PRINT 6021
 6021 FORMAT(//2X,15HTEMPERATURE(OK),6X,4HHEAT,10X,9HMASS FLUX,9X,5HAVGF
     1W//)
      PRINT 6022,T,HEAT,WNEW,AVGFW
 6022 FORMAT(1X,4E16.8)
      PRINT 6032,SUM7
 6032 FORMAT(///1X,36HENTHALPY OF THE REACTING GAS SYSTEM=,1E16.8)
   37 SUM=0.
      DO 111 I=1,KSP
      SUM=SUM+XFW(I)*Y1(I)
  111 CONTINUE
      AVGFW=SUM
 2211 FORMAT(1X,6E14.8/)
  112 CONTINUE
      DO6606 IK=1,NC
      Y(IK)=Y1(IK)
 6606 CONTINUE
      RETURN
      END
```

ENTHALPY	MOLE FRACTION	RATE(I)	FLUXMA(I)
0.	0.24832489E-01	0.10555829E-03	0.68863822E-04
-0.21835453E 05	0.55668452E 00	-0.46370102E-04	0.12350086E-01
-0.20236000E 05	0.35522686E-05	0.14726862E-06	0.14776376E-06
0.88905566E 04	0.15697441E-05	0.12023008E-06	0.60904729E-07
0.52654235E 05	0.82673532E-05	0.37910340E-06	0.29804423E-06
0.19820000E 05	0.98974118E-22	-0.12132990E-25	0.10704271E-22
0.	0.80113050E-01	0.93403076E-12	0.31102993E-02
-0.13468053E 05	0.16792077E-03	-0.18630615E-11	0.39581678E-05
0.	0.86118263E-27	0.14039841E-29	0.38210798E-28
-0.94685054E 05	0.15137768E-01	-0.70199203E-30	0.92353931E-03
-0.27834013E 05	0.12123620E-02	0.13609923E-04	0.47068593E-04
-0.59907508E 05	0.32183853E 00	-0.13609923E-04	0.80325124E-02
0.	0.15449803E 01	0.31466975E-04	0.25706634E-01

TEMPERATURE(CK)	HEAT	MASS FLUX	AVGFW
0.14223403E 04	0.96301310E-03	0.49885977E-01	0.17699366E 02

ENTHALPY OF THE REACTING GAS SYSTEM= -0.15908107E 05

ENTHALPY	MOLE FRACTION	RATE(I)	FLUXMA(I)
0.	0.28116063E-01	0.13815831E-03	0.78117756E-04
-0.21846780E 05	0.55415560E 00	-0.61585103E-04	0.12317341E-01
-0.20236000E 05	0.98663723E-05	0.29181405E-06	0.41119139E-06
0.88491919E 04	0.12417002E-04	0.81772020E-06	0.48299213E-06
0.52601212E 05	0.30056943E-04	0.13353276E-05	0.10856339E-05
0.19820000E 05	0.98291681E-22	-0.24485321E-25	0.10650662E-22
0.	0.79961125E-01	0.21503266E-11	0.31102993E-02
-0.13473978E 05	0.16760221E-03	-0.43006532E-11	0.39581653E-05
0.	0.89811119E-27	0.14243908E-29	0.39925038E-28
-0.94715405E 05	0.15109060E-01	-0.71219539E-30	0.92353931E-03
-0.27933526E 05	0.16393433E-02	0.17696421E-04	0.63766588E-04
-0.59961114E 05	0.32079889E 00	-0.17696421E-04	0.80217772E-02
0.	0.15430168E 01	0.38998958E-04	0.25722736E-01

TEMPERATURE(CK)	HEAT	MASS FLUX	AVGFW
0.14828133E 04	0.12524803E-02	0.49853334E-01	0.17655207E 02

ENTHALPY OF THE REACTING GAS SYSTEM= -0.14854536E 05

ENTHALPY	MOLE FRACTION	RATE(I)	FLUXMA(I)

0.	0.31277198E-01	0.17888312E-03	0.87061729E-04
-0.21847249E 05	0.55167712E 00	-0.82311834E-04	0.12284978E-01
-0.20236000E 05	0.17520340E-04	0.57663911E-06	0.73153223E-06
0.88195344E 04	0.47078513E-04	0.28509407E-05	0.18346373E-05
0.52556908E 05	0.77825992E-04	0.36980169E-05	0.28162257E-05
0.19820000E 05	0.97436288E-22	-0.42760104E-25	0.10577542E-22
0.	0.79813195E-01	0.41837895E-11	0.31102993E-02
-0.13473254E 05	0.16729201E-03	-0.83675789E-11	0.39581619E-05
0.	0.92569896E-27	0.14409323E-29	0.41227708E-28
-0.94741997E 05	0.15081109E-01	-0.72046615E-30	0.92353931E-03
-0.28020883E 05	0.20390736E-02	0.21794521E-04	0.79462159E-04
-0.60004282E 05	0.31980262E 00	-0.21794521E-04	0.80116867E-02
0.	0.15410323E 01	0.46266120E-04	0.25737267E-01

TEMPERATURE(CK)	HEAT	MASS FLUX	AVGFW
0.15350336E 04	0.16531647E-02	0.49824035E-01	0.17613353E 02

