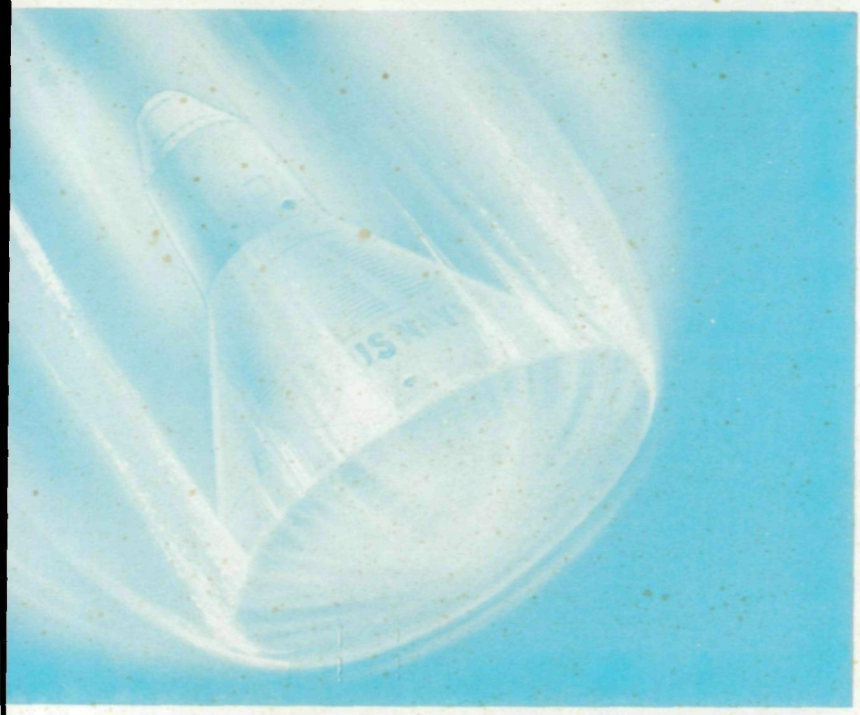

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REACTING FLUIDS LABORATORY

FINAL REPORT
ON
NASA GRANT NGR 19-001-016

EVALUATION OF THE ENERGY TRANSFER IN THE CHAR ZONE DURING ABLATION

Part II: In-Depth Response of Ablative Composites

AUG 1975
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Department of Chemical Engineering

December 15, 1974

Volume II

LOUISIANA STATE UNIVERSITY

IN DEPTH RESPONSE OF

ABLATIVE COMPOSITES

VOLUME II

A Dissertation

Submitted to the Graduate Faculty of the
Louisiana State University and Agricultural
and Mechanical College in partial fulfillment
of the requirements for the degree of
Doctor of Philosophy

in

The Department of Chemical Engineering

by

Eduardo Gonzales del Valle
B.S., Louisiana State University, 1965
M.S., Louisiana State University, 1969

May 1975

PREFACE

This report is the second of two parts and completes the documentation on NASA Grant NGR-19-001-015. It also served as the PhD dissertation for Edwards G. del Valle.

APPENDIX A

EXPLANATION OF THE COMPUTER IMPLEMENTED SOLUTIONS OF THE ENERGY TRANSFER FOR DECOMPOSITION IN-DEPTH OF PLASTIC ABLATORS

The ABLATIN1 and ABLATIN2 systems are general analyses implemented in FORTRAN IV for studying the energy transfer in the combined decomposition/char zone of a charring ablator. Both of these analyses treat the decomposition of the virgin material in the same fashion. Namely, a pseudo-order kinetic expression of the form of Equation (2-1) is used to describe the decomposition process. These analyses differ, however, in the way the chemical generation term is calculated in the char zone. As was explained in Chapter III, there are three chemically distinct flow conditions that are considered, which are, frozen, equilibrium and non-equilibrium flow. The ABLATIN1 analysis considers the pyrolysis gases to be either frozen (not chemical reactions) or, in chemical equilibrium. The frozen flow and equilibrium flow cases give the lower and upper limits of the total energy transfer in the decomposition-char zone, respectively. The ABLATIN2 analysis considers only the gases to be in chemical non-equilibrium: i.e., the rate of reaction is described using finite rate chemistry. Both analyses require that the temperature, the heat flux and the composition

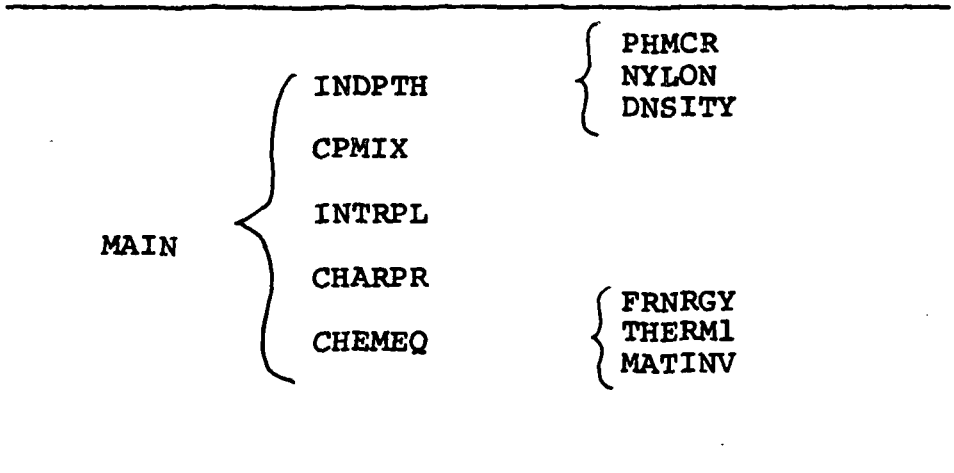
of the pyrolysis gases be specified. Unfortunately, as was said in Chapter III, the current state of the art precludes prediction of the composition of the pyrolysis products from a known combination of plastic composites and therefore it was necessary to specify the pyrolysis gas composition. The boundary conditions selected are written in Equation (3-27).

Once the energy equation is solved, the momentum equation is solved by specifying the front surface pressure. Because the pressure drop is small ($\sim$15 lbs/ft^2), compared to the total pressure ($\sim$2160 lbs/ft^2), the assumption of constant pressure in the solution of the energy equation can be considered valid and the equations can be uncoupled. In both analyses the surface recession velocity is specified and the mass flux of pyrolysis gases is calculated from Equation (3-1). Furthermore, the analyses do not require the arbitrary specification of a char thickness, which is calculated.

The ABLATIN1 System

This analysis provides the lower and upper limits of the total energy transfer in the combined decomposition-char zone by considering the pyrolysis gases to be in frozen, or in chemical equilibrium. This analysis consists of a MAIN program and eleven subroutines. Two of these subroutines are major subroutines in the sense that they control the flow of information to other minor subroutines. A hierarchical diagram of this is shown in Figure A-1. The two major sub-

Figure A-1. Hierarchical System Diagram of ABLATIN1



routines are INDPTH and CHEMEQ and their functions are explained below. The MAIN program has direct access to three other subroutines, which are, CPMIX, INTRPL, and CHARPR. An explanation of each subroutine follows next.

INDPTH: This is one of the two major subroutines. In it the physical properties of the virgin material as a function of temperature are calculated. The thermal conductivity gradient is likewise calculated in this subroutine for use in the general energy equation. In addition, the energy absorbed (BTU/FT^3-sec) due to the degradation of the plastic composites is calculated using the information generated by three minor subroutines, which are: PHMCR, NYLON, and DNSITY. The functions of each one of these subroutines are subsequently explained.

PHMCR: In this subroutine the heat absorbed by the degradation of phenolic resin and phenolic-microballoons is calculated based on the data of Sykes and Nelson (1). The heat term has the units of BTU/lb of each composite.

NYLON: Similar in nature to PHMCR, this subroutine calculates the heat absorbed (in BTU/lb) due to the degradation of nylon based also on the data of Sykes and Nelson (1).

DNSITY: This subroutine calculates the rate of density change of each individual composite (i.e., nylon, phenolic and phenolic-microballoons), which provides the information required to compute the mass flux of pyrolysis gases. In addition, this subroutine is used to control the Runge-Kutta step size while the solution of the energy equation is

marching through the decomposition zone. The density changed (in lbs/ft^3-sec) calculated in this subroutine along with the heat (in BTU/lb) calculated in PHMCR and NYLON are used to generate the q(T) term (in BTU/ft^3-sec) in the general energy equation. (See Equation (3-20)). The calculation of q(T) is performed in subroutine INDPTH.

The first four subroutines just described, PHMCR, NYLON, INDPTH, and DNSITY, constitute the principal subroutines used in describing the physico-chemical changes of the decomposition of nylon-phenolic resin composites. These four subroutines are used when the numerical solution is marching along the decomposition zone. When the decomposition of the virgin material is complete, that is, the virgin material has degraded to gases and char residue, the program has two options. One is to describe the gases with a frozen flow chemistry, in which case the composition of the gases stay constant with temperature, or, to describe the gases with an equilibrium chemistry, in which case the composition of the gases change with temperature and are computed from thermodynamic principles. Both options are explained below.

Frozen Flow Analyses: Under this option the energy equation is solved assuming that there are no chemical reactions taking place in the char zone and hence the chemical composition of the gas mixture does not change. This method of analysis gives the lower bound of the energy absorbed within the char zone. It is the simplest, in terms of numerical solution and the fastest to solve on a machine,

requiring about one minute on an IBM 360/65 computer. Under this option two subroutines are called, these are: CPMIX and CHARPR. An explanation of their functions follows.

CPMIX: This subroutine is called by MAIN to calculate the average heat capacity of a frozen flow mixture. This subroutine is called at every new temperature generated by the Runge-Kutta analysis. The heat capacity of each individual specie is generated by an empirical fit which is read in by MAIN. The thermodynamic data used is given in Appendix C.

CHARPR: The data of Southern Research Institute (2) is used in this subroutine to generate the thermal conductivity, the thermal conductivity gradient and the heat capacity of the char as a function of temperature. Unlike CPMIX, this subroutine is also used by the chemical equilibrium analysis option. The actual data used is presented in Appendix C.

Equilibrium Flow Analysis: This analysis is the second option of the ABLATIN1 system to describe the chemistry in the char zone. The primary difference with the frozen flow analysis is that the equilibrium analysis accounts for concentration changes due to chemical reactions, which are assumed to be in thermodynamic equilibrium. A free energy minimization technique is used to compute the equilibrium composition as a function of temperature. This technique was developed in Chapter IV and the reader is referred to this Chapter for further details. The Equilibrium Flow Analysis uses in addition to CHARPR, five other subroutines which are:

CHEMEQ, which minimizes the free energy; FRNGY, which calculates the free energy function to be minimized; MATINV which inverts the matrix and solves the simultaneous linear equations; THERM1, whose primary function is to calculate the heats of formation of the chemical species; and INTRPL which is used to interpolate the values generated by CHEMEQ and which are needed for the solution of the general energy equation. A more complete explanation of the functions of each subroutine follows next.

CHEMEQ: This is the other major subroutine. This subroutine is called by MAIN when the marching procedure is in the char zone. In this subprogram the equilibrium composition of a multi-component, polyphase system is calculated using free energy minimization technique, which has been explained in Chapter IV. This subroutine is called once throughout the analysis. The equilibrium compositions of each individual species are computed and stored as functions of temperature. In addition, the mass flux, the average molecular weight, the average heat capacity of the mixture and the heat absorbed due to chemical reactions are also stored as functions of temperature. All of these stored values are later used to generate interpolated values needed in the solution of the general energy equation.

To verify the calculations made by this program, several literature examples were used for comparison and the reader is referred to Chapter IV for these comparisons.

FRNRGY: This subroutine supplies the free energy func-

tion to be minimized by CHEMEQ. This subroutine is called at every temperature at which an equilibrium composition calculation is performed. In addition, the heat capacity of each individual species is also calculated.

MATINV: This subroutine is a standard method for solving a set of linear equations by inverting a non-singular nxn matrix. The inversion is performed iteratively by reducing the original matrix to an identity matrix by a series of row operations. The method is then repeated with the resulting identity matrix. The IBM Share Library is the source for this particular program (3). The simultaneous solution of the linear equations (see Table 4-1) gives the Lagrange multipliers which are used to generate the new composition of the gases for the next iteration (see Equation (4-32)). In addition, when there are solid species, the solution of the linearized equations (see Table 4-1) results in the explicit computation of the number of moles of these species directly. This is not the case for the gas species.

THERM1: The calculation of the heat of formation and the entropy of each chemical species is performed in this subroutine. This subroutine is called by CHEMEQ after the species compositions are calculated. The reference temperature used in the calculations is 298.16^{o}K.

INTRPL: This is a general purpose Lagrangian interpolation subprogram with non-equal step size between points. This subprogram is used by MAIN to interpolate the stored values generated by CHEMEQ. In addition, INTRPL is used in

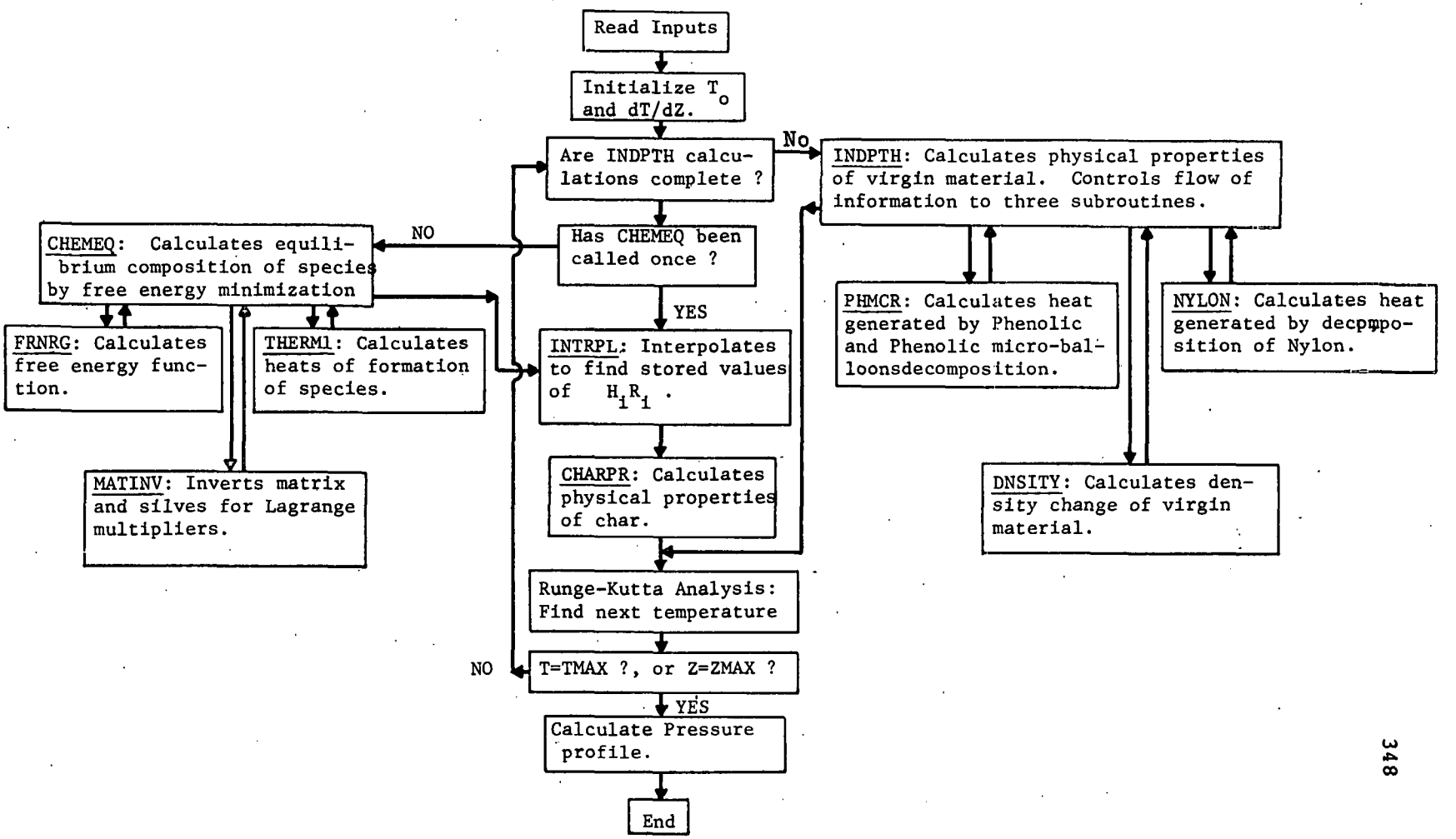
the solution of the uncoupled momentum equation to interpolate values generated during the solution of the energy equation.

The five subroutines just mentioned in addition to CHARPR, constitute the principal subroutines used in describing the physico-chemical changes which occur within the char zone.

Next a brief description of MAIN (the main program) follows. In it the calling sequence of the subroutines for the chemical equilibrium analysis option and the frozen flow analysis are explained.

MAIN: The main program solves the energy equation by using a Runge-Kutta formulae of the form developed in Chapter III. MAIN is assisted in the solution of the energy equation by ten subroutines for the equilibrium analysis, and by two subroutines for frozen flow analysis. As was explained, CHARPR is used by both analyses, so that the total number of subroutines is eleven. A block flow diagram of the main program for the chemical equilibrium option is shown in Figure A-2. After the data is read in and variables are initialized MAIN proceeds to call subroutine INDPTH to generate the physico-chemical properties for the decomposition process. INDPTH interacts with PHMCR, NYLON and DNSITY to obtain the mass flux, heat of reaction and other variables as was previously explained. Once these properties have been calculated MAIN proceeds to calculate the next temperature point in the Runge-Kutta analysis.

Figure A-2. Block Flow Diagram of the ABLATIN1 Program.



This operation is repeated until the virgin material has been totally degraded to gases and char. At this instance MAIN calls CHEMEQ to generate the equilibrium composition of the reacting gases, along with other needed information such as: mass flux of the gases, average molecular weight, the average heat capacity of the mixture and the heat absorbed due to chemical reactions. Unlike subroutine INDPTH, which was called at every new temperature, subroutine CHEMEQ is called only once. This can be done because the equilibrium composition is only a function of temperature and pressure. Pressure is assumed constant through the analysis, and the equilibrium composition, the mass flux, the average molecular weight, the average heat capacity of the mixture and the heat absorbed due to chemical reactions are stored as functions of temperature. Since every new temperature generated by the Runge-Kutta analysis does not coincide with the temperature of the stored information, an interpolation scheme is necessary to generate these values at these intermediate temperatures. This interpolation function is performed by subroutine INTRPL. It was found by this author that storing the equilibrium composition every $10^{o}K$ was sufficient to give accurate interpolated values at intermediate temperature points. After the interpolation is performed CHARPR is called to generate the physical properties for the char. A new temperature is then generated and the procedure is repeated until the temperature of the char reaches the sublimation temperature of carbon at the given

pressure.

For frozen flow the numerical solution while in the decomposition zone is the same. When the marching solution enters the char the primary difference is that CHEMEQ and INTRPL subroutines are bypassed. Instead, MAIN calls CPMIX to generate the heat capacity of the frozen flow mixture and then proceeds to call CHARPR for the physical properties of the char. A new temperature is generated as in the equilibrium case and the process is repeated until the temperature of the char reaches the sublimation temperature of carbon at the given pressure.

Once the temperature profile is established, i.e., the energy equation has been solved, the program proceeds to calculate the pressure profile. More is said about the pressure calculations after the description of the ABLATIN2 System which follows below.

The ABLATIN2 System

This analysis is programmed exclusively for non-equilibrium flow chemistry where the rate of reaction of each species is described by finite rate chemistry. Compared to the chemical equilibrium analysis, the non-equilibrium flow analysis is easy to program. It takes three DO LOOPS and about 20 FORTRAN statements to calculate the rate of reaction of a chemical species which is simultaneously reacting in more than one chemical reaction.

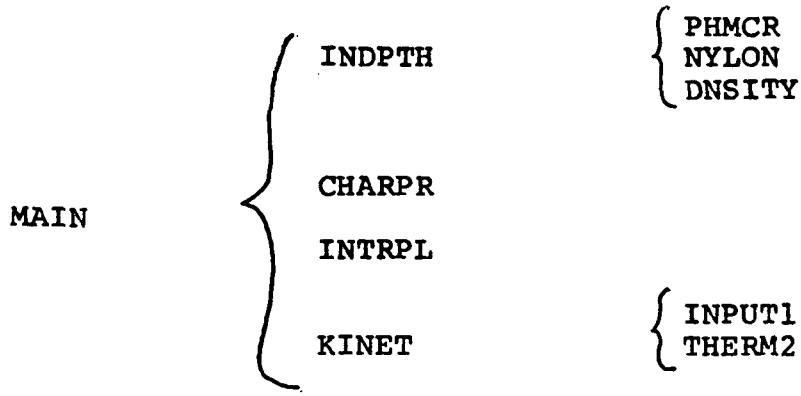
The computing time for the non-equilibrium analysis

however, exceeds that of chemical equilibrium by a factor of about 10. As was explained in Chapter V, this is due in part to the stiffness of the general energy equation caused by very fast chemical reactions taking place in the flow field. This stiffness requires that the step size be of the order of 10^{-7} to 10^{-8} feet to maintain numerical stability. Because the step size was so small many operations had to be made double precision to reduce round-off error. Operations in double precision arithmetic also increased the computing time.

In comparing Figure A-1 and Figure A-3 it is seen that the ABLATIN1 and ABLATIN2 systems use the same subroutines to describe the decomposition process. These subroutines are: INDPTH, PHMCR, NYLON and DNSITY. In addition, CHARPR and INTRPL and the four previously mentioned subroutines perform the same functions in both the ABLATIN1 and ABLATIN2 systems and will not be described again.

Non-Equilibrium Flow Analysis: The primary difference between the equilibrium and non-equilibrium flow analyses is the way the rate of production of chemical species is computed. In the chemical equilibrium analysis the rate of production of species, is computed from thermodynamic principles, while for non-equilibrium, finite rate chemistry is used. The rate of reaction of each species is computed by subroutine KINET. In the non-equilibrium flow analysis, changes in the mole flux of each species with temperature must be calculated as part of the Runge-Kutta analysis. That

Figure A-3 Hierarchical System Diagram of ABLATIN2



is, for each temperature generated in the Runge-Kutta analysis, a corresponding set of concentrations must be calculated. This requires that KINET be called by MAIN at every new increment of temperature. This is necessary because the concentration changes are not only functions of temperature and pressure, but of composition as well. KINET in addition calls two other subroutines, INPUT1 and THERM2 and their functions are subsequently explained.

KINET: This subprogram is the counterpart of CHEMEQ. In it the reaction rate of each species is computed using finite rate data read in by INPUT1. The mole fraction, the total mass flux, the average molecular weight, the heat capacity of the mixture and the heat absorbed due to chemical reactions are also computed and stored for later use in the calculations. In addition, this subroutine controls the step size of the Runge-Kutta analysis to maintain stability. For the CHEMEQ analysis the step size needed to maintain stability is of the order of 10^{-4} to 10^{-5} feet, while for KINET a step size of the order of 10^{-7} to 10^{-8} feet is necessary to maintain stability in regions where rapid chemical changes are occurring.

INPUT1: This subroutine reads in the kinetic data needed to compute finite rate chemistry.

THERM2: This subprogram is similar to THERM1 with the difference that the heat capacity of each species is calculated in addition to the heats of formation. This subprogram is called by KINET at every temperature.

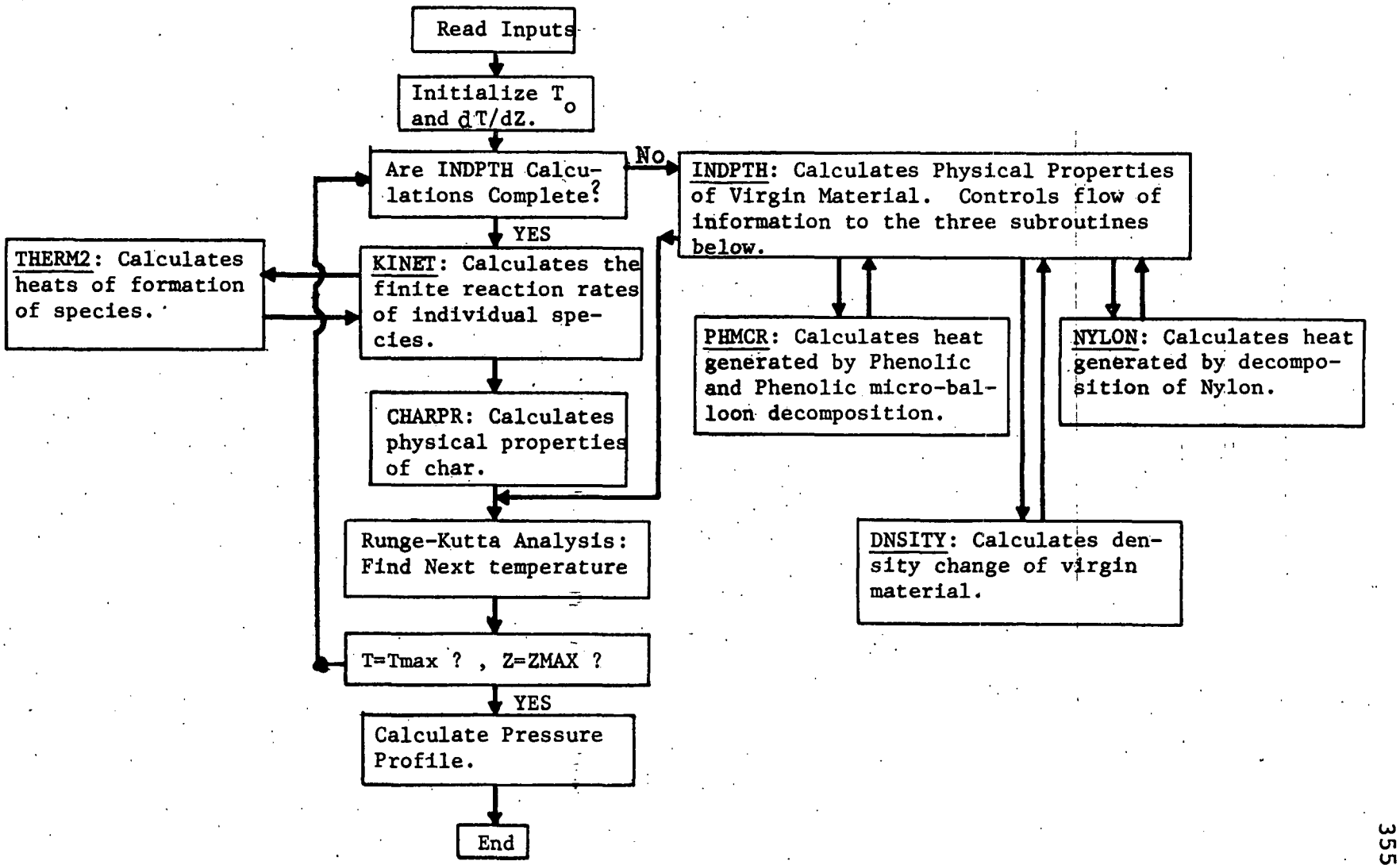
MAIN: The main program of ABLATIN2 performs very similar operations as that for the ABLATIN1 system. In Figure A-4 a block flow diagram of the ABLATIN2 system is given. The principal difference is that in ABLATIN1, MAIN calls CHEMEQ to generate the compositions of the species while in this case KINET is called by MAIN. The rest of the computations are the same as has been explained before.

Calculation of the Pressure Distribution

The pressure distribution through the char zone is calculated by integrating Equation (3-13) using a Simpson's rule integration. Since it was shown in Chapter III that this equation could be uncoupled from the energy equation, its solution is calculated after the temperature distribution is known. Therefore, the integration method for this momentum equation is the same for both the ABLATIN1 and ABLATIN2 system. Interpolation using subprogram INTRPL of both char distance and collision integral as a function of the temperature distribution across the char is required. These operations allow the calculation of the gas mixture viscocity as a function of char distance. The pressure calculation scheme used in this research was developed by April (4).

Simpson's Rule Integration Step: As discussed in Chapter III, the Simpson's Rule formula is used to integrate the pressure equation, Equation (3-13). As with the Runge-Kutta analysis it is necessary to select a step size that gives a fast, yet accurate solution to the equation. April

Figure A-4. Block Flow Diagram of the ABLATIN Program.



(4) made a study of several interval sizes and his results are presented in Table A-1. As noted in this table, April (4) found that the solution of the momentum equation becomes stable with twenty integration steps.

Summary

In this appendix an introduction to the ABLATIN1 and ABLATIN2 systems was given. The ABLATIN1 system was developed to compute the total energy absorbed in the combined decomposition-char zone for a frozen and equilibrium flow model. These two analyses gave the lower and upper limits of the energy absorbed within the combined zones. The ABLATIN2 analysis was developed exclusively for non-equilibrium flow chemistry. This analysis was said to be more time consuming on a computing machine, although it is simpler to program than the other two models. The various functions of each subprogram was explained in detail and block flow diagrams for both the ABLATIN1 and ABLATIN2 systems were given. Finally, a brief explanation on the solution of the pressure equation by MAIN, was given.

In Appendix B a complete listing of the ABLATIN1 and ABLATIN2 systems is presented along with typical input and output data for the frozen, equilibrium and non-equilibrium flow chemistry.

TABLE A-1: Comparison of Various Simpson's Rule Increment Sizes for the Frozen Flow, Variable Physical Properties Analysis After April (4).

Dimensionless Char Distance (Z/L)	Pressure (lb/ft^2) Simpson's Rule Increment Size 20	50	100	200
0.00	2175.5921	2175.5918	2175.5913	2175.5912
0.33	2173.4147	2173.4144	2173.4139	2173.4138
0.67	2168.7373	2168.7368	2168.7364	2168.7364
1.00	2160.0000	2160.0000	2160.0000	2160.0000

Conditions: $W = 0.05\ lb/ft^2\text{-sec}$ $L = 0.0208\ ft$ $\varepsilon = 0.8$

Gas Composition (Mole/Mole Gas):

$CO = 0.245$, $CO_2 = 0.046$, $N_2 = 0.073$, $CH_4 = 0.570$, $C_6H_6 = 0.068$

REFERENCES

1. Sykes, G. F., and J. B. Nelson, "Thermodynamic of Ablation Materials", Preprint 7B, 61st National Meeting, AIChE, Houston, Texas (Feb. 19-23, 1967).

2. Engelke, W. T., C. M. Pyron, Jr., and C. D. Pears, "Thermophysical Properties of a Low Density Phenolic Nylon Ablation Material". NASA CR-809 (July, 1967).

3. Sadaka, R. N., "Double Precision Matrix Inversion with Selective Pivot", IBM Share Library No. 7090-f1, B181 INV2(1965).

4. April, G. C., "Evaluation of the Energy Transfer in the Char Zone During Ablation", PhD. Dissertation, Louisiana State University, Baton Rouge, May 1969.

APPENDIX B

THE ABLATIN1 AND ABLATIN2 ANALYSES

As discussed in Appendix A, the ABLATIN1 and ABLATIN2 programs are general analyses implemented in FORTRAN IV for studying the energy transfer in the decomposition zone and char zone of char forming ablators. The ABLATIN1 analysis was said to consider the pyrolysis gases to be either frozen, or in chemical equilibrium. The ABLATIN2 analysis on the other hand, considers the gases to be in chemical non-equilibrium.

As was shown in Appendix A a great degree of overlap exists in the many common subroutines used by the two analyses. The rationale, however, for keeping the ABLATIN1 and ABLATIN2 analyses as separate programs was due to core restrictions. There were, in addition, other practical considerations regarding input-output which made the separate development of these programs more practical.

A listing of the ABLATIN1 program with all the subroutines is presented in Table B-1. An explanation of the function of each subroutine has been given in Appendix A. Most of the subroutines are self-explanatory with most of the major functions explained through comment cards. The degree of modularity of this program makes it highly flexible, and subject to easy modification in the future. For this reason the author has provided an extensive nomenclature of every

important variable in the program. This was done in the hope of minimizing errors incurred in modifying any subroutine. Furthermore, the listing allows easy cross referencing of variables among subroutines, which will further reduce the possibility of errors.

Communication among subroutines is mostly done by means of labeled common blocks, thus minimizing communication through arguments of a call. This was done to reduce computer time among frequently called subroutines. However, this method of structuring communication can be very error prone and was an additional motivation for providing a nomenclature listing of every important variable. In this way any modification of a variable can be cross checked in the nomenclature listing of every subroutine. A detailed explanation of the input format is also given in this Appendix.

Following the listing and explanation of input format for the ABLATIN1 program, is the listing of ABLATIN2. The ABLATIN2 is listed in Table B-4. In both cases, typical input data and output results are listed.