ENTHALPY OF THE REACTING GAS SYSTEM= -0.13926436E 05

ENTHALPY	MOLE FRACTION	RATE(I)	FLUXMA(I)
0.	0.36405757E-01	0.24917514E-03	0.10164915E-03
-0.21839388E 05	0.54751668E 00	-0.12079509E-03	0.12229847E-01
-0.20236000E 05	0.29178963E-04	0.12864041E-06	0.12220664E-05
0.87941956E 04	0.18668784E-03	0.95402441E-05	0.72975610E-05
0.52512535E 05	0.23728701E-03	0.10313216E-04	0.86129315E-05
0.19820000E 05	0.95738038E-22	-0.72269475E-25	0.10425162E-22
0.	0.79568372E-01	0.79195565E-11	0.31102993E-02
-0.13467270E 05	0.16677854E-03	-0.15839113E-10	0.39581546E-05
0.	0.95838440E-27	0.14570407E-29	0.42837084E-28
-0.94769882E 05	0.15034848E-01	-0.72852036E-30	0.92353931E-03
-0.28112356E 05	0.26314467E-02	0.26539105E-04	0.10286231E-03
-0.60045977E 05	0.31822298E 00	-0.26539105E-04	0.79966430E-02
0.	0.15375523E 01	0.54291780E-04	0.25758160E-01

TEMPERATURE(CK)	HEAT	MASS FLUX	AVGFW
0.15889111E 04	0.24392515E-02	0.49782484E-01	0.17539373E 02

ENTHALPY OF THE REACTING GAS SYSTEM= -0.12914062E 05

T(1)= 500.000000 DT(1)= 25252.399902

T(L)	DT(L)	XAXIS(L)	YAXIS(L)	CAPAC(L)	
500.00000	25252.39990	0.00000	0.00000	0.56901	1
505.25250	25252.39990	0.01000	0.00263	0.56901	2
510.58553	26030.03564	0.02000	0.00529	0.57053	3
516.08235	26827.36865	0.03000	0.00804	0.57210	4

521.74709	27644.66919	0.04000	0.01087	0.57371	5
527.58393	28482.20044	0.05000	0.01379	0.57537	6
533.59710	29340.21729	0.06000	0.01680	0.57708	7
539.79089	30218.96582	0.07000	0.01990	0.57885	8
546.16963	31118.68311	0.08000	0.02308	0.58066	9
552.73772	32039.59668	0.09000	0.02637	0.58254	10
559.49958	32981.92383	0.10000	0.02975	0.58446	11
566.45969	33945.87061	0.11000	0.03323	0.58645	12
573.62257	34931.63281	0.12000	0.03681	0.58848	13
580.99277	35939.39404	0.13000	0.04050	0.59058	14
588.57489	36969.32568	0.14000	0.04429	0.59274	15
596.37355	38021.58691	0.15000	0.04819	0.59496	16
604.39342	39096.32373	0.16000	0.05220	0.59724	17
612.63918	40193.66846	0.17000	0.05632	0.59958	18
621.11555	41313.74022	0.18000	0.06056	0.60198	19
629.82727	42456.64355	0.19000	0.06491	0.60445	20
638.77910	43622.46875	0.20000	0.06939	0.60698	21
647.97581	44811.29102	0.21000	0.07399	0.60958	22
657.42219	46023.17090	0.22000	0.07871	0.61224	23
667.12304	47258.15332	0.23000	0.08356	0.61497	24
677.08318	48516.26758	0.24000	0.08854	0.61776	25
687.30740	49797.52686	0.25000	0.09365	0.62063	26
697.80054	51101.92871	0.26000	0.09890	0.62356	27
708.56741	52429.45459	0.27000	0.10428	0.62656	28
719.61279	53780.06885	0.28000	0.10981	0.62963	29
730.94151	55153.71924	0.29000	0.11547	0.63276	30
742.55833	56550.33789	0.30000	0.12128	0.63597	31
754.46803	57969.83887	0.31000	0.12723	0.63924	32
766.67535	59412.12061	0.32000	0.13334	0.64258	33
779.18504	60877.06396	0.33000	0.13959	0.64599	34
792.00177	62364.53271	0.34000	0.14600	0.64947	35
805.13023	63874.37451	0.35000	0.15257	0.65301	36
818.57504	65406.41943	0.36000	0.15929	0.65662	37
832.34081	66960.48145	0.37000	0.16617	0.66029	38
846.43211	68536.35742	0.38000	0.17322	0.66403	39
860.85343	70133.82910	0.39000	0.18043	0.66784	40
875.60925	71752.66113	0.40000	0.18780	0.67171	41
890.70399	73392.60254	0.41000	0.19535	0.67564	42
906.14201	75053.38672	0.42000	0.20307	0.67963	43
921.92762	76734.73145	0.43000	0.21096	0.68368	44