TABLE B-1. Listing of ABLATIN1 Program

```
C
C
C
C-----INDEPTH RESPONSE OF AN ABLATIVE COMPOSITE
C     EQUILIBRIUM ANALYSIS.
C     ABLATIN1 SYSTEM
C
C
C
C
      COMMON/KA/S1(6),S2(6),S3(6),S4(6),S5(6),S6(6),A11(6),
     1A22(6),A33(6),A44(6),A55(6),A66(6),AA(30,6),JCODE(6)
      COMMON/KB/AI(30),BI(30),CI(30),DI(30),EI(30),FI(30),
     1GI(30),AII(30),BII(30),CII(30),DII(30),EII(30),
     2FII(30),GII(30),TLOW(30)
      COMMON/KC/ICODE(30),Y(30),FW(30)
      COMMON/KCC/SPCIE1 (30),SPCIE2(30),TABLE(353,25)
      COMMON/KE/XTKE(100),ZOMGA(100),EK(100),SIG(100)
      COMMON/KEE/PL,RR,TZERO,EPS,KEY,NN,NQ,MM
      COMMON/KI/W,KMAX,KOUNT
      COMMON/KJ/DELTK,TVAR
      COMMON/KF/CPS,CDO,DCDO,JCHAR,TC
      COMMON/KK/IP
      COMMON/KL/WTOTAL,RHOII
      COMMON/KM/XMOL(30)
      COMMON/KNN/TFMAX
C
C
C
      DIMENSION TOK(200),CHARDN(200),Z1(200),T1(200),ZX(41),ZY(41),
     1                TP(41),P(41),WFLUX(41),TT(21),PROD(21),
     2YCOMP(30,41),PRODCP(21),PRODR(21),COND(30),CV(30),
     3VIS(30),YI(30)
C
```

```
C
      DOUBLE PRECISION ZZ,H11,ZLL,TTTT,DTCC
C
C
C
C-----DEFINE THE ARITHMETIC STATEMENT FUNCTIONS FOR THE
C     RUNGE-KUTTA ANALYSIS.
C
C
      F(A)=+GROUP*A
      G(A)=A
C
C
C
C
C     RR=GAS CONSTANT(1.98726BTU/(LB-MOLE OR)
C     TZERO=REFERENCE TEMPERATURE
C     TFMAX=MAXIMUM ALLOWABLE TEMPERATURE FOR THIS MODEL (OF)
C
      RR=1.98726
C
C
C     HSIMPI=SIMPSON'S RULE INCREMENT SIZE(FT) USED
C            IN THE SOLUTION OF THE MOMENTUM EQUATION
C
      FR2=778.16/32.2
C
C
C     NC=NO. OF GAS SPECIES
C     NNS=NO. OF LIQUID OR SOLID SPECIES
C     NS=NC+NNS(TOTAL NUMBER OF SPECIES)
C     MM=NO. OF ELEMENTS
C     KODE=1 CONDUCTIVITY OF CHAR WITH GAS IN PORES
C     KODE=2 CONDUCTIVITY OF CHAR WITH PORES EVACUATED
```

```
C       KEY=1(FROZEN),=2(EQUILIBRIUM)=3(NON-EQUILIBRIUM)
C       PL=PRESSURE AT Z=L(LB/FT2)
C       DELTK=TEMPERATURE INCREMENT
C       TO=TEMPERATURE AT Z=0
C       EPS=CHAR POROSITY
C       ZL=ABLATOR THICHKNESS(IN FEET)
C       HI=INITIAL RUNGE-KUTTA INCREMENT SIZE(FT) USED
C          IN THE SOLUTION OF THE ENERGY EQUATION.
C       ALPHA=VISCOUS COEFFICIENT IN DARCY'S EQUATION(1/FT)
C       BETA=INERTIAL COEFFICIENT IN DARCY'S EQUATION(1/FT2)
C       SIGMA=STEPHAN-BOLTZMAN CONSTANT(0.481X10-12 BTU/FT2-SEC-OF4)
C       EMIS=CHAR EMISIVITY.
C       QFLUXI=INITIAL BACK SURFACE HEAT FLUX.
C       TCHAR=BACK SURFACE TEMPERATURE OF CHAR
C
C
        FR=0.1666667
C
C
C-----READ INPUT PARAMETERS
C
C
 10     READ11,NC,NNS,MM,KODE,KEY
 11     FORMAT(6I6)
  12    FORMAT(F10.3,10X,5F10.3)
        READ 12,PL,TO,EPS,ZL,HI,TFMAX
        READ21,ALPHA,BETA,SIGMA,EMIS
        READ13,DTC,TCHAR,VR
 13     FORMAT(7E10.3)
        NN=NC
        NS=NC+NNS
        NQ=NS
        QFLUX=QFLUXI
C
```

```
C
C     S1...S6(APPLY BETWEEN 1000-6000 OK)
C     A11...A66(APPLY BETWEEN 300-1000 OK)
C     JCODE(J)=0 THE REFERENCE ELEMENT IS IN THE GAS STATE.
C     JCODE(J)=1  THE REFERENCE ELEMENT IS IN THE SOLID STATE.
C     AI...EI(HEAT CAPACITY CONSTANTS...1000-6000 OK)
C     FI,GI(NEEDED TO CALCULATE THE ENTHALPY,ENTROPY
C     AND FREE ENERGY....1000-6000 OK)
C     AII...GII(300-1000 OK)
C     AA=FORMULA NUMBER. GIVES THE ATOMS OF ELEMENT J
C        IN SPECIE I.
C
C     TLOW(I)=MINIMUM TEMPERATURE AT WHICH THE HIGH TEMPERATURE
C             FIT IS APPLICABLE.
C     FW(I)=MOLECULAR WEIGHT OF SPECIE I.
C     YI(I)=MOLE FRACTION OF SPECIE I.
C     SPCIE1 AND SPCIE2 ARE THE SPECIES IDENTIFICATION
C     ICODE(I)=0 SPECIE IS A GAS
C     ICODE(I)=1 SPECIE IS A SOLID
C
C
C
C
C-----READ EMPIRICAL CONSTANTS TO CALCULATE THE SENSIBLE
C     ENTHALPY CHANGE OF THE CONSTITUENT ELEMENTS.
C
C
      DO 9 J=1,MM
      READ 18,S1(J),S2(J),S3(J),S4(J),S5(J),S6(J),JCODE(J)
      READ 18,A11(J),A22(J),A33(J),A44(J),A55(J),A66(J)
 9    CONTINUE
      DO15I=1,NS
      READ 14,TLOW(I),FW(I),YI(I),SPCIE1(I),SPCIE2(I),ICODE(I)
 14   FORMAT(10X,3E10.3,2X,2A3,I4)
```

```
C
C
C-----READ EMPIRICAL CONSTANTS TO CALCULATE THE HEAT
C     CAPACITY OF THE SOLID PLUS TWO ADDITIONAL CONSTANTS
C     TO CALCULATE THE ENTHALPY,THE ENTROPY AND THE FREE
C     ENERGY OF THE SYSTEM
C
C
      READ13,AI(I),BI(I),CI(I),DI(I),EI(I),FI(I),GI(I)
      READ13,AII(I),BII(I),CII(I),DII(I),EII(I),FII(I),GII(I)
C
C
C-----READ IN THE FORMULA NUMBERS
C
C
 15   READ13,(AA(I,J),J=1,MM)
C
C
C
C     EK=POTENTIAL PARAMETER/BOLTZMAN CONSTANT.
C     SIG=COLLISION DIAMETER(ANGSTRONG UNITS).
C     THESE CONSTANTS ARE USED TO DETERMINE THE
C     VISCOCITY AND THERMAL CONDUCTIVITY OF THE
C     REACTING GAS MIXTURE.
C
C     NDATA=NO. OF XTKE VS. ZOMGA DATA POINTS
C     XTKE=PRODUCT OF TEMPERATURE AND 1/EK VALUE
C     ZOMGA=COLLISION INTEGRAL TABULATED VS XTKE
C
C
C
      READ16,(EK(I),SIG(I),I=1,NC)
 16   FORMAT(2F15.5)
      READ11,NDATA
```

```
      READ17,(XTKE(I),ZOMGA(I),I=1,NDATA)
 17   FORMAT(2F15.5)
 18   FORMAT(6E10.4,I3)
 21   FORMAT(3E15.5,F15.5)
C
C
C
C-----INITIALIZATION OF PARAMETERS
C
C
C
C     N=COUNTER OF RUNGE KUTTA STEPS
C
      N=1
C
C     TO=INITIAL TEMPERATURE OF BACK SURFACE(OF)
C     IT IS A SPECIFIED BOUNDARY CONDITION.
      TC=TO
C
C     TC=INSTANTANEOUS TEMPERATURE OF THE SYSTEM(OF)
C
      K1=1
C
C-----K1=GIVES THE TOTAL NUMBER OF DATA POINTS STORED.
C     SHOULD NOT EXCEED THE DIMENSION OF VARIABLES.
C
      KOUNT=1
C
C
C-----KOUNT IS A CODE. IT IS USED TO DETERMINE WHETHER
C     THE CHEMEQ SUBROUTINE SHOULD BE CALLED OR BYPASSED.
C     THE LOGIC IN THIS PROGRAM IS SUCH THAT CHEMEQ IS
C     CALLED ONLY ONCE. THIS IS POSSIBLE BECAUSE AT EQUILIBRIUM
C     THE COMPOSITION IS ONLY A FUNCTION OF TEMPERATURE AND
```

```
C     PRESSURE AND NOT A FUNCTION OF RESIDENCE TIME AS IS IN
C     THE KINETICS CASE.  WHEN KOUNT=2 CHEMEQ IS BYPASSED.
C
      ROCHAR=13.
      TZERO=298.159
      K1=0
      IND=0
      K10=0
      DELTFF=0.
C
      REAC1=0.
C     REAC1=RATE OF HEAT ABSORBED BY THE CHEMICAL REACTIONS IN
C     (BTU/FT**2-SEC)
C
C
      CPB1=0.
C     CPB1=RATE OF HEAT ABSORBED BY THE FLOWING GASES IN
C     (BTU/FT**2-SEC)
C
C
      CPB2=0.
C     CPB2=RATE OF HEAT ABSORBED BY THE SOLIDS(BTU/FT**2-SEC)
C
      DCDOV=0.
      DCDO=0.
      DELTK=0.
C
C
C-----NN5 GIVES THE NUMBER OF VARIABLES STORED IN TABLE(I,J).
C
C
      NN4=NC+5
      NN5=NN4+NNS
C
```

```
C
C
C-----THE FIRST FIVE VARIABLES ARE.....
C
C
C          1) THE TEMPERATURE(IN OK)
C          3) THE AVERAGE MOLECULAR WEIGHT
C          4) THE MASS FLUX(LBS/FT2-SEC)
C          2) THE HEAT TERM( UNITS? )
C          5) THE HEAT CAPACITY OF THE MIXTURE(CPMX)
C          6) THE REST OF THE VARIABLES ARE THE MOLE
C     FRACTIONS. FOR THE SOLIDS, THE TERM STORED
C     IS THE RATIO OF MOLES OF SOLID TO MOLE OF
C     GASES.
C
C
C     HI=INITIAL RUNGE-KUTTA STEP SIZE
      H=HI
C
C
C
C-----CALCULATE THE INITIAL AVERAGE MOLECULAR WEIGHT OF THE GAS
C
C
C
      SUMY=0.
      DO 1 I=1,NN
 1    SUMY=SUMY+YI(I)
      AVGFW=0.
      DO31I=1,NS
      XMOL(I)=YI(I)/SUMY
      Y(I)=YI(I)
      IF(ICODE(I).EQ.1)GOTO31
      AVGFW=AVGFW+Y(I)*FW(I)
```

```
 31   CONTINUE
C
C
C     W=MASS FLUX(LBS/FT**2(TOTAL)-SEC)
      W=WI
C
C
C-----THE UNITS OF MASS FLUX FOR THE PRESSURE PROFILE ARE:
C                                          (LBS/FT**2(VOIDS)-SEC)
C
C
C
      Z=0.
C     Z=DISTANCE IN FEET
C     ZL=THICKNESS OF CHAR IN INCHES
C     ZINC=INCREMENTS OF DISTANCE AT WHICH VARIABLES
C          SHOULD BE STORED.
C
C
      Z2=0.
C     Z2=VARIABLE USED TO COMPARE WHETHER THE DISTANCE
C     AT WHICH VARIABLES ARE STORED HAS BEEN REACHED.
C
C
      TVAR=(TC+459.69)/1.8
C     TVAR=TEMPERATURE IN OK.
C
      ZZ=0.
      ZLL=ZL/12.
      PRINT 51,ZLL,H
 51   FORMAT(1X,'ZLL='D20.10,'  H='E15.7)
C
C
C
```

```
C-----INDEPTH RESPONSE OF ABLATIVE COMPOSITES.
C     FOR BACK SURFACE TEMPERATURE AND HEAT
C     FLUX SPECIFIED. THE EQUATION OF ENERGY
C     IS A SECOND ORDER, NON-LINEAR, ORDINARY DIFFERENTIAL
C     EQUATION WITH VARIABLE COEFFICIENTS.
C     THE NUMERICAL TECHNIQUE USED IS A 4TH ORDER
C     VARIABLE STEP RUNGE-KUTTA ANALYSIS.
C
C
C
C
C     TCHAR=TEMPERATURE AT WHICH ALL OF THE VIRGIN
C     MATERIAL HAS DECOMPOSED.
C
      ZINC=1.2E-5
      ZINC=2.2E-4
      DELZ=H
      H11=H
      IF(TVAR.GT.TCHAR)GOTO32
C
C
      CALL INDPTH(TC,CDOV,DCDOV,GASCP,Q,CPV,RHO,TVAR,
     1DELTK,N,DELZ,VR,W,H)
C
C
C
C     CDOV=THERMAL CONDUCTIVITY OF VIRGIN MATERIAL(
C     BTU/(FT-SEC-OF)
C     DCDOV=THE DERIVATIVE OF CDOV WITH TEMPERATURE(BTU/(FT-2EC))
C     GASCP=HEAT CAPACITY OF MIXTURE(BTU/LB-OF)
C     Q=HEAT ABSORBED BY DEPOLYMERIZATION OF THE
C     VIRGIN PLASTIC COMPOSITE(BTU/FT3-SEC)
C     CPV=HEAT CAPACITY OF VIRGIN COMPOSITE(BTU/LB-OF)
C     RHO=DENSITY OF VIRGIN COMPOSITE
```

```
C     DELTK=TEMPERATURE DIFFERENCE IN OK FOR A DISTANCE H.
C     N=NUMBER OF INTEGRATION STEPS
C     DELZ=INCREMENT OF DISTANCE(FT)
C     VR=SURFACE RECESSION VELOCITY(FT/SEC)
C     W=MASS FLUX(LBS/FT2-SEC)
C     H=RUNGE-KUTTA INTEGRATION STEP SIZE(FT)
C
C
      WI=W
C
      QCZI=CDOV*DTC
      DTCII=DTC
      PRINT 1390,QCZI
 1390 FORMAT(1X,'QCZ='F15.5)
C
C
C-----CALCULATE THE HEAT CAPACITY OF THE PYROLYSIS GASES
C
C
      CALL CPMIX(TVAR,NN,CPMX)
      GASCP=CPMX/AVGFW
      GOTO113
C
C
 32   CALL CHARPR
C
C
C
C
C-----THIS SUBROUTINE CALCULATES THE THERMO-PHYSICAL
C     PROPERTIES OF THE CHAR
C
C
      DELZ=H
```

```
      Z1(1)=0.
      T1(1)=TO
      ZLL=0.0208333
      GOTO103
 101  TVAR=(TC+459.69)/1.8
      IF(TVAR.GT.TCHAR)GOTO102
      CALL INDPTH(TC,CDOV,DCDOV,GASCP,Q,CPV,RHO,TVAR,DELTK,
     1N,DELZ,VR,W,H)
C
C
C-----FOR EXPLANATION OF THE VARIABLES IN THE ARGUMENT SEE
C     PREVIOUS CALL INDPTH STATEMENT.
C
C
C
C
C-----CALCULATE THE HEAT CAPACITY OF THE PYROLYSIS GASES
C
C
      CALL CPMIX(TVAR,NN,CPMX)
      GASCP=CPMX/AVGFW
      H11=H
      WI=W
      ZLL=ZZ+0.0208333
      PRINT 139,TC,TVAR,DTC,GASCP,DCDOV,CPV,Q,CDOV,ZZ
 139  FORMAT(1X,'T='F9.4,' TK='F9.4,' DT='E11.4,' CP='F6.3,' DKE='E11.4,
     1' CPP='E11.4,' Q='E11.4,' KE='E11.4,D15.7)
      PRINT 1390,QCZI
      QCZI=CDOV*DTC
      GOTO113
C
C
C-----USE SUBROUTINE CHARPR TO GENERATE NEEDED PHYSICAL PROPERTY
C     DATA FOR THE CHAR ZONE(HEAT CAPACITY OF THE CHAR AND THE
```

```
C     OVER ALL EFFECTIVE THERMAL CONDUCTIVITY OF THE GAS AND CHAR).
C
C
 102  CALL CHARPR
      IF(IND.EQ.0)DTC=QCZI/CDO
      IND=1
 103  IF(KEY.EQ.2)GOTO104
C
C
C-----CALCULATE THE HEAT CAPACITY OF A FROZEN FLOW MIXTURE
C
C
      CALL CPMIX(TVAR,NN,CPMX)
      GASCP=CPMX/AVGFW
C
      GOTO111
 104  IF(KOUNT.EQ.2)GOTO105
      CALL CHEMEQ
      GO TO 300
C
C-----CHEMEQ SUBROUTINE CALCULATES THE EQUILIBRIUM COMPOSITION
C     OF THE REACTING GASES. IT ALSO CALCULATES THE HEAT ABSORBED
C     OR RELEASE DUE TO THE CHEMICAL REACTION. IN ADDITION IT
C     FURNISHES THE NEEDED AVERAGE MOLECULAR WEIGHT AND HEAT
C     CAPACITY OF THE MIXTURE.
C
 105  DO110KL=2,5
      CALL OMEGA(TVAR,TABLE(1,1),TABLE(1,KL),KMAX,VARY)
C     OMEGA IS AN INTERPOLATION ROUTINE. SEE BEGINNING
C     OF PROGRAM FOR EXPLANATION OF VARIABLES STORED IN TABLE(I,J)
      II=KL-1
      GOTO(106,107,108,109),II
 106  REACT=VARY
C     REACT=HEAT EFFECT DUE TO CHEMICAL REACTIONS. THIS
```

```
C       VARIABLE IS USE IN GROUP TERM BELOW. THE
C       UNITS OF REACT ARE(BTU/FT2-SEC-OF)
        GOTO110
 107    AVGFW=VARY
C       AVGFW=AVERAGE MOLECULAR WEIGHT OF THE GAS MIXTURE.
        GOTO110
 108    W=VARY*EPS
C       W=MASS FLUX(LBS/FT**2-TOTAL-SEC)
        GOTO110
 109    CPMX=VARY
C       CPMX=HEAT CAPACITY OF THE MIXTURE(BTU/LB-MOLE-OF)
        GASCP=CPMX/AVGFW
C       GASCP=HEAT CAPACITY(BTU/LB-OF)
 110    CONTINUE
        REAC1=REAC1+REACT*DELTFF
        CPB1=CPB1+W*EPS*GASCP*DELTFF
        CPB2=CPB2+CPS*RHO*VR*(1.-EPS)*DELTFF
        IF(KEY.GT.1)GOTO112
 111    ROCHAR=(WTOTAL-W)/VR
        CONVEG=W*GASCP
        CPB1=CPB1+CONVEG*DELTFF
        CONVES=CPS*ROCHAR*VR
        CPB2=CPB2+CONVES*DELTFF
        GROUP=(CONVEG+CONVES-DCDO*DTC)/CDO
C
C       DCDO=DERIVATIVE OF CDO WITH TEMPERATURE(BTU/FT-SEC-OF2)
C       CDO=EFFECTIVE THERMAL CONDUCTIVITY(BTU/FT-SEC-OF)
C       DTC=GRADIENT OF TEMPERATURE WITH DISTANCE(OF/FT)
C-----THE ABOVE GROUP TERM IS FOR FROZEN CONDITION
C
        GOTO114
C
C
C-----CALCULATE THE BULK DENSITY OF THE CHAR
```

```
C
C
 112  ROCHAR=(WTOTAL-W)/VR
C     ROCHAR=BULK DENSITY OF THE CHAR(LBS/FT**3)
      CONVEG=W*GASCP
      CPB1=CPB1+CONVEG*DELTFF
      CONVES=CPS*ROCHAR*VR
      CPB2=CPB2+CONVES*DELTFF
      REAC1=REAC1+REACT*DELTFF
      GROUP=(CONVEG+CONVES+REACT-DCDO*DTC)/CDO
C
C     VR=SURFACE RECESSION VELOCITY(FT/SEC)
C     THE ABOVE GROUP TERM HOLDS FOR EQUILIBRIUM IN THE CHAR
      GOTO114
 113  GROUP=(W*GASCP+CPV*RHO*VR+Q/DTC-DCDOV*DTC)/CDOV
C
C-----THE ABOVE GROUP TERM IS USED DURING THE DEPOLYMERIZATION OF
C     THE VIRGIN PLASTIC COMPOSITE.
C
 114  A=DTC
      DELG1=H*G(A)
      DELF1=H*F(A)
      DELG2=H*G(A+DELF1/2.)
      DELF2=H*F(A+DELF1/2.)
      DELG3=H*G(A+DELF2/2.)
      DELF3=H*F(A+DELF2/2.)
      DELG4=H*G(A+DELF3)
      DELF4=H*F(A+DELF3)
      DTC=DTC+(DELF1+2.*(DELF2+DELF3)+DELF4)/6.
      IF(IND.EQ.0)GOTO115
      QCZ=CDO*DTC
 115  TPREV=TC
      IF(H.LT.0.8E-8)GOTO117
      TC=TC+(DELG1+2.*(DELG2+DELG3)+DELG4)/6.
```

```
      GOTO118
 117  IF(K10.EQ.0)TTTT=TC
      K10=1
      DTCC=DTC
      TTTT=TTTT+H11*DTCC
      TC=TTTT
 118  DELTFF=TC-TPREV
      DELTK=DELTFF/1.8
C
C-----COMPARE THE TEMPERATURE CALCUALTED WITH THE MAXIMUM VALUE.
C
C
 138  ZPREV=ZZ
      ZZ=ZZ+H11
      IF(TC.GT.1000.)H=2.E-5
      IF(KEY.EQ.1)GOTO141
      IF(TC.GT.1500.)H=2.E-6
        IF(TC.GT.3000.)H=1.E-6
      IF(TC.GT.3500.)H=0.5E-6
      H11=H
      Z=ZZ
 141  IF(TC.GT.TFMAX)GOTO150
      N=N+1
      IF(TVAR.LE.TCHAR)Z2=ZZ
      IF(TVAR.LE.TCHAR)GOTO101
      IF(Z2.GT.ZZ)GOTO101
  140 PRINT 142,TC,H,DTC,GASCP,DCDO,GROUP,REACT,CDO
  142 FORMAT(1X,'TF='F9.4,' H='E14.6,  ' DT='E11.5,' CP='F6.4,' DKE='E11
     1.5,' GRP='E12.5,' Q='E11.4,' KE='E11.5)
      PRINT 1140,AVGFW,W,CPMX,TVAR,KMAX,CPS,GASCP,RHO,QCZ
 1140 FORMAT(1X,'AVGFW='F 7.3,' W='F 7.5,' CPMX='E9.2,' TVAR='F7.2,
     1' KMAX='I5,' CPS='F 6.3,' GASCP='F 6.4,' RHO='F8.4,' QCZ='F10.2)
      IF(TC.GT.2600.)ZINC=1.2E-5
      Z2=Z2+ZINC
```

```
      Z1(K1)=ZPREV
      T1(K1)=TPREV
      CHARDN(K1)=ROCHAR
      TOK(K1)=TVAR
C
C
C-----STORE THE TEMPERATURE PROFILE FOR LATER USE IN THE SOLUTION
C     OF THE MOMENTUM EQUATION.
C
C
      PRINT 153,REAC1,CPB1,CPB2,ZPREV,K1
  153 FORMAT(1X,'REAC1='E15.7,' CPB1='E15.7,' CPB2='E15.7,
     1' ZPREV='E15.7,I5/)
      K1=K1+1
      IF(K1.GT.199)K1=199
      GOTO101
  150 TL=TC
C     TL=FINAL TEMPERATURE
      PRINT 1140,AVGFW,W,CPMX,TVAR,KMAX,CPS,GASCP,RHO,QCZ
      PRINT 142,TC,H,DTC,GASCP,DCDO,GROUP,REACT,CDO
      PRINT 153,REAC1,CPB1,CPB2,ZPREV,K1
      T1(K1)=TL
C     THE TEMPERATURE PROFILE HAS BEEN DEFINED
      DELTT=TL-T1(1)
C     DELTT=TEMPERATURE DROP ACROSS THE CHAR(OF)
      Z1(K1)=ZZ
      CHARDN(K1)=ROCHAR
      TOK(K1)=(TC+459.69)/1.8
      PRINT 154
  154 FORMAT(1H1, 7X,'T(OF)', 9X,'T(OK)', 11X,'Z')
      DO 156 I=1,K1
      PRINT 155,T1(I),TOK(I),Z1(I)
  155 FORMAT(1X,4E15.7)
  156 CONTINUE
```

```
      DISTAN=Z1(K1)-Z1(1)
C     DISTAN IS THE THICKNESS OF THE CHAR.
C
C-----CALCULATION OF THE PRESSURE PROFILE IN THE
C     CHAR USING SIMPSON'S RULE FOR THE INTEGRATION
C     OF THE MOMENTUM EQUATION FOLLOWS.
C
      JS=39
C     JS=NUMBER OF SLICES IN THE CHAR
      HS=DISTAN/FLOAT(JS)
C     HS=INCREMENT OF GRID(IN FEET)
C-----INITIALIZE
      SIMP1=0.
      SIMP2=0.
      ITEMP=K1
C     ITEMP=TOTAL NUMBER OF TEMPERATURE POINTS STORED
      LS=JS+1
      WFLUX(1)=WI
      ZX(LS)=Z1(K1)
      TP(LS)=TL
      P(LS)=PL
C
C-----THE INTEGRATION OF THE MOMENTUM EQUATION IS PERFORMED
C     FROM THE FRONT SURFACE OF THE CHAR TO THE BACK SURFACE
C     THE INTEGRATION OF THE ENERGY EQUATION, ON THE OTHER
C     HAND, WAS PERFORMED FROM THE VIRGIN MATERIAL TO THE FRONT
C     SURFACE OF THE CHAR. BECAUSE THE DIRECTION OF INTEGRATION
C     OF BOTH EQUATIONS ARE DIFFERENT IT IS NECESSARY TO RE-
C     DEFINE Z=0. AT THE FRONT SURFACE OF THE CHAR.
C
      ACON1=2.6693E-3
      ACON5=2.42/3600.
      ACON7=778.16/32.2
      MS=20
```

```
      HSIMPI=HS/FLOAT(MS)
      MP=MS+1
      DO260N=1,JS
      NBAR=N-1
      HN=NBAR
      LO=LS-NBAR
      ZX(LO)=ZX(LS)-HN*HS
      ZY(MP)=ZX(LO)
C     DEFINE MP AS THE TOTAL NO. OF POINT OVER WHICH SIMPSONS'S
C     RULE IS TO BE APPLIED
      DO241M=1,MP
      MBAR=M-1
      HM=MBAR
      MO=MP-MBAR
      ZY(MO)=ZY(MP)-HM*HSIMPI
      ZVAR=ZY(MO)
      IF(ZVAR.LT.Z1(1))ZVAR=Z1(1)
C
C-----FOR A SPECIFIED CHAR DISTANCE OBTAIN THE
C     CORRESPONDING TEMPERATURE FROM THE TEMPE-
C     RATURE PROFILE
C
      CALL OMEGA(ZVAR,Z1,T1,ITEMP,TVIS)
C     TVIS IS THE INTERPOLATED TEMPERATURE IN OF
C     WHICH CORRESPONDS TO THE VALUE OF ZVAR
      TK=(459.69+TVIS)/1.8
C     TK=TEMPERATURE IN KELVIN
      DO205I=1,NC
      TKE=TK/EK(I)
C
C
C-----FOR THE VALUE OF INTERPOLATED TEMPERATURE FIND
C     THE CORRESPONDING COLLISION INTEGRAL TO CALCULATE
C     THE PURE GAS VISCOCITY USING THE METHOD OF WILKE-JOHNSON
```

```
C
      CALL OMEGA(TKE,XTKE,ZOMGA,NDATA,OMGA)
C
C     OMGA=COLLISION INTEGRAL
C
 205  VIS(I)=2.6693E-3*SQRT(FW(I)*TK)/(SIG(I)**2*OMGA)
      IF(NC.EQ.1)GOTO237
      IF(KEY.GT.1)GOTO206
      VMIX=0.
      WFLUX(LO)=WI
      GO TO 222
 206  TVAR=TK
      DO218KL=3,NN5
C
C     THE FIFTH VARIABLE STORED IN TABLE IS CPMX.  THIS
C     VARIABLE IS NOT USED IN THE SOLUTION OF THE MOMENTUM
C     EQUATION. SO ITS INTERPOLATION IS BYPASSED.
C
      IF(KL.EQ.5)GOTO218
C
C     INTERPOLATE FOR THE DATA GENERATED IN CHEMEQ
C
      CALL OMEGA(TVAR,TABLE(1,1),TABLE(1,KL),KMAX,VARY1)
      IF(KL.GT.5)GOTO216
C
C     KMAX=NUMBER OF DATA POINTS STORED
C
      IF(KL.EQ.4)GOTO215
      AVGFW=VARY1
      GOTO218
 215  W=VARY1
      GOTO217
 216  Y(KL-5)=VARY1
      IF(VARY1.GT.0.)GOTO217
```

```
      Y(KL-5)=1.E-10
217   IF(M.GT.1)GOTO218
      TP(LO)=TVIS
      WFLUX(LO)=W
      KYCOMP=KL-5
      YCOMP(KYCOMP,LO)=Y(KYCOMP)
218   CONTINUE
      VMIX=0.
      GOTO224
222   IF(M.GT.1)GOTO224
      DO 223 I=1,NS
      YCOMP(I,LO)=XMOL(I)
      WFLUX(LO)=W
223   TP(LO)=TVIS
224   DO 236 J=1,NC
      TERM=1.
      DO230L=1,NC
      IF(L.EQ.J)GOTO230
      TOPV=(1.+SQRT(VIS(J)/VIS(L))*SQRT(SQRT(FW(L)/FW(J))))**2
      BOTV=  SQRT(2.)*SQRT(1.+FW(J)/FW(L))*2.
      PHIV=TOPV/BOTV
      TERM=TERM+PHIV*(Y(L)/Y(J))
230   CONTINUE
      VMIX=VMIX+VIS(J)/TERM
236   CONTINUE
      GOTO238
237   VISCOS=VIS(I)*ACON5
C     ACON5=2.42/3600.
      GOTO239
238   VISCOS=VMIX*ACON5
239   PROD(MO)=TVIS*VISCOS*W/AVGFW
      TT(MO)=TVIS/AVGFW*(W**2)
241   CONTINUE
      ZX(LO-1)=ZX(LO)-HS
```

```
C     INTEGRATE USING SIMPSONS RULE
      SUM1=0.
      SUM2=0.
      SUM3=0.
      SUM4=0.
      MODD=MP-2
      DO255KP=3,MODD,2
      SUM1=SUM1+2.*PROD(KP)
 255  SUM3=SUM3+2.*TT(KP)
      MEVEN=MP-1
      DO256KP=2,MEVEN,2
      SUM2=SUM2+4.*PROD(KP)
 256  SUM4=SUM4+4.*TT(KP)
      SIMP1=(HSIMPI/3.0)*(PROD(1)+SUM1+SUM2+PROD(MP))+SIMP1
      SIMP2=(HSIMPI/3.0)*(TT(1)+SUM3+SUM4+TT(MP))+SIMP2
C     FR2=778.16/32.2
      P(LO-1)=SQRT(PL**2+(2.*RR)*FR2*(ALPHA*SIMP1+BETA*SIMP2))
 260  CONTINUE
C
C
C-----CALCULATE THE SURFACE HEAT FLUX,QL,THE RERADIATION,QR,
C     AND THE TOTAL AERODYNAMIC HEATING,QA.
C
C
      IF(KEY.GT.1)GOTO261
      QL=QCZ
      GOTO262
 261  QL=QCZ
 262  QR=EMIS*SIGMA*(TL+459.69)**4
      QA=QL+QR
C
      TP(1)=T1(1)
C     PRINT INPUT PARAMETERS
C
```

```
2603 PRINT 597
597  FORMAT(1H1////////)
     IF(KEY.EQ.2)GOTO5982
     PRINT 5981
5981 FORMAT(35X,'INDEPTH FLOW ANALYSIS(FROZEN FLOW)'//)
5982 PRINT 5984
5984 FORMAT(35X,'INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)'//)
5986 PRINT 5990
5990 FORMAT(12X,51H                                          THEORETICAL/
    1/)
     PRINT600,T1(1),NC
600  FORMAT(18X,'CHAR BACK TEMPERATURE (OF)='F7.1,13X,'NUMBER OF GAS CO
    1MPONENTS='I3/)
     PRINT 601,DTCII,RHOII
601  FORMAT(18X,'INITIAL SLOPE(OF/FT)='F8.1,12X,'INITIAL DENSITY OF COM
    1POSITE(LBS/FT**3)='F6.2/)
     THICK=DISTAN*12.
     THICK1=Z1(1)*12.
     PRINT 602,THICK,THICK1
602  FORMAT(18X,'THICKNESS OF CHAR(INCHES)='F8.6,6X,'THICKNESS OF DECOM
    1POSITION ZONE='F8.6/)
     QCZZ=QCZ-QCZI
     PRINT 604,WTOTAL,WFLUX(LS)
604  FORMAT(18X,'TOTAL MASS FLUX(LBS/FT2-SEC)='F7.6,6X,29HGAS MASS FLUX
    1 AT THE SURFACE=,1X,F7.6/)
     PRINT 611,TFMAX,VR
611  FORMAT(18X,'FRONT SURFACE TEMPERATURE(OF)='F6.1,5X,'SURFACE RECESS
    1ION VELOCITY(FT/SEC)='F7.5/)
     PRINT 603,QCZZ,QCZI
603  FORMAT(25X,'RATE OF HEAT ABSORBED IN THE CHAR ZONE(BTU/FT**2-SEC)=
    1'F9.3,//25X,'RATE OF HEAT ABSORBED IN THE DECOMPOSITION ZONE(BTU/F
    1T2-SEC=)'F9.3/)
     HCHAR=QCZZ/QCZ*100.
     HDECOM=QCZI/QCZ*100.
```

```
      SUM=REAC1+CPB1+CPB2
      HGAS=CPB1/SUM*100.
      HSOLID=CPB2/SUM*100.
      HREACT=REAC1/SUM*100.
      PRINT 605,HCHAR
 605  FORMAT(25X,'PERCENT OF TOTAL HEAT ABSORBED IN THE CHAR ZONE='E15.7
     1/)
      PRINT 606,HDECOM
 606  FORMAT(25X,'PERCENT OF TOTAL HEAT ABSORBED IN DECOMP-ZONE='E15.7/)
      PRINT 607,HGAS
 607  FORMAT(25X,'PERCENT OF HEAT ABSORBED BY THE GAS IN THE CHAR ZONE='
     1E15.7/)
      PRINT 608,HSOLID
 608  FORMAT(25X,'PERCENT OF HEAT ABSORBED BY THE SOLIDS IN THE CHAR ZON
     1E='E15.7/)
      PRINT 610,HREACT
 610  FORMAT(25X,'PERCENT OF HEAT ABSORBED BY REACTION IN THE CHAR ZONE=
     1'E15.7/)
      PRINT586
 586  FORMAT(1H1)
C
C--------PRINT OUTPUT PARAMETERS CORRESPONDING TO JS, GRID SIZE
C
      IKE=1
      MIKE=5
      LIKE=1
 2602 PRINT 597
 2662 PRINT 5984
      IF(LIKE.GT.1)GO TO 265
      PRINT2650,DELTT
 2650 FORMAT(35X,23HTEMPERATURE DROP (OF) =,1X,F20.1/)
      DELP=(P(1)-PL)
      PRINT2651,DELP
 2651 FORMAT(35X,24HPRESSURE DROP (LB/FT2) =,1X,F19.1/)
```

```
      PRINT2652,QL
 2652 FORMAT(35X,33HSURFACE HEAT FLUX (BTU/FT2-SEC) =,1X,F10.2/)
      PRINT2653,QR
 2653 FORMAT(35X,32HRADIANT HEAT FLUX BTU/FT2-SEC)=,1X,F11.2/)
      PRINT2654,QA
 2654 FORMAT(35X,35HAERODYNAMIC HEAT FLUX(BTU/FT2-SEC)=,1X,F8.2//)
 265  PRINT2720,(ZX(KK),KK=IKE,MIKE)
 2720 FORMAT(14X,15HCHAR DEPTH (FT),6X,5F13.4)
      PRINT2721,(TP(KK),KK=IKE,MIKE)
 2721 FORMAT(14X,16HTEMPERATURE (OF),5X,5F13.1)
      PRINT2730,(P(KK),KK=IKE,MIKE)
 2730 FORMAT(14X,17HPRESSURE (LB/FT2),4X,5F13.1)
      PRINT2723,(WFLUX(KK),KK=IKE,MIKE)
 2723 FORMAT(14X,21HMASS FLUX(LB/FT2-SEC),5F13.4/)
      PRINT2724
 2724 FORMAT(14X,66H  GAS COMPONENT                          COMPOSITION (
     1MOLE/MOLE GAS)/)
      IF(KEY.GT.1)GOTO2727
      DO 2728 KICK=1,LS
      DO2728LL=1,NS
      YCOMP(LL,KICK)=YI(LL)
 2728 CONTINUE
 2727 DO2729LL=1,NS
      YCOMP(LL,1)=YI(LL)
      PRINT 2725,LL,SPCIE1(LL),SPCIE2(LL),(YCOMP(LL,KK),KK=IKE,MIKE)
 2725 FORMAT(12X,I2,2X,2A3,11X,5E13.4)
 2729 CONTINUE
      IF(MIKE.GE.LS)GO TO 2800
      LIKE=LIKE+1
      MIKE=MIKE+5
      IKE=IKE+5
      GO TO 2602
 2800 PRINT586
  300 STOP
```

END

851

```
      SUBROUTINE INDPTH(TC,CDOV,DCDOV,GASCP,Q,CPV,RHO,TVAR,
     1 DELTKK,N,DELZ,VR,W,H)
C
C
C
      DIMENSION DRHODT(5)
C
C-----INDPTH SUBROUTINE CALCULATES THE PHYSICAL PROPER-
C     TIES FOR THE VIRGIN MATERIAL AND PYROLYSIS GASES.
C
C     T=TEMPERATURE IN FARENHEIT.
      IF(N.GT.1)GOTO2
      DCDOV=.338983E-8
      READ 1,A,B,C,D,E
C     A THROUGH E ARE CONSTANT FOR THE HEAT CAPACITY OF THE
C     VIRGIN MATERIAL.
    1 FORMAT(5E12.6)
C     CDOV=THERMAL CONDUCTIVITY OF THE VIRGIN MATERIAL
C          (BTU/(FT-SEC-OF))
    2 CDOV=1.266102E-5+.338983E-8*TC
      PRINT 10,H,DELZ
 10   FORMAT(1X,'IN INDPTH      H='E15.7,' DELZ='E15.7)
C     DCDOV=RATE OF CHANGE OF CDOV WITH THEMPERATURE.
      T=TC
      IF(T.GT.750.)GOTO3
      T2=TC*T
      T3=TC*T2
      T4=TC*T3
C
C     CPV=HEAT CAPACITY OF THE VIRGIN MATERIAL(BTU/LB-OF)
      CPV=A+B*T+C*T2+D*T3+E*T4
    3 GASCP=0.62
C
      CALL PHMCR(TVAR,DELTKK,QPHNLC,QMICRO,N)
```

```
C
      IF(TVAR.GE.789.)GOTO200
C
      CALL NYLON(TVAR,DELTKK,QNYLON)
        GOTO210
  200 QNYLON=0.
C
  210 CALL DNSITY(RHO,TVAR,DELZ,VR,N,DRHODT,W,H)
      Q=(QNYLON*DRHODT(1)+QPHNLC*DRHODT(2)+QMICRO*DRHODT(3))*(-1.8)
      RETURN
      END
```

```
      SUBROUTINE PHMCR(T,DELT,QPHNLC,QMICRO,K6)                         PHMC   1
C                                                                       PHMC   2
C                                                                       PHMC   3
      DIMENSION A(4),B(4),C(4),D(4),E(4),A1(4),B1(4),C1(4),D1(4),E1(4)  PHMC   4
C                                                                       PHMC   5
C                                                                       PHMC   6
C-----THIS SUBROUTINE COMPUTES THE HEAT OF PYROLYSIS OF PHENOLIC,       PHMC   7
C                                                                       PHMC   8
C                                                                       PHMC   9
C     BASED ON THE DATA OF SYKES AND NELSON(THERMOANALYSIS OF           PHMC  10
C     ABLATION MATERIALS)                                               PHMC  11
      IF(K6.GT.1)GOTO4                                                  PHMC  12
      NUMBER=4                                                          PHMC  13
      AREA=1350.                                                        PHMC  14
      AREA1=1464.                                                       PHMC  15
C     READ1,NUMBER,AREA,AREA1                                           PHMC  16
    1 FORMAT(I6,2E10.8)                                                 PHMC  17
      DO2I=1,NUMBER                                                     PHMC  18
      READ3,A(I),B(I),C(I),D(I),E(I)                                    PHMC  19
    2 READ3,A1(I),B1(I),C1(I),D1(I),E1(I)                               PHMC  20
    3 FORMAT(5E12.8)                                                    PHMC  21
    4 IF(T.LT.623.)GOTO5                                                PHMC  22
      IF(T.GT.1073.)GOTO5                                               PHMC  23
      I=1                                                               PHMC  24
      IF(T.GT.748..AND.T.LT.798.)I=2                                    PHMC  25
      IF(T.GT.798..AND.T.LT.898.)I=3                                    PHMC  26
      IF(T.GT.898.)I=4                                                  PHMC  27
      DT=(T-623.)                                                       PHMC  28
      DT2=DT*DT                                                         PHMC  29
      DT3=DT2*DT                                                        PHMC  30
      DT4=DT3*DT                                                        PHMC  31
C     CALCULATE THE HEAT OF PYROLYSIS OF PHENOLIC(QPHNOL)               PHMC  32
      H=A(I)+B(I)*DT+C(I)*DT2+D(I)*DT3+E(I)*DT4                         PHMC  33
      QPHNLC=H*DELT*69.312/AREA                                         PHMC  34
```

```
C                                                                       PHMC  35
C     69.312=TOTAL HEAT ABSORBED BY THE DECOMPOSITION OF                PHMC  36
C     PHENOLIC IN CAL/GRAM.                                             PHMC  37
C                                                                       PHMC  38
C     CALCULATE THE HEAT OF PYROLYSIS OF PHENOLIC MICRO-                PHMC  39
C     BALLOONS(QMICRO)                                                  PHMC  40
      I=1                                                               PHMC  41
      IF(T.GT.713..AND.T.LT.798.)I=2                                    PHMC  42
      IF(T.GT.798..AND.T.LT.913.)I=3                                    PHMC  43
      IF(T.GT.913.)I=4                                                  PHMC  44
      H=A1(I)+B1(I)*DT+C1(I)*DT2+D1(I)*DT3+E1(I)*DT4                    PHMC  45
      QMICRO=H*DELT*90.822/AREA1                                        PHMC  46
C     90.822=TOTAL HEAT ABSORBED BY THE DECOMPOSITION OF                PHMC  47
C     PHENOLIC MICRO-BALLOONS IN CAL/GRAM.                              PHMC  48
      RETURN                                                            PHMC  49
    5 QPHNLC=0.                                                         PHMC  50
      QMICRO=0.                                                         PHMC  51
  6   RETURN                                                            PHMC  52
      END                                                               PHMC  53
```

```
      SUBROUTINE NYLON(T,DELT,QNYLON)                                   NYLO   1
C                                                                       NYLO   2
C                                                                       NYLO   3
C-----THIS SUBROUTINE COMPUTES THE HEAT OF PYROLYSIS OF NYLON           NYLO   4
C     BASED ON THE DATA OF SYKES AND NELSON(THERMOANALYSIS OF           NYLO   5
C     ABLATION MATERIALS)                                               NYLO   6
C                                                                       NYLO   7
C     SLOPE=SLOPE OF LINE OBTAIN FROM SYKES AND NELSON'S DATA.          NYLO   8
      QNYLON=0.                                                         NYLO   9
      SLOPE=0.6086957                                                   NYLO  10
C                                                                       NYLO  11
      AREA=1122.                                                        NYLO  12
C     AREA=AREA UNDER CURVE OF FIGURE-2(DIFFERENTIAL THERMAL            NYLO  13
C     ANALYSIS) BY SYKES AND NELSON                                     NYLO  14
      CONST=150.5738/AREA                                               NYLO  15
      IF(T.LT.647.)GOTO4                                                NYLO  16
      IF(T.GT.699.)GOTO2                                                NYLO  17
      IF(T.GE.689..AND.T.LE.699.)GOTO1                                  NYLO  18
      H=SLOPE*(T-647.)                                                  NYLO  19
      GOTO3                                                             NYLO  20
 1    H=24.4                                                            NYLO  21
      GOTO3                                                             NYLO  22
 2    DH=SLOPE*(T-693.)                                                 NYLO  23
      H=28.0-DH                                                         NYLO  24
      IF(T.GE.739.)H=0.                                                 NYLO  25
 3    QNYLON=DELT*H*CONST                                               NYLO  26
 4    RETURN                                                            NYLO  27
      END                                                               NYLO  28
```

```
      SUBROUTINE OMEGA (VAR,X,F,IMAX,SOM)                               OMEG   1
C                                                                       OMEG   2
C                                                                       OMEG   3
C                                                                       OMEG   4
C-----THIS PROGRAM PERFORMS LAGRANGIAN INTERPOLATION                    OMEG   5
C     WITH NON-EQUAL STEP SIZE BETWEEN POINTS                           OMEG   6
C     F=DEPENDANT VARIABLE                                              OMEG   7
C     X=INDEPENDENT VARIABLE                                            OMEG   8
C     VAR-VALUE OF X FOR WHICH CORRESPONDING VALUE OF                   OMEG   9
C     F IS DESIRED BY INTERPOLATION                                     OMEG  10
C     IMAX=NUMBER OF POINTS IN ARRAY X OR F                             OMEG  11
C     SOM=VALUE OF INTERPOLATED DEPENDENT VARIABLE                      OMEG  12
C     NPTS=NUMBER OF POINTS USED FOR INTERPOLATION                      OMEG  13
C                                                                       OMEG  14
      DIMENSION X(  1),F(  1),XN(350),FN(350)                           OMEG  15
      COMMON/KK/IP                                                      OMEG  16
      NPTS=3                                                            OMEG  17
 607  XUP=1.E30                                                         OMEG  18
      DO611I=1,IMAX                                                     OMEG  19
      T=VAR-X(I)                                                        OMEG  20
      IF(T.GE.0.)GOTO609                                                OMEG  21
 608  T=-T                                                              OMEG  22
 609  IF(T.GE.XUP)GOTO611                                               OMEG  23
 610  IP=I                                                              OMEG  24
      XUP=T                                                             OMEG  25
 611  CONTINUE                                                          OMEG  26
      IN=1                                                              OMEG  27
      NPP=NPTS+1                                                        OMEG  28
      DO618I=1,NPP                                                      OMEG  29
      FN(I)=F(IP)                                                       OMEG  30
      XN(I)=X(IP)                                                       OMEG  31
      IF(IN.GT.0)GOTO613                                                OMEG  32
 612  IQ=IP-I                                                           OMEG  33
      GOTO615                                                           OMEG  34
```

```
613   IQ=IP+I                                                    OMEG  35
      IF(IMAX.GE.IQ)GOTO615                                      OMEG  36
614   IP=IP-1                                                    OMEG  37
      GOTO618                                                    OMEG  38
615   IF(IQ.GT.0)GOTO617                                         OMEG  39
616   IP=IP+1                                                    OMEG  40
      GOTO618                                                    OMEG  41
617   IP=IQ                                                      OMEG  42
      IN=-IN                                                     OMEG  43
618   CONTINUE                                                   OMEG  44
      SOM=0.                                                     OMEG  45
      FACT=1.                                                    OMEG  46
      DO620J=1,NPTS                                              OMEG  47
      SOM=SOM+FACT*FN(1)                                         OMEG  48
      DO619I=J,NPTS                                              OMEG  49
      IQ=I-J+1                                                   OMEG  50
619   FN(IQ)=(FN(IQ+1)-FN(IQ))/(XN(I+1)-XN(IQ))                  OMEG  51
620   FACT=FACT*(VAR-XN(J))                                      OMEG  52
      RETURN                                                     OMEG  53
      END                                                        OMEG  54
```

```
      SUBROUTINE THERM1                                                 THER   1
C     THIS SUBPROGRAM CALCULATES THE HEAT OF FORMATION AND              THER   2
C     THE ENTROPY OF EACH CHEMICAL SPECIE                               THER   3
      COMMON/KA/S1(6),S2(6),S3(6),S4(6),S5(6),S6(6),A11(6),             THER   4
     1A22(6),A33(6),A44(6),A55(6),A66(6),AA(30,6),JCODE(6)              THER   5
      COMMON/KB/AI(30),BI(30),CI(30),DI(30),EI(30),FI(30),GI(30),       THER   6
     2AII(30),BII(30),CII(30),DII(30),EII(30),FII(30),GII(30),          THER   7
     3TLOW(30)                                                          THER   8
      COMMON/KC/ICODE(30),Y(30),XMW(30)                                 THER   9
      COMMON/KEE/PL,RR,TZERO,EPS,KEY,NN,NQ,MM                           THER  10
      COMMON/KG/ENT(30),S(30),ENT1(30),T                                THER  11
C     S1....S6=EMPIRICAL CONSTANTS FOR THE HIGH TEMPERATURE             THER  12
C     ENTHALPY FIT OF THE CONSTITUENT ELEMENTS                          THER  13
C     A11..A66=EMPIRICAL CONSTANTS FOR THE LOW TEMPERATURE              THER  14
C     ENTHALPY FIT OF THE CONSTITUENT ELEMENTS                          THER  15
C     AI....GI=EMPIRICAL CONSTANTS FOR THE HIGH TEMPERATURE             THER  16
C     FIT OF THE CHEMICAL SPECIES                                       THER  17
C     AII..BII=EMPIRICAL CONSTANTS FOR THE LOW TEMPERATURE              THER  18
C     FIT OF THE CHEMICAL SPECIES                                       THER  19
      DIMENSION CPDT1(6)                                                THER  20
C     ENT(I)=HEAT OF FORMATION AT ANY TEMPERATURE T                     THER  21
C     ENT1(I)=SENSIBLE ENTHALPY GAIN+CHEMICAL ENERGY(HEAT               THER  22
C     OF FORMATION AT 298.16 OK)                                        THER  23
C     CPDT1(J)=SENSIBLE ENTHALPY GAIN OF THE ELEMENTS                   THER  24
C     TLOW(I)=TEMPERATURE AT WHICH ONE MUST CHANGE FROM ONE FIT         THER  25
C     TO THE OTHER OR, THE MIN TEMP OF HIGH TEMP FIT.                   THER  26
C     S=ENTROPY                                                         THER  27
C     NN=NUMBER OF GAS SPECIES                                          THER  28
C     NQ=NUMBER OF GAS+SOLID SPECIES                                    THER  29
C     MM=NUMBER OF CONSTITUENT ELEMENTS                                 THER  30
C     T=TEMPERATURE IN OK.                                              THER  31
      T1=T                                                              THER  32
      T2=T1*T                                                           THER  33
      T3=T2*T                                                           THER  34
```

```
      T4=T3*T                                                           THER  35
      T5=T4*T                                                           THER  36
      A1=T1                                                             THER  37
      A2=T2/2.                                                          THER  38
      A3=T3/3.                                                          THER  39
      A4=T4/4.                                                          THER  40
      A5=T5/5.                                                          THER  41
C     CALCULATE THE HEAT OF FORMATION,ENT,AND THE ENTROPY S.            THER  42
      DO 8 I=1,NQ                                                       THER  43
      IF(T.LT.TLOW(I))GOTO3                                             THER  44
      ENT1(I)=(AI(I)*A1+BI(I)*A2+CI(I)*A3+DI(I)*A4+EI(I)*A5             THER  45
     1+FI(I))*RR                                                        THER  46
      S(I)=(AI(I)*ALOG(T)+BI(I)*A1+CI(I)*A2+DI(I)*A3+EI(I)*A4+GI(I))*RR THER  47
      IF(I.GT.1)GOTO5                                                   THER  48
      DO2 J=1,MM                                                        THER  49
 2    CPDT1(J)=(S1(J)*A1+S2(J)*A2+S3(J)*A3+S4(J)*A4+S5(J)*A5+S6(J))*RR  THER  50
      GOTO5                                                             THER  51
 3    ENT1(I)=(AII(I)*A1+BII(I)*A2+CII(I)*A3+DII(I)*A4+EII(I)*A5        THER  52
     1+FII(I))*RR                                                       THER  53
      S(I)=(AII(I)*ALOG(T)+BII(I)*A1+CII(I)*A2+DII(I)*A3+EII(I)*A4      THER  54
     1+GII(I))*RR                                                       THER  55
      IF(I.GT.1)GOTO5                                                   THER  56
      DO4J=1,MM                                                         THER  57
 4    CPDT1(J)=(A11(J)*A1+A22(J)*A2+A33(J)*A3+A44(J)*A4+A55(J)*A5       THER  58
     1+A66(J))*RR                                                       THER  59
 5    RSUM=0.                                                           THER  60
C     RSUM IS THE SENSIBLE ENTHALPY OF THE CONSTITUENT ELEMENTS         THER  61
C     OF THE ITH SPECIE(AT TEMPERATURE T(OK) WITH RESPECT TO THE        THER  62
C     STANDARD STATE P=1 ATM AND T=298.16 OK).                          THER  63
      DO7J=1,MM                                                         THER  64
      IF(JCODE(J).EQ.1)GOTO6                                            THER  65
C     WHEN JCODE(J)=0, THE CONSTITUENT ELEMENT HAS BEEN ASSUMED TO BE   THER  66
C     IN ITS BI-MOLECULAR FORM. FOR EXAMPLE HYDROGEN IS TAKEN TO BE     THER  67
C     H2. WHEN JCODE(J)=1,THE CONSTITUENT ELEMENT HAS BEEN ASSUMED TO   THER  68
```

```
C       BE ITS UNI-MOLECULAR,OR ATOMIC FORM. FOR EXAMPLE CARBON IS TAKEN  THER  69
C       TO BE C.                                                          THER  70
C       AA(I,J) IS THE FORMULA NUMBER. IT GIVES THE GRAM-ATOMS OF         THER  71
C       ELEMENT J IN SPECIE I. EXAMPLE,CH4(METHANE),AA(I,J) FOR           THER  72
C       CARBON IS 1. FOR HYDROGEN IS 4.                                   THER  73
        RSUM=RSUM+0.500*AA(I,J)*CPDT1(J)                                  THER  74
        GOTO7                                                             THER  75
  6     RSUM=RSUM+AA(I,J)*CPDT1(J)                                        THER  76
  7     CONTINUE                                                          THER  77
        ENT(I)=ENT1(I)-RSUM                                               THER  78
        IF(ABS(ENT(I)).LT.3.)ENT(I)=0.                                    THER  79
  8     CONTINUE                                                          THER  80
        RETURN                                                            THER  81
        END                                                               THER  82
```

```
      SUBROUTINE DNSITY(RHO,T,DELZ,VR,K6,DRHODT,W,H)
C
C
C-----THIS SUBROUTINE CALCULATES THE DENSITY OF PHENOLIC-NYLON
C     COMPOSITES AS A FUNCTION OF TEMPERATURE--BASED ON DATA
C     OF SYKES AND NELSON(THERMOANALYSIS OF ABLATION MATERIALS)
C
C
      COMMON/KL/WTOTAL,RHOII
      DIMENSION RHOI(5),RHOT(5),RHOC(5),A(7),E(7),RATER(7),
     1DRHODT(5),XN(5,7),FRAC(5),RHOVOL(5)
      DIMENSION MASFRC(5),MASFLX(5),VOLUME(5),VOLFRC(5),DELFLX(5)
      DIMENSION RHOCC(5),DRHO(5)
      INTEGER COMPST
      REAL MASFRC,MASFLX
      IF(K6.GT.1)GOTO7
C
C
C-----READ INPUT
C
C
      READ 1,COMPST,NREACT
    1 FORMAT(2I6)
C
C     COMPST=NUMBER OF COMPOSITE MATERIALS DEGRADING DURING
C     ABLATION.
C     NREACT=NUMBER OF PSEUDO-KINETIC REACTIONS USED TO DES-
C     CRIBE THE DEGRADATION OF THE ABLATIVE COMPOSITES.
C
C
C
C-----INITIALIZATION OF XN(I,J),WHICH IS THE ORDER OF THE
C     REACTION
C
```

```
C
      DO2J=1,NREACT
      DO2I=1,COMPST
    2 XN(I,J)=0.
C
C     A(J)=FREQUENCY FACTOR(SEC-1)
C     E(J)=ENERGY OF ACTIVATION(JOULE/(MOLE))
C
C
      R=8.314
C     R=8.314(JOULES/(MOLE-OK))
C
C
C     RHOI(1)=68.6(NYLON)
C     RHOI(2)=80.0(PHENOLIC RESIN)
C     RHOI(3)=17.8(PHENOLIC-MICROBALLOONS)
C     RHOC(1)=68.6*0.075=5.145
C     RHOC(2)=80.0*0.541=43.28
C     RHOC(3)=17.8*542=9.6476
C
C
C     MASFRC(1)=0.4
C     MASFRC(2)=0.25
C     MASFRC(3)=0.35
C
C
C
C-----INITIALIZE
C
C
C
C     XN(I,J)=ORDER OF THE KINETIC EXPRESSION.
C
      DO3J=1,NREACT
```

```
    3 READ 4,I,A(J),E(J),XN(I,J)                                        DNSI  69
    4 FORMAT(4X,I6,3E10.8)                                              DNSI  70
      READ 5,(RHOI(I),RHOC(I),MASFRC(I),I=1,COMPST)                     DNSI  71
    5 FORMAT(3E10.4)                                                    DNSI  72
C                                                                       DNSI  73
C                                                                       DNSI  74
C     RHOI(I)=INITIAL DENSITY OF COMPOSITE I                            DNSI  75
C     RHOC(I)=RESIDUAL DENSITY OF COMPOSITE I                           DNSI  76
C     RHOT(I)=DENSITY OF THE COMPOSITE I AT ANY TEMPERATURE             DNSI  77
C                                                                       DNSI  78
C                                                                       DNSI  79
C                                                                       DNSI  80
C-----LET RHOT(I)=RHOI(I) AS INITIAL CONDITION                          DNSI  81
C                                                                       DNSI  82
C                                                                       DNSI  83
      DO 6 I=1,COMPST                                                   DNSI  84
      RHOCC(I)=RHOC(I)+0.001*RHOC(I)                                    DNSI  85
      MASFLX(I)=0.                                                      DNSI  86
    6 RHOT(I)=RHOI(I)                                                   DNSI  87
      SUMVOL=0.                                                         DNSI  88
      DO 60 I=1,COMPST                                                  DNSI  89
      VOLUME(I)=MASFRC(I)/RHOT(I)                                       DNSI  90
   60 SUMVOL=SUMVOL+VOLUME(I)                                           DNSI  91
      DO 65 I=1,COMPST                                                  DNSI  92
   65 VOLFRC(I)=VOLUME(I)/SUMVOL                                        DNSI  93
      RHO=1./SUMVOL                                                     DNSI  94
      RHOII=RHO                                                         DNSI  95
      WTOTAL=RHOII*VR                                                   DNSI  96
      PRINT 66,RHO,WTOTAL                                               DNSI  97
   66 FORMAT(1X,'INITIAL DENSITY OF COMPOSITE(LBS/FT**3)='F10.5,2X,     DNSI  98
     1'WTOTAL(LBS/FT**2-SEC)='E15.7/)                                   DNSI  99
    7 RRR=1000./(R*T)                                                   DNSI 100
      RHOPRV=RHO                                                        DNSI 101
      DO 9 I=1,COMPST                                                   DNSI 102
```

```
      SUM=0.                                                            DNSI 103
      DO 8 J=1,NREACT                                                   DNSI 104
      IF(XN(I,J).EQ.0.)GOTO8                                            DNSI 105
C                                                                       DNSI 106
C     RATER(J)=SPECIFIC REACTION VELOCITY                               DNSI 107
      IF(RHOT(I).LE.RHOC(I))RHOT(I)=RHOCC(I)                            DNSI 108
      RATER(J)=-RHOI(I)*((RHOT(I)-RHOC(I))/RHOI(I))**XN(I,J)*A(J)*EXP(- DNSI 109
     1E(J)*RRR)                                                         DNSI 110
      SUM=SUM+RATER(J)                                                  DNSI 111
 8    CONTINUE                                                          DNSI 112
      DRHODT(I)=SUM                                                     DNSI 113
      IF(RHOT(I).LE.RHOCC(I))DRHODT(I)=0.                               DNSI 114
    9 CONTINUE                                                          DNSI 115
      PRINT 900,H,DELZ                                                  DNSI 116
 900  FORMAT(1X,' IN DENSITY     H='E15.7,' DELZ='E15.7)                DNSI 117
C                                                                       DNSI 118
C-----CONTROLLING STEP SIZE FOR STABILITY                               DNSI 119
C                                                                       DNSI 120
      TEST=0.                                                           DNSI 121
      DO 90 I=1,COMPST                                                  DNSI 122
      DRHO(I)=-DELZ*DRHODT(I)/VR                                        DNSI 123
   90 TEST=AMAX1(TEST,DRHO(I))                                          DNSI 124
      IF(TEST.GT.0.5)H=H/2.                                             DNSI 125
      IF(TEST.LT..1)H=H*2.                                              DNSI 126
      IF(H.GT.2.08E-4)H=2.08E-4                                         DNSI 127
C     DELZ=STEP SIZE IN FEET                                            DNSI 128
      DELZ=H                                                            DNSI 129
      RHO=0.                                                            DNSI 130
      W=0.                                                              DNSI 131
      DO10I=1,COMPST                                                    DNSI 132
      DELFLX(I)=-DELZ*DRHODT(I)                                         DNSI 133
C                                                                       DNSI 134
C     DELFLX(I)=CHANGE IN MASS FLUX DUE TO A CHANGE IN THE              DNSI 135
C     DENSITY OF THE COMPOSITES.                                        DNSI 136
```

```
C                                                                       DNSI 137
      RHOT(I)=RHOT(I)-DELFLX(I)/VR                                      DNSI 138
      RHOVOL(I)=RHOT(I)*VOLFRC(I)                                       DNSI 139
      RHO=RHO+RHOVOL(I)                                                 DNSI 140
C     RHO=BULK DENSITY OF THE COMPOSITE                                 DNSI 141
      MASFLX(I)=MASFLX(I)+DELFLX(I)                                     DNSI 142
   10 W=W+MASFLX(I)                                                     DNSI 143
      W1=(RHOII-RHO)*VR                                                 DNSI 144
      W=W1                                                              DNSI 145
      DO 100 I=1,COMPST                                                 DNSI 146
  100 MASFRC(I)=RHOVOL(I)/RHO                                           DNSI 147
      PRINT 11,RHO,DELZ,VR,T,W                                          DNSI 148
  11  FORMAT(1X,'RHO(OVERALL DENSITY OF ='E10.4,' DELZ='E10.4,'V='E10.4,DNSI 149
     1' T='E10.4,' W='E13.5)                                            DNSI 150
      PRINT 12                                                          DNSI 151
   12 FORMAT(8X,'VIRGIN MATERIAL)')                                     DNSI 152
      DO 14 I=1,COMPST                                                  DNSI 153
      PRINT 13,I,RHOT(I),I,DRHODT(I),I,DRHO(I),I,MASFRC(I)              DNSI 154
  13  FORMAT(1X,'RHOT('I1,')='E12.6,' DRODT('I1,')='E12.6,' DRHO('I1,')=DNSI 155
     1'E12.6,' MASFRC('I1,')='E12.6)                                    DNSI 156
  14  CONTINUE                                                          DNSI 157
      RETURN                                                            DNSI 158
      END                                                               DNSI 159
```

```
      SUBROUTINE CHARPR                                                 CHAR   1
C     CHARPR SUBROUTINE CALCULATES THE EFFECTIVE THERMAL                CHAR   2
C     CONDUCTIVITY AND HEAT CAPACITY OF THE CHAR.                       CHAR   3
C                                                                       CHAR   4
C                                                                       CHAR   5
      COMMON/KF/CPS,CDO,DCDO,JCHAR,TC                                   CHAR   6
C     T=TEMPERATURE IN RANKINE                                          CHAR   7
C     TC=TEMPERATURE IN FARENHEIT                                       CHAR   8
C     CPS=HEAT CAPACITY OF CHAR(BTU/LB-OF)                              CHAR   9
C     CDO=EFFECTIVE THERMAL CONDUCTIVITY(BTU/FT-SEC-OF)                 CHAR  10
C     DCDO=RATE OF CHANGE OF CDO WITH TEMPERATURE                       CHAR  11
      TC2=TC*TC                                                         CHAR  12
      TC3=TC2*TC                                                        CHAR  13
      IF(TC.GT.2500.)GOTO507                                            CHAR  14
      T=TC+459.7                                                        CHAR  15
      CPS=0.43+3.6E-5*T-87.2E3/(T*T)                                    CHAR  16
      IF(TC.LT.1000.)CPS=0.39                                           CHAR  17
  507 CPS=0.52                                                          CHAR  18
      CDO=11.57E-5+5.3E-15*TC3                                          CHAR  19
      DCDO=15.9E-15*TC2                                                 CHAR  20
      RETURN                                                            CHAR  21
      END                                                               CHAR  22
```

```
      SUBROUTINE CPMIX(T,NN,CPMX)                                       CPMI   1
C                                                                       CPMI   2
C                                                                       CPMI   3
C-----THIS SUBROUTINE COMPUTES THE MOLAL HEAT CAPACITY                  CPMI   4
C     OF A NON-REACTING GAS.  IT IS ONLY USE FOR THE                    CPMI   5
C     FROZEN FLOW CASE.                                                 CPMI   6
C                                                                       CPMI   7
C                                                                       CPMI   8
      COMMON/KB/AI(30),BI(30),CI(30),DI(30),EI(30),FI(30),              CPMI   9
     1GI(30),AII(30),BII(30),CII(30),DII(30),EII(30),                   CPMI  10
     2FII(30),GII(30),TLOW(30)                                          CPMI  11
      COMMON/KM/XMOL(30)                                                CPMI  12
      DIMENSION CP(30)                                                  CPMI  13
      RR=1.98726                                                        CPMI  14
C                                                                       CPMI  15
C     CPMX=HEAT CAPCITY(BTU/LB-MOLE-OF)                                 CPMI  16
C                                                                       CPMI  17
C                                                                       CPMI  18
C                                                                       CPMI  19
C-----CALCULATE THE HEAT CAPACITY OF EACH INDIVIDUAL SPECIE.            CPMI  20
C                                                                       CPMI  21
C                                                                       CPMI  22
      CPMX=0.                                                           CPMI  23
      DO 3 I=1,NN                                                       CPMI  24
      IF(T.GT.TLOW(I))GOTO1                                             CPMI  25
      CP(I)=(AII(I)+(((EII(I)*T+DII(I))*T+CII(I))*T+BII(I))*T)*RR        CPMI  26
      GOTO2                                                             CPMI  27
 1    CP(I)=(AI(I)+(((EI(I)*T+DI(I))*T+CI(I))*T+BI(I))*T)*RR            CPMI  28
 2    CPMX=CPMX+CP(I)*XMOL(I)                                           CPMI  29
 3    CONTINUE                                                          CPMI  30
      RETURN                                                            CPMI  31
      END                                                               CPMI  32
```

```
      SUBROUTINE CHEMEQ                                                 CHEM   1
C                                                                       CHEM   2
C                                                                       CHEM   3
C                                                                       CHEM   4
C-----THIS SUBPROGRAM COMPUTES COMPLEX CHEMICAL EQUILIBRIUM             CHEM   5
C     FOR A MULTICOMPONENT,POLYPHASE SYSTEM BY FREE ENERGY              CHEM   6
C     MINIMIZATION.(J.CHEM.PHYS.VOL.28.NO.5,751-58,MAY 1958).           CHEM   7
C                                                                       CHEM   8
C                                                                       CHEM   9
      COMMON/KA/S1(6),S2(6),S3(6),S4(6),S5(6),S6(6),A11(6),             CHEM  10
     1A22(6),A33(6),A44(6),A55(6),A66(6),AA(30,6),JCODE(6)              CHEM  11
      COMMON/KB/AI(30),BI(30),CI(30),DI(30),EI(30),FI(30),              CHEM  12
     1GI(30),AII(30),BII(30),CII(30),DII(30),EII(30),                   CHEM  13
     2FII(30),GII(30),TLOW(30)                                          CHEM  14
      COMMON/KC/ICODE(30),Y(30),XMW(30)                                 CHEM  15
      COMMON/KCC/SPCIE1 (30),SPCIE2(30),TABLE(353,25)                   CHEM  16
      COMMON/KGG/FORT(30),CP(30)                                        CHEM  17
      COMMON/KEE/PL,RR,TZERO,EPS,KEY,NN,NQ,MM                           CHEM  18
      COMMON/KI/WEPS,KPT3,KOUNT                                         CHEM  19
      COMMON/KJ/DELTK,TVAR                                              CHEM  20
      COMMON/KG/ENT(30),S(30),ENT1(30),T                                CHEM  21
      COMMON/KNN/TFMAX                                                  CHEM  22
      DIMENSION PERC(30),PERC1(30),XMOL(30),XMOL1(30)                   CHEM  23
      DIMENSION X(30),FY(30),C(30),BB(8),FSUM(30),YSUM(30),             CHEM  24
     1XMASS(30),XLAM(30),FLUX(350,25),                                  CHEM  25
     2DFLUX(350,25),R(6,6),B(6,1),PI(6),DELT(30)                        CHEM  26
C                                                                       CHEM  27
C                                                                       CHEM  28
C     PL=PRESSURE IN LBS/FT2                                            CHEM  29
C     RR=1.987(CAL/GM-MOLE-OK)                                          CHEM  30
C     TZERO=298.16 OK                                                   CHEM  31
C     EPS=POROSITY OF THE MATRIX                                        CHEM  32
C     KEY=2 FOR EQUILIBRIUM FLOW                                        CHEM  33
C     NN=NUMBER OF GAS COMPONENTS                                       CHEM  34
```

```
C       NQ=NUMBER OF SOLID+GAS COMPONENTS                                CHEM  35
C       TABLE(I,J)STORES THE VALUES OF THE TEMPERATURE(J=1)IN            CHEM  36
C       OK,THE HEAT ABSORBED OR RELEASED BY CHEMICAL REACTIONS           CHEM  37
C       (J=2)(BTU/FT**3-SEC),THE AVERAGE MOLECULAR WEIGHT OF THE         CHEM  38
C       MIXTURE(J=3),THE MASS FLOW RATE OF THE GASES(LBS/FT2-SEC),       CHEM  39
C       AND THE AVERAGE HEAT CAPACITY OF THE MIXTURE.                    CHEM  40
C       FROM J=5 ON,THE VALUES OF MOLES,Y(I),OF EACH INDIVIDUAL          CHEM  41
C       ARE STORED. I IS THE NUMBER OF TEMPERATURE POINTS                CHEM  42
C                                                                        CHEM  43
        W1=WEPS/EPS                                                      CHEM  44
        W=WEPS/EPS                                                       CHEM  45
        XT=TVAR                                                          CHEM  46
        CRIT=0.0001                                                      CHEM  47
        TMAX=(TFMAX+459.69)/1.8                                          CHEM  48
        TINC=(TMAX-XT)/346.                                              CHEM  49
        IF(TINC.LT.7.5)TINC=7.5                                          CHEM  50
        TINC=200.                                                        CHEM  51
        TMAX=TMAX+4.*TINC                                                CHEM  52
        READ 7,IPRINT                                                    CHEM  53
 7      FORMAT(I1)                                                       CHEM  54
        NS=NQ                                                            CHEM  55
        NC=NN                                                            CHEM  56
C                                                                        CHEM  57
C       XT=INITIAL TEMPERATURE(OK)                                       CHEM  58
C       TMAX=FINAL TEMPERATURE(OK)                                       CHEM  59
C       TINC=INCREMENT OF TEMPERATURE                                    CHEM  60
C       CRIT=CRITERIA FOR CONVERGENCE                                    CHEM  61