938.06506	78436.34180	0.44000	0.21903	0.68779	45
954.55851	80157.90723	0.45000	0.22728	0.69196	46
971.41209	81899.10449	0.46000	0.23571	0.69619	47
988.62986	83659.59863	0.47000	0.24431	0.70047	48
1006.21579	85439.04199	0.48000	0.25311	0.70480	49
1024.17378	87237.07813	0.49000	0.26209	0.70919	50
1042.50766	89053.34082	0.50000	0.27125	0.71363	51
1061.22119	90887.45703	0.51000	0.28061	0.71812	52
1080.31804	92739.04688	0.52000	0.29016	0.72267	53
1099.80180	94607.72656	0.53000	0.29990	0.72726	54
1119.67599	96493.11133	0.54000	0.30984	0.73190	55
1139.94405	98394.81738	0.55000	0.31997	0.73660	56
1160.60933	100312.46191	0.56000	0.33030	0.74134	57
1181.67509	102245.67090	0.57000	0.34084	0.74614	58
1203.14456	104194.07813	0.58000	0.35157	0.75099	59
1225.02084	106157.33105	0.59000	0.36251	0.75589	60
1247.30699	108135.09473	0.60000	0.37365	0.76085	61
1270.00600	110127.05566	0.61000	0.38500	0.76587	62
1293.12079	112132.92676	0.62000	0.39656	0.77096	63

1316.65422	114152.45313	0.63000	0.40833	0.77612	64
1340.60912	116185.39355	0.64000	0.42030	0.78134	65
1364.98819	118230.76660	0.65000	0.43249	0.78632	66
1389.79390	120287.65723	0.66000	0.44490	0.79133	67
1415.02861	122355.66406	0.67000	0.45751	0.79636	68
1440.69458	124434.39160	0.68000	0.47035	0.80142	69
1466.79431	126523.45215	0.69000	0.48340	0.80650	70
1493.32901	128622.46484	0.70000	0.49666	0.81160	71
1520.30161	130731.05566	0.71000	0.51015	0.81671	72
1547.71375	132848.85938	0.72000	0.52386	0.82184	73
1575.56732	134975.52148	0.73000	0.53778	0.82699	74
1603.86414	137110.69531	0.74000	0.55193	0.83214	75
1632.60593	139254.04492	0.75000	0.56630	0.83730	76
1661.79436	141405.24414	0.76000	0.58090	0.84247	77
1691.43102	143563.97852	0.77000	0.59572	0.84765	78
1721.51746	145729.94531	0.78000	0.61076	0.85282	79
1752.05515	147902.85156	0.79000	0.62603	0.85800	80
1783.04549	150082.41797	0.80000	0.64152	0.86318	81
1814.48985	152268.37891	0.81000	0.65724	0.86835	82
1846.38954	154460.48438	0.82000	0.67319	0.87351	83
1878.74580	156658.50000	0.83000	0.68937	0.87867	84
1911.55984	158862.21484	0.84000	0.70578	0.88381	85
1944.83284	161071.44336	0.85000	0.72242	0.88894	86
1978.56592	163286.03906	0.86000	0.73928	0.89406	87
2012.76018	165505.90234	0.87000	0.75638	0.89916	88
2047.41672	167731.00977	0.88000	0.77371	0.90425	89
2082.53662	169961.45117	0.89000	0.79127	0.90931	90
2118.12103	172197.48242	0.90000	0.80906	0.91435	91
2154.17117	174439.60742	0.91000	0.82709	0.91937	92
2190.68835	176688.70508	0.92000	0.84534	0.92436	93
2227.67419	178946.18555	0.93000	0.86384	0.92932	94
2265.13065	181214.22852	0.94000	0.88257	0.93426	95
2303.06024	183496.11133	0.95000	0.90153	0.93917	96
2341.46631	185796.69531	0.96000	0.92073	0.94405	97
2380.35345	188123.14258	0.97000	0.94018	0.94890	98
2419.72806	190485.91797	0.98000	0.95986	0.95372	99
2459.59921	192900.24219	0.99000	0.97980	0.95852	100
2499.97977	195388.35938	1.00000	0.99999	0.95852	101

TEMPERATURE PROFILE DEFINED

(I)	ZX(I)	TP(I)	P(I)
1	0.000010	500.250668	2178.869598
2	0.006940	783.832504	2175.997925
3	0.013870	1406.974976	2170.710266
4	0.020800	2500.000000	2160.000000

TEMPERATURE-PRESSURE PROFILES DEFINED. HEAT FLUX CALCULATED.

NON-EQUILIBRIUM FLOW RESULTS

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