C       KEY=2(EQUILIBRIUM)                                               CHEM  62
C                                                                        CHEM  63
        MA=1                                                             CHEM  64
        M=MA                                                             CHEM  65
C                                                                        CHEM  66
C-----CALCULATE THE SIZE OF THE MATRIX R.                                CHEM  67
C                                                                        CHEM  68
```

```
      NA=MM+1+NQ-NN                                                     CHEM  69
      N=NA                                                              CHEM  70
      P=PL/2160.                                                        CHEM  71
      KPT=0                                                             CHEM  72
C                                                                       CHEM  73
C     KPT COUNTS THE NUMBER OF TEMPERATURE POINTS                       CHEM  74
C                                                                       CHEM  75
      MAXNT=100                                                         CHEM  76
C     MAXNT=MAXIMUM NUMBER OF ITERATIONS ALLOWED                        CHEM  77
C     BEFORE INCREASING CRIT(CRIT=CRITERIA FOR CONVERGENCE)             CHEM  78
      KCODE=0                                                           CHEM  79
C     KCODE=0(NO SOLIDS ),KCODE=1(SOLIDS ARE ASSUMED PRESENT)           CHEM  80
      T=XT                                                              CHEM  81
      KOS=NQ+5                                                          CHEM  82
C                                                                       CHEM  83
C     KOS IS THE TOTAL NUMBER OF VARIABLES STORED                       CHEM  84
C     IN TABLE(I,J)(J=1...KOS)                                          CHEM  85
C     ENT(I)=HEAT OF FORMATION OF SPECIE I                              CHEM  86
C     FORT(I)=FREE ENERGY FUNCTION(F/RT)                                CHEM  87
C     FORT IS CALCULATED IN SUBROUTINE FRNERG                           CHEM  88
      LL=NN+1                                                           CHEM  89
      XBETA=CRIT                                                        CHEM  90
C                                                                       CHEM  91
C-----CALCULATE THE GRAM-ATOMS OF EACH ELEMENT,BB(J).                   CHEM  92
C     BB(J)IS THE MATERIAL BALANCE CONSTRAINT ON THE                    CHEM  93
C     FREE ENERGY EQUATION.                                             CHEM  94
C                                                                       CHEM  95
      DO320J=1,MM                                                       CHEM  96
      BB(J)=0.                                                          CHEM  97
      DO 320 I=1,NQ                                                     CHEM  98
      BB(J)=BB(J)+AA(I,J)*Y(I)                                          CHEM  99
  320 CONTINUE                                                          CHEM 100
      DO433I=1,NQ                                                       CHEM 101
      IF(ICODE(I).EQ.0)GOTO433                                          CHEM 102
```

```
      KCODE=1                                                           CHEM 103
 433  CONTINUE                                                          CHEM 104
C                                                                       CHEM 105
C-----TEST TO DETERMINE WHETHER THERE ARE SOLIDS IN THE                 CHEM 106
C     SYSTEM OF SPECIES ASSUMED.                                        CHEM 107
C                                                                       CHEM 108
  500 IF(IPRINT .EQ. 0) GO TO 501                                       CHEM 109
      PRINT4                                                            CHEM 110
    4 FORMAT(1H1,20X,5HFO/RT,13X,12HINITIAL Y(I))                       CHEM 111
C                                                                       CHEM 112
C-----CALL THE FREE ENERGY SUBPROGRAM                                   CHEM 113
C                                                                       CHEM 114
 501  NT=1                                                              CHEM 115
      CALL FRNERG(T,NQ)                                                 CHEM 116
C                                                                       CHEM 117
C-----THE ABOVE SUBPROGRAM CALCULATES THE FREE ENRGY FUNCTION FORT.     CHEM 118
C                                                                       CHEM 119
      IF(IPRINT .EQ. 0) GO TO 300                                       CHEM 120
      DO206I=1,NQ                                                       CHEM 121
 206  PRINT14,I,SPCIE1(I),SPCIE2(I),FORT(I),Y(I),XMW(I)                 CHEM 122
 14   FORMAT(1X,I2,2X,2A3,3E20.7)                                       CHEM 123
  300 YBAR=0.0                                                          CHEM 124
      DO50I=1,NN                                                        CHEM 125
C                                                                       CHEM 126
C                                                                       CHEM 127
C     YBAR IS THE TOTAL NUMBER OF MOLES OF GAS SPECIES                  CHEM 128
C                                                                       CHEM 129
   50 YBAR=YBAR+Y(I)                                                    CHEM 130
      DO10I=1,NN                                                        CHEM 131
      C(I)=FORT(I)+ALOG(P)                                              CHEM 132
      FAC=Y(I)/YBAR                                                     CHEM 133
      IF(FAC.LT.1.E-73)FAC=1.E-73                                       CHEM 134
C                                                                       CHEM 135
C-----CALCULATE THE FREE ENERGY PARAMETER OF THE GAS SPECIES            CHEM 136
```

```
C      TO BE MINIMIZE                                                    CHEM 137
C                                                                        CHEM 138
       FY(I)=Y(I)*(C(I)+ALOG(FAC))                                       CHEM 139
    10 CONTINUE                                                          CHEM 140
       IF(KCODE.EQ.0)GOTO111                                             CHEM 141
C                                                                        CHEM 142
C                                                                        CHEM 143
C-----IF THERE ARE NO SOLIDS PROCEED TO STATEMENT 111                    CHEM 144
C                                                                        CHEM 145
C                                                                        CHEM 146
C-----CALCULATION OF THE FREE ENERGY PARAMENTER FOR SOLIDS               CHEM 147
C                                                                        CHEM 148
       DO 11 I=LL,NQ                                                     CHEM 149
       FY(I)=Y(I)*FORT(I)                                                CHEM 150
    11 CONTINUE                                                          CHEM 151
C                                                                        CHEM 152
C-----FROM STATEMENT 111 TO 1050 OPERATIONS ARE PERFORMED TO CONSTRUCT   CHEM 153
C      THE R MATRIX AND THE B VECTOR                                     CHEM 154
C                                                                        CHEM 155
C                                                                        CHEM 156
   111 DO30J=1,MM                                                        CHEM 157
       DO30K=1,MM                                                        CHEM 158
       SUM=0.                                                            CHEM 159
       DO20I=1,NN                                                        CHEM 160
    20 SUM=SUM+AA(I,J)*AA(I,K)*Y(I)                                      CHEM 161
       R(J,K)=SUM                                                        CHEM 162
    30 CONTINUE                                                          CHEM 163
       GSUM1=0.                                                          CHEM 164
       DO 1022 I=1,NQ                                                    CHEM 165
       GSUM1=GSUM1+FY(I)                                                 CHEM 166
  1022 CONTINUE                                                          CHEM 167
  3000 JJ=MM+1                                                           CHEM 168
       DO 103 K=1,MM                                                     CHEM 169
       SUM=0.                                                            CHEM 170
```

```
      DO 101 I=1,NN                                                     CHEM 171
  101 SUM=SUM+AA(I,K)*Y(I)                                              CHEM 172
      R(K,JJ)=SUM                                                       CHEM 173
      R(JJ,K)=SUM                                                       CHEM 174
  103 CONTINUE                                                          CHEM 175
      KL=NS-NC+JJ                                                       CHEM 176
      DO 1044 J=JJ,KL                                                   CHEM 177
      DO 1045 K=JJ,KL                                                   CHEM 178
 1045 R(J,K)=0.0                                                        CHEM 179
 1044 CONTINUE                                                          CHEM 180
      DO70J=1,MM                                                        CHEM 181
      SUM=0.                                                            CHEM 182
      DO130I=1,NN                                                       CHEM 183
  130 SUM=SUM+AA(I,J)*FY(I)                                             CHEM 184
   70 B(J,1)=SUM+BB(J)                                                  CHEM 185
      SUM=0.                                                            CHEM 186
      DO80I=1,NN                                                        CHEM 187
   80 SUM=SUM+FY(I)                                                     CHEM 188
      B(JJ,1)=SUM                                                       CHEM 189
      IF(KCODE.EQ.0)GOTO1050                                            CHEM 190
      KK=MM+1                                                           CHEM 191
      DO 29 I=LL,NQ                                                     CHEM 192
      KK=KK+1                                                           CHEM 193
      DO 29 J=1,MM                                                      CHEM 194
      R(J,KK)=AA(I,J)                                                   CHEM 195
      R(KK,J)=R(J,KK)                                                   CHEM 196
   29 CONTINUE                                                          CHEM 197
      KM=MM+1                                                           CHEM 198
      DO 1053 I=LL,NQ                                                   CHEM 199
      KM=KM+1                                                           CHEM 200
 1053 B(KM,1)=FORT(I)                                                   CHEM 201
 1050 CONTINUE                                                          CHEM 202
      IF(KCODE.EQ.0)R(JJ,JJ)=0.                                         CHEM 203
C                                                                       CHEM 204
```

```
C-----MATRIX INVERSION IS CALLED TO SOLVE THE SET OF SIMULTANEOUS
C     LINEARIZED EQUATIONS.
C
C
      CALL MATINV(R,NA,B,MA)
C
C
C-----FROM THE SOLUTION OF THE MATRIX THE VALUES OF THE LAGRANGIAN
C     MULTIPLIERS AND THE MOLES OF THE SOLID SPECIES ARE OBTAINED
C
C
      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)
C
C-----CALCULATE THE MOLES OF GASEOUS SPECIES
C
  110 X(I)=FSUM(I)+YSUM(I)
C
C-----CALCUALTE THE CONVERGENCE PARAMENTE XLAMBD
```

```
C
      XLAMBD=1.0
      DO 86 I=1,NQ
      DELT(I)=X(I)-Y(I)
      IF(DELT(I).GE.0.)GOTO86
      IF(X(I).GT.0.)GOTO86
      XLAM(I)=-Y(I)/DELT(I)
      XLAMBD=AMIN1(XLAMBD,XLAM(I))
      XLAMBD=0.99*XLAMBD
   86 CONTINUE
      XLAM1=XLAMBD
      IF(XLAM1.EQ.0.)XLAM1=1.E-5
      DEBAR=0.
      DO87I=1,NN
   87 DEBAR=DEBAR+DELT(I)
C
C
C-----DETERMINE THE SIZE OF THE UNIT VECTOR XLAMBD.
C     APPLY THE CORRECTIONS TO OBTAIN A NEW SET OF ESTIMATES FOR THE
C     NEXT ITERATION. WHEN THE VALUE OF XLAMBD IS VERY SMALL SET THE
C     VALUES OF Y(I) EQUAL TO X(I) TO AVOID USING THE SAME VALUES OF
C     Y(I) AS WAS USED IN THE PREVIOUS ITERATION
C
C
C
C-----CALCUALTE THE FREE NERGY GRADIENT DFDL. IF IT IS POSITIVE
C     REDUCE THE VALUE OF XLAMBD UNTIL DFDL IS NEGATIVE.
C
   93 DFDL=0.
      DO88I=1,NQ
      IF(ICODE(I).EQ.1)GOTO83
   96 FAC=(Y(I)+XLAMBD*DELT(I))/(YBAR+XLAMBD*DEBAR)
   98 IF(FAC.GT.0.)GOTO82
  991 XLAMBD=.9*XLAMBD
```

```
      IF(XLAMBD.GT.1.0E- 6)GOTO96                                       CHEM 273
      IF(FAC.LT.1.E-73)FAC=1.E-73                                       CHEM 274
   82 DFDL=DFDL+DELT(I)*(C(I)+ALOG(FAC))                                CHEM 275
      GOTO88                                                            CHEM 276
   83 DFDL=DFDL+DELT(I)*FORT(I)                                         CHEM 277
   88 CONTINUE                                                          CHEM 278
      IF(DFDL.LT.0.000)GOTO89                                           CHEM 279
      XLAMBD=.9*XLAMBD                                                  CHEM 280
      IF(XLAMBD.GT.1.0E- 6)GOTO93                                       CHEM 281
C                                                                       CHEM 282
C-----CALCULATE THE NEW AND IMPROVED VALUE OF THE MOLES OF THE SPECIES. CHEM 283
C                                                                       CHEM 284
   89 DO76I=1,NQ                                                        CHEM 285
      IF(XLAMBD.GT.1.E-6)GOTO90                                         CHEM 286
      IF(DFDL.LT.0.)GOTO90                                              CHEM 287
      IF(XLAM1.LT.1.E-6)XLAM1=1.E-6                                     CHEM 288
      Y(I)=Y(I)+XLAM1*DELT(I)*.1                                        CHEM 289
      GOTO900                                                           CHEM 290
   90 CONTINUE                                                          CHEM 291
      Y(I)=Y(I)+XLAMBD*DELT(I)                                          CHEM 292
  900 CONTINUE                                                          CHEM 293
      IF(Y(I).LT.0.)Y(I)=1.E-73                                         CHEM 294
 76   CONTINUE                                                          CHEM 295
      SUMY=0.                                                           CHEM 296
      SUM=0.                                                            CHEM 297
      DO370I=1,NN                                                       CHEM 298
 370  SUMY=SUMY+Y(I)                                                    CHEM 299
      DO371I=LL,NQ                                                      CHEM 300
 371  SUM=SUM+Y(I)                                                      CHEM 301
      SUMY1=SUMY+SUM                                                    CHEM 302
      DO340I=1,NQ                                                       CHEM 303
      XMOL1(I)=Y(I)/SUMY1                                               CHEM 304
      PERC1(I)=XMOL1(I)*100.                                            CHEM 305
      XMOL(I)=Y(I)/SUMY                                                 CHEM 306
```

```
 340  PERC(I)=XMOL(I)*100.                                              CHEM 307
      GSUM2=0.                                                          CHEM 308
      DO342I=1,NQ                                                       CHEM 309
      IF(ICODE(I).EQ.1)GOTO341                                          CHEM 310
      FAC=XMOL(I)                                                       CHEM 311
      IF(FAC.LT.1.E-73)FAC=1.E-73                                       CHEM 312
      FY(I)=Y(I)*(C(I)+ALOG(FAC))                                       CHEM 313
      GSUM2=GSUM2+FY(I)                                                 CHEM 314
      GOTO342                                                           CHEM 315
 341  FY(I)=Y(I)*FORT(I)                                                CHEM 316
      GSUM2=GSUM2+FY(I)                                                 CHEM 317
 342  CONTINUE                                                          CHEM 318
 350  BETA=0.                                                           CHEM 319
      DO85I=1,NQ                                                        CHEM 320
C                                                                       CHEM 321
C-----CHECK IF THE MINIMUM HAS BEEN REACHED                             CHEM 322
C                                                                       CHEM 323
 85   BETA=BETA+ABS(DELT(I))                                            CHEM 324
      RESTA=1.0000000-U                                                 CHEM 325
      IF(ABS(RESTA).LT.XBETA)GOTO800                                    CHEM 326
      IF(NT.GE.MAXNT)GOTO600                                            CHEM 327
      NT=NT+1                                                           CHEM 328
      GOTO300                                                           CHEM 329
 600  XBETA=XBETA+0.001                                                 CHEM 330
      MAXNT=MAXNT+10                                                    CHEM 331
      NT=NT+1                                                           CHEM 332
      GOTO300                                                           CHEM 333
C*********************************************************************** CHEM 334
C*********************************************************************** CHEM 335
C-----CONVERGENCE HAS BEEN ACHIEVED                                    * CHEM 336
C*********************************************************************** CHEM 337
C*********************************************************************** CHEM 338
 800  IF(IPRINT .EQ. 0) GO TO 1802                                      CHEM 339
      PRINT16,NT,U                                                      CHEM 340
```

```
 16   FORMAT(//1X,'NT = NO. OF ITERATIONS REQUIRED ='I5,5X,                CHEM 341
     1'U=X/Y='F15.7/ )                                                    CHEM 342
      PRINT2189,(J,BB(J),J=1,MM)                                          CHEM 343
 2189 FORMAT(1X,'BB('I1,')='F15.7)                                        CHEM 344
      PRINT201,BETA                                                       CHEM 345
 201  FORMAT( /1X,'BETA='F15.7/ )                                         CHEM 346
      PRINT202,GSUM2                                                      CHEM 347
 202  FORMAT(1X,'FREE ENERGY FY(I) OF THE SYSTEM AT EQUILIBRIUM'F15.7)    CHEM 348
      PRINT203,P,T                                                        CHEM 349
 203  FORMAT(  /1X,'PRESSURE(ATM)='F10.4,5X,'TEMP(OK)='F13.6/ )           CHEM 350
 1802 XMWGAS=0.                                                           CHEM 351
      DO81I=1,NN                                                          CHEM 352
C                                                                         CHEM 353
C-----CALCULATE THE AVERAGE MOLECULAR WEIGHT OF THE GAS,XMWGAS            CHEM 354
C                                                                         CHEM 355
 81   XMWGAS=XMWGAS+XMOL(I)*XMW(I)                                        CHEM 356
      DO191I=1,NQ                                                         CHEM 357
 191  XMASS(I)=XMW(I)*XMOL(I)/XMWGAS                                      CHEM 358
      CPMX=0.                                                             CHEM 359
      DO781I=1,NN                                                         CHEM 360
 781  CPMX=CPMX+CP(I)*XMOL(I)                                             CHEM 361
      IF(IPRINT .EQ. 0) GO TO 1803                                        CHEM 362
      PRINT 18,CPMX,W                                                     CHEM 363
 18   FORMAT( /1X,'HEAT CAPACITY OF THE MIXTURE'/1X,'IN CALORIES PER GRACHEM 364
     1M MOLE    ='F10.5,10X,'MASS FLUX(LBS/FT2SEC)='F10.5)               CHEM 365
      PRINT17,XMWGAS                                                      CHEM 366
 17   FORMAT( /1X,'MOLECULAR WEIGHT OF THE GAS MIXTURE='F8.5)             CHEM 367
 1803 XBETA=CRIT                                                          CHEM 368
      KPT=KPT+1                                                           CHEM 369
C                                                                         CHEM 370
C                                                                         CHEM 371
C-----REDIFINE MOLE BASIS. THIS OPERATION IS PERFORMED AFTER              CHEM 372
C     THE FIRST EQUILIBRIUM CALCULATION. THIS IS DONE TO MAKE             CHEM 373
C     THE MOLES OF Y(I) CALCULATED BASED ON ONE MOLE OF VIR-              CHEM 374
```

```
C     PLASTIC COMPOSITF COMPATIBLE WITH THE ACTUAL NUMBER                CHEM 375
C     OF MOLES FLOWING THROUGH THE POROUS MATRIX. THIS OPERA-            CHEM 376
C     TION IS PERFORMED ONLY ONCE.                                       CHEM 377
C                                                                        CHEM 378
C                                                                        CHEM 379
      IF(T.NE.XT)GOTO823                                                 CHEM 380
C                                                                        CHEM 381
C-----PROPORTION THE MOLES OF FLOWING GASES IN DIRECT                    CHEM 382
C     RELATION TO THEIR EQUILIBRIUM MOLE FRACTION.                       CHEM 383
C                                                                        CHEM 384
      RIN=0.                                                             CHEM 385
      SUM=0.                                                             CHEM 386
      DO821I=1,NQ                                                        CHEM 387
      IF(ICODE(I).EQ.1)GOTO8210                                          CHEM 388
      Y(I)=W/XMWGAS*XMOL(I)                                              CHEM 389
      SUM=SUM+Y(I)                                                       CHEM 390
      GOTO821                                                            CHEM 391
 8210 Y(I)=XMOL(I)*SUM                                                   CHEM 392
      RIN=RIN+XMOL(I)*XMW(I)/XMWGAS                                      CHEM 393
 821  CONTINUE                                                           CHEM 394
C                                                                        CHEM 395
C-----RIN=THE RATIO OF THE MASS OF THE SOLID MATRIX                      CHEM 396
C     TO THE MASS OF THE FLOWING GASES AT THE                            CHEM 397
C     PREVIOUS TEMPERATURE STATION.                                      CHEM 398
C                                                                        CHEM 399
C                                                                        CHEM 400
C-----ROUT=THE SAME RATIO AT AN INCREMENT OF TEMPERA-                    CHEM 401
C     TURE DOWN THE FLOW FIELD.                                          CHEM 402
C     TO INITIALIZE, ROUT IS SET EQUAL TO RIN.                           CHEM 403
C                                                                        CHEM 404
      ROUT=RIN                                                           CHEM 405
C                                                                        CHEM 406
C-----RECOMPUTE THE MATFRIAL BALANCE CONSTRAINTS.                        CHEM 407
C                                                                        CHEM 408
```

```
      DO79J=1,MM                                                        CHEM 409
      BB(J)=0.                                                          CHEM 410
      DO79I=1,NQ                                                        CHEM 411
 79   BB(J)=BB(J)+AA(I,J)*Y(I)                                          CHEM 412
      GOTO171                                                           CHEM 413
 823  ROUT=0.                                                           CHEM 414
      DO824I=LL,NQ                                                      CHEM 415
 824  ROUT=ROUT+XMOL(I)*XMW(I)/XMWGAS                                   CHEM 416
      RATIO=(1.+RIN)/(1.+ROUT)                                          CHEM 417
C                                                                       CHEM 418
C     RATIO IS THE FRACTION GAIN OR LOSS OF SOLID                       CHEM 419
C     MATERIAL BY THE FLOWING GASES.                                    CHEM 420
C                                                                       CHEM 421
      W=W*RATIO                                                         CHEM 422
      RIN=ROUT                                                          CHEM 423
 171  TABLE(KPT,1)=T                                                    CHEM 424
      TABLE(KPT,3)=XMWGAS                                               CHEM 425
      TABLE(KPT,4)=W                                                    CHEM 426
      PRINT 172,W,T                                                     CHEM 427
 172  FORMAT(1X,'W='E15.7,E20.7)                                        CHEM 428
      TABLE(KPT,5)=CPMX                                                 CHEM 429
C                                                                       CHEM 430
C                                                                       CHEM 431
C-----CALCULATION AND STORAGE OF THE INDIVIDUAL MASS                    CHEM 432
C     FLUXES AT EVERY TEMPERATURE IN VARIABLE FLUX(J,I)                 CHEM 433
C     FOLLOWS. THESE STORED VALUES ARE USED SUBSEQUENT-                 CHEM 434
C     LY TO COMPUTE THE DERATIVE OF FLUX(J,I)WITH TEM-                  CHEM 435
C     PERATURE, WHICH IS DFLUX(J,I). THIS VARIABLE IS                   CHEM 436
C     USED TO COMPUTE A VARIABLE CALL REACT, WHICH ACCOUNTS             CHEM 437
C     FOR THE HEAT EFFECTS OF THE CHEMICAL REACTIONS.                   CHEM 438
C     NOTICE THAT THE REACT TERM HAS TO BE MULTIPLYED BY                CHEM 439
C     THE GRADIENT OF TEMPERATURE WITH DISTANCE. THIS OPE-              CHEM 440
C     RATION IS PERFORMED IN THE MAIN PROGRAM.                          CHEM 441
C                                                                       CHEM 442
```

```
C                                                                       CHEM 443
      IF(IPRINT .EQ. 0) GO TO 1804                                      CHEM 444
      PRINT204                                                          CHEM 445
 204  FORMAT(//6X,'I',21X,'Y(I)',9X,'MOLE FRACTION',5X,                 CHEM 446
     1'MASS FRACTION')                                                  CHEM 447
 1804 DO1712I=1,NQ                                                      CHEM 448
      FLUX(KPT,I)=W*XMASS(I)                                            CHEM 449
      IF(IPRINT .EQ. 0) GO TO 1712                                      CHEM 450
      PRINT19,I,SPCIE1(I),SPCIE2(I),Y(I),XMOL(I),XMASS(I),FLUX(KPT,I)   CHEM 451
 1712 CONTINUE                                                          CHEM 452
 19   FORMAT(1X,I6,3X,2A3,2X,4E18.7)                                    CHEM 453
      DO1713I=6,KOS                                                     CHEM 454
      II=I-5                                                            CHEM 455
C                                                                       CHEM 456
C     THE UNITS OF FLUX(KPT,I) ARE LBS/FT2-SEC.                         CHEM 457
C                                                                       CHEM 458
 1713 TABLE(KPT,I)=XMOL(II)                                             CHEM 459
      IF(T.GE.TMAX)GOTO333                                              CHEM 460
      T=T+TINC                                                          CHEM 461
      GOTO500                                                           CHEM 462
C                                                                       CHEM 463
C-----THE MOLE FRACTIONS AT EVERY TEMPERATURE UP TO TMAX                CHEM 464
C     HAVE BEEN STORED. THESE STORED VALUES WILL NOW BE                 CHEM 465
C     USED TO COMPUTE THE DERIVATIVE OF FLUX. THAT IS, THE              CHEM 466
C     RATE OF CHANGE OF THE MASS FLOW RATE WITH TEMPERATURE.            CHEM 467
C     THIS RATE OF CHANGE WILL BE STORED IN VARIABLE DFLUX(J,I).        CHEM 468
C     THE UNITS OF DFLUX(J,I) ARE, LBS/FT2-SEC OK                       CHEM 469
C                                                                       CHEM 470
 333  KPT3=KPT-3                                                        CHEM 471
      TINC60=1./(60.*TINC)                                              CHEM 472
      KOUNT=2                                                           CHEM 473
      DO1717J=1,KPT3                                                    CHEM 474
      DO1716I=1,NQ                                                      CHEM 475
      IF(J.GT.2)GOTO1715                                                CHEM 476
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      IF(J.GT.1)GOTO1714                                                CHEM 477
      DFLUX(J,I)=(1./(60.*TINC))*(-137.*FLUX(J,I)+300.*FLUX(J+1,I)      CHEM 478
     1-300.*FLUX(J+2,I)+200.*FLUX(J+3,I)-75.*FLUX(J+4,I)                CHEM 479
     2+12.*FLUX(J+5,I))                                                 CHEM 480
      GOTO1716                                                          CHEM 481
 1714 DFLUX(J,I)=TINC60*(-12.*FLUX(J-1,I)-65.*FLUX(J,I)+120.*FLUX(J+1,I)CHEM 482
     1-60.*FLUX(J+2,I)+20.*FLUX(J+3,I)-3.*FLUX(J+4,I))                  CHEM 483
      GO TO 1716                                                        CHEM 484
 1715 DFLUX(J,I)=TINC60*(3.*FLUX(J-2,I)-30.*FLUX(J-1,I)-20.*FLUX(J,I)   CHEM 485
     1+60.*FLUX(J+1,I)-15.*FLUX(J+2,I)+2.*FLUX(J+3,I))                  CHEM 486
 1716 CONTINUE                                                          CHEM 487
 1717 CONTINUE                                                          CHEM 488
C                                                                       CHEM 489
C-----CALCULATE THE HEAT TERM NECESSARY FOR GROUP                       CHEM 490
C                                                                       CHEM 491
C     IN THE MAIN PROGRAM.                                              CHEM 492
      DO1722J=1,KPT3                                                    CHEM 493
      HEAT=0.                                                           CHEM 494
      PRINT 1718,J                                                      CHEM 495
 1718 FORMAT(1X,'J='I3/)                                                CHEM 496
      PRINT 1719,(DFLUX(J,I),I=1,NQ)                                    CHEM 497
 1719 FORMAT(1X,8E15.7)                                                 CHEM 498
      T=TABLE(J,1)                                                      CHEM 499
      CALL THERM1                                                       CHEM 500
      DO1721I=1,NQ                                                      CHEM 501
      IF(I.LE.NN)GOTO1720                                               CHEM 502
      HEAT=HEAT+DFLUX(J,I)*ENT(I)*(1.-EPS)/XMW(I)                       CHEM 503
      GOTO1721                                                          CHEM 504
 1720 HEAT=HEAT+DFLUX(J,I)*ENT(I)*EPS/XMW(I)                            CHEM 505
 1721 CONTINUE                                                          CHEM 506
 1722 TABLE(J,2)=HEAT                                                   CHEM 507
C     THE UNITS OF HEAT ARE BTU/FT2-SEC OF                              CHEM 508
      RETURN                                                            CHEM 509
      END                                                               CHEM 510
```

```
      SUBROUTINE FRNERG(T,NQ)                                           FRNE   1
C                                                                       FRNE   2
C     THIS SUBPROGRAM CALCULATES THE FREE ENERGY FUNCTION               FRNE   3
C     AND THE HEAT CAPACITY OF EACH INDIVIDUAL SPECIE.                  FRNE   4
      COMMON/KB/AI(30),BI(30),CI(30),DI(30),EI(30),FI(30),GI(30),       FRNE   5
     1AII(30),BII(30),CII(30),DII(30),EII(30),FII(30),GII(30),           FRNE   6
     2TLOW(30)                                                          FRNE   7
      COMMON/KGG/FORT(30),CP(30)                                        FRNE   8
      DO2I=1,NQ                                                         FRNE   9
      IF(T.GT.TLOW(I))GOTO1                                             FRNE  10
      FORT(I)=AII(I)*(1.-ALOG(T))-((((EII(I)/20.)*T+DII(I)/12.)*T+      FRNE  11
     1CII(I)/6.)*T+BII(I)/2.)*T+FII(I)/T-GII(I)                         FRNE  12
      CP(I)=AII(I)+(((EII(I)*T+DII(I))*T+CII(I))*T+BII(I))*T            FRNE  13
      GOTO2                                                             FRNE  14
 1    FORT(I)=AI(I)*(1.-ALOG(T))-((((EI(I)/20.)*T+DI(I)/12.)*T+         FRNE  15
     1CI(I)/6.)*T+BI(I)/2.)*T+FI(I)/T-GI(I)                             FRNE  16
      CP(I)=AI(I)+(((EI(I)*T+DI(I))*T+CI(I))*T+BI(I))*T                 FRNE  17
 2    CONTINUE                                                          FRNE  18
      RETURN                                                            FRNE  19
      END                                                               FRNE  20
```

```
      SUBROUTINE MATINV(A,N,B,M)                                        MATI   1
C                                                                       MATI   2
C                                                                       MATI   3
C                                                                       MATI   4
C                                                                       MATI   5
C     MATRIX INVERSION WITH ACCOMPANYING SOLUTION OF LINEAR EQUATIONS   MATI   6
C                                                                       MATI   7
C                                                                       MATI   8
      DIMENSION A(6,6),B(6,1),IPIVOT(6),INDEX(6,2)                      MATI   9
      EQUIVALENCE (IROW,JROW), (ICOLUM,JCOLUM), (AMAX,T,SWAP)           MATI  10
C                                                                       MATI  11
C     INITIALIZATION                                                    MATI  12
C                                                                       MATI  13
    5 ISCALE=0                                                          MATI  14
    6 R1=10.0**18                                                       MATI  15
    7 R2=1.0/R1                                                         MATI  16
   10 DETERM=1.0                                                        MATI  17
   15  DO 20 J=1,N                                                      MATI  18
   20 IPIVOT(J)=0                                                       MATI  19
   30 DO 550 I=1,N                                                      MATI  20
C                                                                       MATI  21
C     SEARCH FOR PIVOT ELEMENT                                          MATI  22
C                                                                       MATI  23
   40 AMAX=0.0                                                          MATI  24
   45 DO 105 J=1,N                                                      MATI  25
   50 IF (IPIVOT(J)-1)60,105,60                                         MATI  26
   60 DO 100 K=1,N                                                      MATI  27
   70 IF (IPIVOT(K)-1)80,100,740                                        MATI  28
   80 IF (ABS(AMAX)-ABS(A(J,K)))85,100,100                              MATI  29
   85 IROW=J                                                            MATI  30
   90 ICOLUM=K                                                          MATI  31
   95 AMAX=A(J,K)                                                       MATI  32
  100 CONTINUE                                                          MATI  33
  105 CONTINUE                                                          MATI  34
```

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      IF (AMAX)110,106,110                                              MATI  35
  106 DETERM=0.0                                                        MATI  36
      ISCALE=0                                                          MATI  37
      GO TO 740                                                         MATI  38
  110 IPIVOT(ICOLUM)=IPIVOT(ICOLUM)+1                                   MATI  39
C                                                                       MATI  40
C     INTERCHANGE ROWS TO PUT PIVOT ELEMENT ON DIAGONAL                 MATI  41
C                                                                       MATI  42
  130 IF (IROW-ICOLUM)140,260,140                                       MATI  43
  140 DETERM=-DETERM                                                    MATI  44
  150 DO 200 L=1,N                                                      MATI  45
  160 SWAP=A(IROW,L)                                                    MATI  46
  170 A(IROW,L)=A(ICOLUM,L)                                             MATI  47
  200 A(ICOLUM,L)=SWAP                                                  MATI  48
  205 IF(M)260,260,210                                                  MATI  49
  210 DO 250 L=1,M                                                      MATI  50
  220 SWAP=B(IROW,L)                                                    MATI  51
  230 B(IROW,L)=B(ICOLUM,L)                                             MATI  52
  250 B(ICOLUM,L)=SWAP                                                  MATI  53
  260 INDEX(I,1)=IROW                                                   MATI  54
  270 INDEX(I,2)=ICOLUM                                                 MATI  55
  310 PIVOT=A(ICOLUM,ICOLUM)                                            MATI  56
C                                                                       MATI  57
C     SCALE THE DETERMINANT                                             MATI  58
C                                                                       MATI  59
 1000 PIVOTI=PIVOT                                                      MATI  60
 1005 IF(ABS(DETERM)-R1)1030,1010,1010                                  MATI  61
 1010 DETERM=DETERM/R1                                                  MATI  62
      ISCALE=ISCALE+1                                                   MATI  63
      IF(ABS(DETERM)-R1)1060,1020,1020                                  MATI  64
 1020 DETERM=DETERM/R1                                                  MATI  65
      ISCALE=ISCALE+1                                                   MATI  66
      GO TO 1060                                                        MATI  67
 1030 IF(ABS(DETERM)-R2)1040,1040,1060                                  MATI  68
```

```
 1040 DETERM=DETERM*R1                                                  MATI  69
      ISCALE=ISCALE-1                                                   MATI  70
      IF(ABS(DETERM)-R2)1050,1050,1060                                  MATI  71
 1050 DETERM=DETERM*R1                                                  MATI  72
      ISCALE=ISCALE-1                                                   MATI  73
 1060 IF(ABS(PIVOTI)-R1)1090,1070,1070                                  MATI  74
 1070 PIVOTI=PIVOTI/R1                                                  MATI  75
      ISCALE=ISCALE+1                                                   MATI  76
      IF(ABS(PIVOTI)-R1)320,1080,1080                                   MATI  77
 1080 PIVOTI=PIVOTI/R1                                                  MATI  78
      ISCALE=ISCALE+1                                                   MATI  79
      GO TO 320                                                         MATI  80
 1090 IF(ABS(PIVOTI)-R2)2000,2000,320                                   MATI  81
 2000 PIVOTI=PIVOTI*R1                                                  MATI  82
      ISCALE=ISCALE-1                                                   MATI  83
      IF(ABS(PIVOTI)-R2)2010,2010,320                                   MATI  84
 2010 PIVOTI=PIVOTI*R1                                                  MATI  85
      ISCALE=ISCALE-1                                                   MATI  86
  320 DETERM=DETERM*PIVOTI                                              MATI  87
C                                                                       MATI  88
C     DIVIDE PIVOT ROW BY PIVOT ELEMENT                                 MATI  89
C                                                                       MATI  90
  330 A(ICOLUM,ICOLUM)=1.0                                              MATI  91
  340 DO 350 L=1,N                                                      MATI  92
  350 A(ICOLUM,L)=A(ICOLUM,L)/PIVOT                                     MATI  93
  355 IF(M) 380,380,360                                                 MATI  94
  360 DO 370 L=1,M                                                      MATI  95
  370 B(ICOLUM,L)=B(ICOLUM,L)/PIVOT                                     MATI  96
C                                                                       MATI  97
C     REDUCE NON-PIVOT ROWS                                             MATI  98
C                                                                       MATI  99
  380 DO 550 L1=1,N                                                     MATI 100
  390 IF(L1-ICOLUM)400,550,400                                          MATI 101
  400 T=A(L1,ICOLUM)                                                    MATI 102
```

```
  420 A(L1,ICOLUM)=0.0                                                  MATI 103
  430 DO 450 L=1,N                                                      MATI 104
  450 A(L1,L)=A(L1,L)-A(ICOLUM,L)*T                                     MATI 105
  455 IF(M) 550,550,460                                                 MATI 106
  460 DO 500 L=1,M                                                      MATI 107
  500 B(L1,L)=B(L1,L)-B(ICOLUM,L)*T                                     MATI 108
  550 CONTINUE                                                          MATI 109
C                                                                       MATI 110
C     INTERCHANGE COLUMNS                                               MATI 111
C                                                                       MATI 112
  600 DO 710 I=1,N                                                      MATI 113
  610 L=N+1-I                                                           MATI 114
  620 IF(INDEX(L,1)-INDEX(L,2))630,710,630                              MATI 115
  630 JROW=INDEX(L,1)                                                   MATI 116
  640 JCOLUM=INDEX(L,2)                                                 MATI 117
  650 DO 705 K=1,N                                                      MATI 118
  660 SWAP=A(K,JROW)                                                    MATI 119
  670 A(K,JROW)=A(K,JCOLUM)                                             MATI 120
  700 A(K,JCOLUM)=SWAP                                                  MATI 121
  705 CONTINUE                                                          MATI 122
  710 CONTINUE                                                          MATI 123
  740 RETURN                                                            MATI 124
      END                                                               MATI 125
```

ABLATIN1 ANALYSIS NOMENCLATURE

MAIN

AA(I,J): Formula number. Gives the gram atoms of element J in species I.

AI...GI: These are the seven empirical constants for the high temperature fit (1000°K-6000°K) for the free energy functions. The first five constants (AI through EI) are used in the heat capacity fit.

AII...GII: These are the seven empirical constants for the low temperature fit (300°K-1000°K) for the free energy function.

A11...A66: These are the six empirical constants for the enthalpy fit of the constituent elements (300°K-1000°K).

ALPHA: Viscous coefficient in Darcy's equation (FT^{-1}).

AVGFW: Average molecular weight of the gas mixture.

BETA: Inertial coefficient in Darcy's equation ($1/FT^2$).

CDO: Thermal conductivity of the char (BTU/FT-sec-°F).

CDOV: Thermal conductivity of the virgin material, (BTUft/sec-°F).

CPB1: Total rate of heat absorbed by the gases in the char zone (BTU/ft^2-sec).

CPB2: Total rate of heat absorbed by the solids in the char zone (BTU/ft^2-sec).

CPS: Heat capacity of the char (BTU/lb-°F).

CPV: Heat capacity of the virgin material (BTU/lb-^{o}F).

DCDO: Rate of change of the thermal conductivity of the char with temperature (BTU/ft-sec-^{o}F^{2}).

DCDOV: Rate of change of the thermal conductivity of the virgin material with temperature (BTU/ft-sec-^{o}F^{2}).

DELTF: Differential change in temperature in ^{o}F for an increment of distance H.

DELTK: Differential change in temperature in ^{o}K for an increment of distance H.

DELTP: Pressure drop across the char (lbs/ft^{2}).

DELZ: Increment of distance (in feet).

DISTAN: Char thickness in feet.

DT: Temperature gradient (^{o}F/ft).

DTC: Temperature gradient in the char (^{o}F/ft).

DTCC: Temperature gradient in double precision arithmetic in the char (^{o}F/ft).

DTCI: Temperature gradient in the virgin material (^{o}F/ft).

EK: Potential parameter /Boltzman constant.

EMIS: Char emissivity.

EPS: Porosity of the char (ft^{2}voids/ft^{2} total).

FW(I): Molecular weight of species I.

GASCP: Is the heat capacity of the gas mixture in (BTU/lb-^{o}F).

GROUP: This is the bracketted term of Equation (3-36) (1/ft).

H: Runge-Kutta step size (in feet).

H11: Runge-Kutta step size in double precision arithmetic (in feet).

HCHAR: Percent of total heat absorbed in the char zone.

HDECOM: Percent of total heat absorbed in the decomposition zone.

HGAS: Percent of heat absorbed by the gas in the char zone.

HI: Initial value of Runge-Kutta step (in feet).

HREACT: Percent of heat absorbed by the reactions in the char zone.

HSOLID: Percent of heat absorbed in the solids in the char zone.

ICODE(I): Is a code to identify whether a species is a gas, or a solid. If ICODE is zero, the species is a gas. If ICODE is one, the species is a solid.

IMAX: Number of data points for EK.

ITEMP: Total number of temperature points stored in temperature profile.

JCODE(J): Is a code used to determine whether the reference state of the constituent element J is in the gas or in the solid state.

JS: Total number of slices in which the char is divided for the solution of the momentum equation.

K1: Is a counter for the number of temperature points stored during the solution of the energy equation.

MM: Is the number of elements.

NC: Number of gas species read in.

NDATA: Number of collision integral points tabulated versus XTKE.

NN: Number of gas species in the system.

NN5: Is the total number of variables stored in Table (I,J).

NNS: Is the number of solid species in the system.

NQ: Is the total number of gas and solid species in the system.

NS: Is the total number of gas and solid species read in.

OMGA: Interpolated value of XTKE.

P: Pressure in lbs/ft^2.

PL: Pressure at the front surface of the char (lbs/ft^2).

Q: Is the rate of heat absorbed in the decomposition zone in (BTU/ft^3-sec).

Q2: It equals Q/DTC (BTU/ft^2-sec-^oF).

QA: Aerodynamic heating rate (BTU/ft^2-sec). Equals QL+QR .

QCZ: Heat flux in the char zone (BTU/ft^2-sec).

QCZI: Heat flux in the decomposition zone (BTU/ft^2-sec).

QL: Is the total heat flux at the surface (BTU/ft^2-sec).

QR: Is the rate of re-radiation from the surface of the char (BTU/ft^2-sec).

REAC1: Is the total rate of heat absorbed by the chemical reactions (BTU/ft^2-sec).

REAC2: Heat absorbed by the chemical reactions (BTU/ft^2-sec).

REACT: Equals REAC2/DTC (BTU/ft^2-sec-^{o}F).

RHO: Bulk density of the virgin material (lbs/ft^3).

ROCHAR: Bulk density of the char material (lbs/ft^3).

RR: Gas constant: 1.98726 (BTU/lb-mole^{o}R).

S1...S6: These are six empirical constants for the enthalpy fit of the constituent elements (1000°K-6000°K).

SIG: Collision diameter (Angstrongs).

SIGMA: Stephan-Boltzman constant (4.81×10^{-13} BTU/ft^2-sec-^{o}F^4).

T1(K1): Variable in which the temperature profile is stored versus distance Z. K1 is a counter.

TC: Temperature in ^{o}F.

TCHAR: Temperature at which all the virgin material has degraded to gas and char. (^{o}K).

TFMAX: Maximum specified temperature of the front surface of the char (^{o}F).

THICK: Is the thickness of the char zone, in inches.

THICK1: Is the thickness of the decomposition zone in inches.

TK: Interpolated value of the temperature (in ^{o}K) at a distance Z in the char.

TL: Front surface temperature of the char (^{o}F) when the temperature profile has been defined.

TLOW(I): Maximum temperature of low temperature fit for species I. (^{o}K).

TO: Initial temperature (^{o}F) at Z=0.

TPREV: Temperature (^{o}F) at the previous step.

TTTT: This is the temperature (^{o}F) in double precision arithmetic. A provision has been made in the program that if the step size is less than 8. x10^{-9} ft., the Runge-Kutta analysis is calculated in double precision arithmetic to reduce round-off error.

TVAR: Temperature in ^{o}K.

TVIS: Interpolated value of the temperature profile (^{o}F) at a distance Z along the char.

VISCOS: Viscocity of the gas (in centipoise).

VR: Surface recession velocity (ft/sec).

W: Mass flux based on the total area (lbs/ft^2-sec).

WI: Mass flux of the gases entering the char based on the total area (lbs/ft^2-sec).

XTKE: Product of the temperature in ^{o}K and 1/EK.

YCOMP(I,J): Array to store the concentration profile.

Y(I): Mole fraction of species I.

YI(I): Initial mole fraction of species I.

Z: Distance along the decomposition zone or the char zone (ft).

ZINC: Increment of distance at which the temperature profile is stored (ft).

ZMAX: Maximum allowable thickness of the char zone. (Usually 0.25 inches).

ZZ: Distance of Z in double precision arithmetic (ft).

INDPTH

This subroutine calculates the physical properties of

the virgin material and the pyrolysis gases.

A...E: These are five empirical constants for the heat capacity of the virgin material.

TELTKK: Increment of temperature (^{o}K).

PHMCR

This subroutine computes the heat absorbed by the decomposition of the phenolic resin and phenolic microballoons.

AREA: This is the area generated by a plot of calories versus temperature (^{o}K) by the decomposition of phenolic resin during a differential thermal analysis (1350 cal/^{o}K).

AREA1: This is the area generated by a plot of calories versus temperature (^{o}K) by the decomposition of phenolic microballoons during a differential thermal analysis (1464 cal/^{o}K).

A(I)...E(I): These are five empirical constants used to fit a curve through a portion of the plot of calories versus temperature for the phenolic microballoons.

DT: Is the temperature difference in ^{o}K from a base temperature of 350°C(623°K). Below 350°C, decomposition of the virgin material has not been initiated.

DELT: Is the temperature increment (^{o}K) for an increment of the Runge-Kutta Step.

H: Is the height (in calories) for the plot of calories versus temperature (^{o}K).

K6: Is a code used to bypass the read statements. When K6 is one, the data is read in. When K6 is two, the read

statements are bypassed.

NUMBER: Is the number of fits used for the plots of calories versus temperature.

QMICRO: Heat absorbed by the decomposition of the phenolic microballoons (calories/gram).

QPHNLC: Heat absorbed by the decomposition of the phenolic resin (calories/gram).

NYLON:

This subroutine calculates the heat ab sorbed by the decomposition of nylon.

AREA: This is the area generated by a plot of calories versus temperature (^{o}K) for the decomposition of nylon (1122 calories / ^{o}K) during a differential thermal analysis.

QNYLON: Heat absorbed by the decomposition of nylon (calories/gram).

DNSITY:

This subroutine calculates the density change of phenolic nylon and the mass flux of the pyrolysis gas.

A(J): Frequency factor of reaction J (sec^{-1}).

COMPST: Is an integer variable giving the number of composite in the ablator. In the case of phenolic nylon, it is three.

DELFLX(I): Is the change in mass flux of composite I due to degradation (lbs/ft^2-sec).

DRHO: Differential change in density due to degradation.

This variable is used as a criteria for stability while the solution is marching through the decomposition zone (lbs/ft^3).

DRHODT(I): Rate of gas generation by the degradation of composite I (lbs/ft^3-sec).

E(J): Energy of activation of reaction J used to describe the degradation of the composite (Joules/gram-mole).

MASFLX(I): Rate of change of mass flux due to the degradation of composite I (lbs/ft^2-sec).

MASFRC(I): Mass fraction of each composite in the mixture of virgin material.

NREACT: Number of pseudo-order kinetic reactions used to describe the decomposition of the virgin material composite.

RATER(J): Is specific reaction velocity of reaction J (lbs/ft^3-sec).

RHO: Bulk density of the composite (lbs/ft^3).

RHOC(I): Residual density of composite I (lbs/ft^3).

RHOCC(I): Lowest value of residual density of composite I (lbs/ft^3).

RHOI(I): Initial density of composite I (lbs/ft^3).

RHOII: Initial density of the virgin composite (lbs/ft^3).

RHOT(I): Density of composite I at temperature T (lbs/ft^3).

VOLFRC(I): Volume fraction of each composite I.

CHARPR:

This subroutine calculates the effective thermal conductivity and the heat capacity of the char.

T: Temperature in ^{o}R.

INTRPL:

This program performs Lagrangian interpolation with non-equal step size between points.

F: Dependent variable array.

IMAX: Number of points in array.

SOM: Value of the interpolated dependent variable.

VAR: Value of X for which corresponding value of F is derived by interpolation.

X: Independent variable array.

THERM1:

This subroutine calculates the heat of formation of each chemical specie, the heat capacity of the mixture and the heat absorbed by the chemical reactions.

CPDT1: Is the sensible enthalpy gain by the constituent elements from a reference temperature of 298.16^{o}K (calories/gram-mole).

CPMX: Heat capacity of the gas mixture (calories/gram-mole ^{o}K).

ENT1(I): Enthalpy of species I (calories/gram-mole).

ENT(I): Heat of formation of species I (calories/gram-mole).

HEAT1: Rate of heat generated, or absorbed, by the chemical reactions (calories/cm^3-sec).

KINET:

This program computes the rate of reaction of each chemical species.

AEF(J): Activation energy of reaction J (calories/gram-mole.

AF(J): Frequency factor of reaction J (sec^{-1}).

DELZZ: Runge-Kutta step size (cm.).

DLFLUX(I): Differential change in molal flux due to the chemical reaction of species I. This variable is used for the purpose of controlling the step size (gram-mole/cm^2-sec).

FLUXMO(I): Molal flux of each chemical species I (gram-moles/cm^2-sec).

HEAT: Rate of heat generated or absorbed by the chemical reactions (BTU/ft^3-sec).

K2: Is a counter to keep track of the number of temperature points stored in Table (I,J).

K7: When K7 is one, initialization occurs and subroutine INOUT is called. When it is 2, this is bypassed.

KOS: Total number of variables stored in the Table (I,J) array.

KSP: Number of gas components in the chemical system.

KSP1: Number of gas and solid species in the chemical system.

NPEX(I,J): Power on the concentration of product I in

reaction J.

P: Pressure of the system in atmosphere.

PERCE(J): Mole percent of species J.

PSC(I,J): Stochiometric coefficient of the product I in reaction J.

R: Gas constant (82.06 cm^3-atm/gram-mole ^oK).

RATE(J): Rate of formation of species I (gram-moles/ cm^3-sec).

RATER(J): Specific reaction velocity of reaction J (gram-moles/cm^3-sec).

RK(J): Reverse reaction rate constant of reaction J.

RR: Gas constant (1.98726 calories/gram-mole ^oK).

SF(J): Power on the temperature of the Arrhenius type kinetic expression.

SPCIE1(J): Specie identification name.

T: Temperature (^oK).

TABLE(I,J): Is an array where I represents the number of variables stored and J the number of temperature points. The variables stored are in the following order: T, HEAT, WNEW, AVGFW AND KSP1 values of Y1(I).

TESS: Is the absolute maximum value of DLFLUX(I). This variable is used in controlling the step size for stability.

TF: Temperature (^oF).

TPREV: Is the previous value of the temperature (^oK).

WNEW: Total mass flux of the gases (lbs/ft^2-sec).

XMW (I): Molecular weight of species I.

Y1(I): Mole fraction of species I.

INPUT:

This subroutine reads in the kinetic data.

AK(J): Empirical constant for the fit of the equilibrium constant with temperature.

BK(J): Empirical constant for the fit of the equilibrium constant with temperature.

EKMAX(J): Maximum allowable value for the equilibrium constant of reaction J.

EKMIN(J): Minimum allowable value for the equilibrium constant of reaction J.

NCOEF(J): Is the sum of the stochiometric coefficient of the products minus the reactants.

INPUT FORMAT: A Typical Input for Equilibrium Flow.*

CARD-1:	FORMAT (5I6)	COLUMNS:
NC = 19		1-6
NNS = 1		7-12
MM = 4		13-18
KODE = 1		19-24
KEY = 2		25-30

CARD-2:	FORMAT (F10.3, 10X, 4F10.3)	
PL = 2160.		1-10
TO = 500		21-30
EPS = .8		31-40
ZL = .35		41-50
HI = .000007		51-60

CARD-3:	FORMAT(3EL5.5, F15.5)	
ALPHA = .5E9		1-15
BETA = .5E5		16-30
SIGMA = .48E-12		31-45
EMIS = .90		46-60

CARD-4	FORMAT (3E10.3)	
DTC = 3000.		1-10
TCHAR = 1073.		11-20
VT = 1.E-3		21-30

*See Table B-2 for the complete input data set.

CARD-5 FORMAT (6E10.3, I3)	COLUMNS
S1(1) = 1.363250E0	1-10
S2(1) = 1.85605E-3	11-20
S3(1) = -7.6675E-7	21-30
S4(1) =.151043E-9	31-40
S5(1) = -1.139E-14	41-50
S6(1) = -6.46972E2	51-60
JCODE(1) = 1	61-63

CARD-6 FORMAT (6E10.3)	
A11(1) = -.712442E0	1-10
A22(1) = 7.34065E-3	11-20
A33(1) = -5.5262E-6	21-30
A44(1) = 1.51400E-9	31-40
A55(1) = -2.382E-14	41-50
A66(1) = -6.80533E1	51-60

CARD-5 and CARD-6 are read sequentially MM times as is specified in CARD-1. For this particular example MM = 4.

CARD-7 FORMAT (10X, 3E10.3, 2X, 2A3, I4)	
TLOW (1) = 1000.	11-20
FW(1) = 1.008	21-30
YI(1) = .739503E-7	31-40
SPCIE 1(1) =	43-45
SPCIE 2 (1) = H	46-48
ICODE(1) = 0	49-52

CARD-8 FORMAT (7E10.3)	COLUMNS
AI(1) = 2.500000E0	1-10
BI(1) = 0.	11-20
CI(1) = 0.	21-30
DI(1) = 0.	31-40
EI(1) = 0.	41-50
FI(1) = 2.547050E4	51-60
GI(1) = -4.6001E-1	61-70

CARD-9 FORMAT (7E10.3)	
AII(1) = 2.500000E0	1-10
BII(1) = 0.	11-20
CII(1) = 0.	21-30
DII(1) = 0.	31-40
EII(1) = 0.	41-50
FII(1) = 2.547050E-4	51-60
GII(1) = 4.6001E-1	61-70

CARD-10 FORMAT (4E10.3)	
AA(1,1) = 0.	1-10
AA(1,2) = 1.	11-20
AA(1,3) = 0.	21-30
AA(1,4) = 0.	31-40

CARD-7, CARD-8, CARD-9 and CARD-10 are read in sequentially as a group, (NC+NNS) number of times. Only the data for Specie 1, in this case hydrogen atoms, is presented.

	COLUMNS
CARD-11 FORMAT (2F15.5)	
EK(1) = 33.3	1-15
SIG(1) = 2.986	16-30

CARD-11 is read NC number of times as specified by CARD-1.

CARD-12 FORMAT (I6)	
NDATA = 34	1-6

CARD-13 FORMAT (2F15.5)	
XTKE(1) = 0.30	1-15
ZOMGA(1) = 2.785	16-30

CARD-13 is repeated NDATA number of times as specified by CARD-12.

CARDS-1 through 13 are read in the MAIN program. These cards define the physical conditions of the system. In addition they provide the thermodynamic data and the physical constants for the pyrolysis species. CARDS-14 through 19 provide the thermophysical information for the virgin material and also the kinetic data for the degradation of the polymer.

CARD-14 FORMAT (5E12.6)	
A = 0.37000070E0	1-12
B = 0.7367133E-4	13-24
C = 0.1532518E-5	25-36
D = -.1962704E-8	37-48
E = .8857809E-12	49-60

CARD-14 is read in subroutine INDPTH.

CARD-15	FORMAT (5E12.8)	COLUMNS
A(1) = 0.10561790E0		1-12
B(1) = -1.836062E-2		13-24
C(1) = 1.7580490E-3		25-36
D(1) = -1.678598E-5		37-48
E(1) = 4.7310570E-8		49-60

CARD-16	FORMAT (5E12.8)	
A1(1) = -.35642660E-1		1-12
B1(1) = 4.5790730E-2		13-24
C1(1) = 1.2298170E-4		25-36
D1(1) = -.8277667E-7		37-48
E1(1) = -.2279748E-7		49-60

CARD-15 and CARD-16 are read sequentially four times in subroutine PHMCR. For a thorough explanation on the sources of data for the phenolic resin see Appendix C.

CARD-17	FORMAT (2I6)	
COMPST = 3		1-6
NREACT = 7		6-12

Card-17 is read in subroutine DNSITY as well as CARDS 18 and 19.

CARD-18	FORMAT (4X, I6, 3E10.8)	
I = 1		5-10
A(1) = 8.3000E14		11-20
E(1) = 232.0		21-30

	COLUMNS
XN(I,1) = 1.0	31-40

CARD-18 is read NREACT number of times and the index in I changes from 1 through 3 depending on whether the data is for nylon or for phenolic or for the microballoons.

CARD-19 FORMAT (3E10.3)

RHOI(1) = 68.6	1-10
RHOC(1) = 5.145	11-21
MASFR(1) = 0.4	21-30

CARD-19 is repeated COMPST number of times.

CARD-20 FORMAT (I1)

IPRINT = 1

CARD-20 is read in subroutine CHEMEQ.

TABLE B-2. Typical Input Data for Equilibrium Analysis

```
                                                                                DATA   1
    19     1     4     1     2                                                  DATA   2
     2160.                500.        .8 0.3500000 .00000700 5500.              DATA   3
       .50000E9       .50000E5   .4805555E-12   0.90                            DATA   4
  3000.0E0   1073.00     2.E-3                                                  DATA   5
1.363252E01.85605E-3-7.6675E-7.151043E-9-1.139E-14-6.49672E2  1                 DATA   6
-.712442E07.34065E-3-5.5262E-61.51400E-9-2.382E-14-6.80533E1                    DATA   7
3.043690E06.11871E-4-7.3994E-9-2.033E-112.4594E-15-8.54910E2  0                 DATA   8
2.846085E04.19321E-3-9.6119E-69.51227E-9-3.309E-12-9.67253E2                    DATA   9
2.854576E01.59763E-3-6.2566E-7.113158E-9-7.690E-15-8.90174E2  0                 DATA  10
3.691615E0-1.3333E-32.65031E-6-.97688E-9-9.977E-14-1.06283E3                    DATA  11
3.597613E07.81456E-4-2.2387E-74.2490E-11-3.346E-15-1.19279E3  0                 DATA  12
3.718995E0-2.5167E-38.58374E-6-8.2999E-92.7082E-12-1.10577E3                    DATA  13
             1000.E0   1.008E0.739503E-7       H   0                            DATA  14
2.500000E0 0.00000E0 0.00000E0 0.00000E0 0.00000E02.547050E4-4.6001E-1          DATA  15
2.500000E0 0.00000E0 0.00000E0 0.00000E0 0.00000E02.547050E4-4.6001E-1          DATA  16
0.000000E0 1.00000E0 0.00000E0 0.00000E0                                        DATA  17
             1000.E0   2.016E0  4.577835      H2   0                            DATA  18
3.04369E00 6.1187E-4 -7.399E-9 -2.03E-11 2.459E-15-8.5491E02 -1.648E00          DATA  19
2.846085E04.1932E-03-9.6119E-69.5123E-09-3.309E-12-9.67254E2 -1.4118E0          DATA  20
0.000000E0 2.00000E0 0.00000E0 0.00000E0                                        DATA  21
             1000.E0  15.035E0.103791E-6     CH3   0                            DATA  22
2.802766E06.25045E-3-2.2892E-63.8993E-10-2.528E-141.578749E45.684117E0          DATA  23
3.399505E04.26783E-32.03327E-7-1.1548E-94.1288E-131.564979E42.703747E0          DATA  24
1.000000E0 3.00000E0 0.00000E0 0.00000E0                                        DATA  25
             1000.E0  16.043E0  .1604671     CH4   0                            DATA  26
 1.18000E0 1.0950E-2-4.0620E-6 7.137E-10-4.749E-14-9.8556E03 1.2506E01          DATA  27
4.249768E0-6.9127E-3 3.1602E-5-2.9715E-89.5103E-12-1.01866E4-9.1755E-1          DATA  28
 1.00000E0 4.0000E00 0.0000E00 0.0000E00                                        DATA  29
             1000.E0  26.038E0.390335E-7    C2H2   0                            DATA  30
 4.4966E00 5.2698E-3-1.840E-063.1054E-10-2.000E-142.5637E004-3.14481E0          DATA  31
7.90333E-1 2.3466E-2-3.5542E-5 2.7951E-8-8.448E-12 2.6255E04 1.4005E01          DATA  32
 2.00000E0 2.00000E0 0.00000E0 0.00000E0                                        DATA  33
             1000.E0  28.054E0.286425E-5    C2H4   0                            DATA  34
```

```
 3.5023E00 1.159E-02-4.4745E-6 7.945E-10-5.323E-14 4.5439E03 2.4667E00  DATA   35
1.120244E0 1.3906E-2 2.6568E-6-1.1560E-85.2387E-125.332889E3 1.58378E1  DATA   36
 2.00000E0 4.00000E0 0.00000E0 0.00000E0                                DATA   37
             1000.E0  30.070E0.208273E-5    C2H6   0                   DATA   38
.1430799E1.188898E-1-.70440E-5.118720E-8-.7445E-13-.114311E5.1401321E2  DATA   39
.2882039E1.103219E-1.119142E-4-.14832E-7.44749E-11-.116209E5.7597900E1  DATA   40
 2.00000E0 6.00000E0 0.00000E0 0.00000E0                                DATA   41
             1000.E0  28.016E0 0.1880617      N2   0                   DATA   42
2.854576E0 1.5976E-3-6.2566E-71.1316E-10-7.69E- 15-8.90174E2 6.39029E0  DATA   43
3.691615E0-1.3333E-32.65031E-6-9.769E-10-9.977E-14-1.06283E3 2.28750E0  DATA   44
0.000000E0 0.00000E0 2.00000E0 0.00000E0                                DATA   45
             1000.E0  17.032E0.261467E-3     NH3   0                   DATA   46
2.149399E06.49285E-3-2.2695E-63.7394E-10-2.361E-14-6.40196E3 9.23891E0  DATA   47
3.77162E00-4.8621E-49.8742E-06-9.5679E-93.1313E-12-6.72810E3 1.4654E00  DATA   48
0.00000E00 3.00000E0 1.00000E0 0.00000E0                                DATA   49
             1000.E0  27.027E0.206307E-4     HCN   0                   DATA   50
3.653803E03.44363E-3-1.2585E-62.1692E-10-1.430E-141.442180E42.372602E0  DATA   51
2.168115E01.07290E-2-1.5088E-51.19330E-8-3.700E-121.468290E49.281020E0  DATA   52
1.000000E0 1.00000E0 1.00000E0 0.00000E0                                DATA   53
             1000.E0  18.016E0 0.1063185     H20   0                   DATA   54
 2.67075E0 3.0317E-3 -8.535E-7 1.179E-10-6.197E-15-2.9889E04 6.88383E0  DATA   55
4.15650E00-1.7244E-35.6982E-06-4.5930E-91.4234E-12-3.02888E4-6.8616E-1  DATA   56
0.000000E0 2.00000E0 0.00000E0 1.00000E0                                DATA   57
             1000.E0  17.008E0 1.0000E-9      OH   0                   DATA   58
2.889554E09.98350E-4-2.1880E-71.9803E-11-3.845E-163.881179E35.559701E0  DATA   59
3.823470E0-1.1187E-31.24668E-6-2.103E-10-5.254E-143.585278E35.8253E-01  DATA   60
0.000000E0 1.00000E0 0.00000E0 1.00000E0                                DATA   61
             1000.E0  44.011E0 .02711201     CO2   0                   DATA   62
 4.4129E003.1923E-03 -1.298E-6 2.415E-10-1.674E-14-4.8944E04-7.2876E-1  DATA   63
2.170100E0 1.0378E-2-1.0734E-56.34592E-9-1.628E-12-4.83526E4 1.06644E1  DATA   64
 1.00000E0 0.00000E0 0.00000E0 2.00000E0                                DATA   65
             1000.E0  28.011E0 0.1077713      CO   0                   DATA   66
 2.9512E00 1.5526E-3-6.1911E-7 1.135E-10-7.788E-15-1.4232E04 6.5314E00  DATA   67
3.787133E0-2.171E-035.07573E-6-3.4738E-97.7217E-13-1.43635E4 2.63355E0  DATA   68
```

```
 1.00000E0 0.00000E0 0.00000E0 1.00000E0                                DATA  69
             1000.E0  26.019E0 1.0000E-9      CN   0                    DATA  70
3.602263E03.40862E-49.71624E-8-1.582E-11-4.142E-164.731037E43.552052E0  DATA  71
3.852814E0-2.7632E-36.85704E-6-5.413E-091.4906E-124.740969E42.971802E0  DATA  72
1.000000E0 0.00000E0 1.00000E0 0.00000E0                                DATA  73
             1000.E0  25.030E0 1.0000E-9     C2H   0                    DATA  74
.3513479E1.358906E-2-.13231E-5.230520E-9-.1530E-13.5788759E5.4523285E1  DATA  75
.3006269E1.553788E-2-.35112E-5.124860E-8-.1896E-12.5796960E5.6920349E1  DATA  76
2.000000E0 1.00000E0 0.00000E0 0.00000E0                                DATA  77
             1000.E0  37.041E0 1.0000E-9     C3H   0                    DATA  78
.3964709E1.620030E-2-.22655E-5.371712E-9-.2262E-13.6283285E5.3467072E1  DATA  79
.2473840E1.117509E-1-.80448E-5.272896E-8-.3544E-12.6307721E5.1054254E2  DATA  80
3.000000E0 1.00000E0 0.00000E0 0.00000E0                                DATA  81
             1000.E0  39.052E0 1.0000E-9     C4H   0                    DATA  82
.5873679E1.740338E-2-.27289E-5.443720E-9-.2637E-13.7605163E5-.401004E1  DATA  83
.2695820E1.226768E-1-.24508E-4.131474E-7-.2673E-11.7648881E5.1039807E2  DATA  84
4.000000E0 1.00000E0 0.00000E0 0.00000E0                                DATA  85
             1000.E0  36.033E0 1.0000E-9      C3   0                    DATA  86
4.712474E02.90265E-3-1.2142E-62.2847E-10-1.599E-149.375270E4-2.53044E0  DATA  87
2.632587E09.41857E-3-9.5932E-65.57955E-9-1.424E-129.431148E48.078826E0  DATA  88
3.000000E0 0.00000E0 0.00000E0 0.00000E0                                DATA  89
             1000.E0  12.011E0  7.125731       C   1                    DATA  90
1.36325E001.85605E-3-7.6675E-71.5104E-10-1.139E-14-6.4967E02-7.9890E00  DATA  91
-7.1244E-17.34065E-3-5.5262E-6 1.514E-09-2.382E-14-6.80533E1 2.79326E0  DATA  92
 1.0000E00 0.00000E0 0.0000E00 0.0000E00                                DATA  93
           33.3          2.986     H                                   DATA  94
           33.3          2.986    H2                                   DATA  95
          136.5          3.822   CH3                                   DATA  96
          136.5          3.822   CH4                                   DATA  97
          185.0          4.221  C2H2                                   DATA  98
          205.0          4.232  C2H4                                   DATA  99
          230.0          4.418  C2H6                                   DATA 100
           91.5          3.681    N2                                   DATA 101
          356.0          2.649   H2O                                   DATA 102
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        335.          4.31    HCN                                  DATA 103
        312.0         3.432   NH3                                  DATA 104
        113.0         3.433    OH                                  DATA 105
        190.0         3.996   CO2                                  DATA 106
        110.0         3.590    CO                                  DATA 107
        335.          4.31     CN                                  DATA 108
        185.0         4.221  C2H                                   DATA 109
        185.0         4.221  C3H                                   DATA 110
        185.0         4.221  C4H                                   DATA 111
        185.0         4.221   C3                                   DATA 112
34                                                                 DATA 113
0.30          2.785                                                DATA 114
0.35          2.628                                                DATA 115
0.40          2.492                                                DATA 116
0.45          2.368                                                DATA 117
0.50          2.257                                                DATA 118
0.55          2.156                                                DATA 119
0.60          2.065                                                DATA 120
0.65          1.982                                                DATA 121
0.70          1.908                                                DATA 122
0.75          1.841                                                DATA 123
0.80          1.780                                                DATA 124
0.85          1.725                                                DATA 125
0.90          1.675                                                DATA 126
0.95          1.629                                                DATA 127
1.00          1.587                                                DATA 128
1.10          1.514                                                DATA 129
1.20          1.452                                                DATA 130
1.30          1.399                                                DATA 131
1.50          1.314                                                DATA 132
1.70          1.248                                                DATA 133
1.90          1.197                                                DATA 134
2.2           1.138                                                DATA 135
2.6           1.081                                                DATA 136
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    3.2             1.022                                                   DATA 137
  200.0             0.5320                                                  DATA 138
  400.0             0.4811                                                  DATA 139
0.3700070E0 0.7367133E-4 .1532518E-5-.1962704E-8.8857809E-12                DATA 140
0.1056179E0 -1.836062E-2 1.758049E-3-1.678598E-5 4.731057E-8                DATA 141
-.3564266E-1 4.579073E-2 1.229817E-4-.8277667E-7-.2279748E-7                DATA 142
173.99268E0 -4.816270E0 .50990242E-1-2.383797E-4 4.135187E-7                DATA 143
-50.09959E0  1.707140E0 -.1945725E-1 .9382376E-4-.1648646E-6                DATA 144
52.578338E0 -.8655753E0 .51867970E-2-.1242327E-4 .1021600E-7                DATA 145
-169.8485E0  3.907641E0 -.3215650E-1 .1127232E-3-.1410145E-6                DATA 146
    7.0             0.8727                                                  DATA 147
   10.0             0.8242                                                  DATA 148
   20.0             0.7432                                                  DATA 149
   40.0             0.6718                                                  DATA 150
   70.0             0.6194                                                  DATA 151
  100.0             0.5882                                                  DATA 152
    4.0             0.9700                                                  DATA 153
     5.0             0.9269                                                 DATA 154
-1731.992E0 20.881448E0 -.9146933E-1 .1739896E-3-.1218719E-6                DATA 155
     3     7                                                                DATA 156
         1 8.3000E14 232.000E0 1.00000E0                                    DATA 157
         2 5.10000E8 114.000E0 3.00000E0                                    DATA 158
         2 2.50000E5 100.000E0 1.30000E0                                    DATA 159
         2 2.00000E7 140.000E0 3.10000E0                                    DATA 160
         3 2.00000E5  70.000E0 2.00000E0                                    DATA 161
         3 9.70000E6 122.000E0 2.00000E0                                    DATA 162
         3 1.3000E10 172.000E0 3.00000E0                                    DATA 163
 68.6000E0 5.14500E0 0.4000E0                                               DATA 164
 80.0000E0 43.2800E0 0.2500E0                                               DATA 165
 17.8000E0 9.64760E0 0.3500E0                                               DATA 166
1                                                                           DATA 167
-855.3400E0 10.103099E0 -.4343457E-1 .8122788E-4-.5603327E-7                DATA 168
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TABLE B-3. Typical Output for Equilibrium Analysis

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INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)

THEORETICAL

CHAR BACK TEMPERATURE (OF)= 1524.8          NUMBER OF GAS COMPONENTS= 19
INITIAL SLOPE(OF/FT)=  3000.0          INITIAL DENSITY OF COMPOSITE(LBS/FT**3)= 34.94
THICKNESS OF CHAR(INCHES)=0.022392     THICKNESS OF DECOMPOSITION ZONE=0.053250
TOTAL MASS FLUX(LBS/FT2-SEC)=.034942    GAS MASS FLUX AT THE SURFACE= .074805
FRONT SURFACE TEMPERATURE(OF)=5500.0    SURFACE RECESSION VELOCITY(FT/SEC)=0.00100
      RATE OF HEAT ABSORBED IN THE CHAR ZONE(BTU/FT**2-SEC)=16872.277
      RATE OF HEAT ABSORBED IN THE DECOMPOSITION ZONE(BTU/FT2-SEC=)   20.638
      PERCENT OF TOTAL HEAT ABSORBED IN THE CHAR ZONE=  0.9987781E 02
      PERCENT OF TOTAL HEAT ABSORBED IN DECOMP-ZONE=  0.1221668E 00
      PERCENT OF HEAT ABSORBED BY THE GAS IN THE CHAR ZONE=  0.4576713E 00
      PERCENT OF HEAT ABSORBED BY THE SOLIDS IN THE CHAR ZONE=  0.8026010E-01
      PERCENT OF HEAT ABSORBED BY REACTION IN THE CHAR ZONE=  0.9946208E 02
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INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)

TEMPERATURE DROP (OF) = 3981.0

PRESSURE DROP (LB/FT2) = 9.6

SURFACE HEAT FLUX (BTU/FT2-SEC) = 16892.92

RADIANT HEAT FLUX BTU/FT2-SEC)=, 547.71

AERODYNAMIC HEAT FLUX(BTU/FT2-SEC)= 17440.63

CHAR DEPTH (FT)	0.0044	0.0045	0.0045	0.0046	0.0046
TEMPERATURE (OF)	1524.8	1533.0	1542.2	1552.3	1563.3
PRESSURE (LB/FT2)	2169.6	2169.5	2169.4	2169.3	2169.2
MASS FLUX(LB/FT2-SEC)	0.0216	0.0266	0.0266	0.0265	0.0264

	GAS COMPONENT	COMPOSITION (MOLE/MOLE GAS)				
1	H	0.7395E-07	0.2825E-07	0.3112E-07	0.3528E-07	0.4074E-07
2	H2	0.4578E 01	0.8869E 00	0.8880E 00	0.8894E 00	0.8908E 00
3	CH3	0.1038E-06	0.3446E-07	0.3658E-07	0.3952E-07	0.4299E-07
4	CH4	0.1605E 00	0.2709E-01	0.2605E-01	0.2476E-01	0.2355E-01
5	C2H2	0.3903E-07	0.1627E-07	0.1794E-07	0.2036E-07	0.2353E-07
6	C2H4	0.2864E-05	0.7532E-06	0.7683E-06	0.7881E-06	0.8090E-06
7	C2H6	0.2083E-05	0.3445E-06	0.3289E-06	0.3097E-06	0.2919E-06
8	N2	0.1881E 00	0.3549E-01	0.3545E-01	0.3539E-01	0.3534E-01
9	NH3	0.2615E-03	0.4901E-04	0.4783E-04	0.4634E-04	0.4489E-04
10	HCN	0.2063E-04	0.7020E-05	0.7429E-05	0.7995E-05	0.8661E-05
11	H2O	0.1063E 00	0.3443E-02	0.3247E-02	0.3010E-02	0.2797E-02
12	OH	0.1000E-08	0.5333E-12	0.5719E-12	0.6259E-12	0.6912E-12
13	CO2	0.2711E-01	0.1753E-03	0.1630E-03	0.1484E-03	0.1356E-03
14	CO	0.1078E 00	0.4684E-01	0.4700E-01	0.4719E-01	0.4736E-01
15	CN	0.1000E-08	0.3660E-14	0.4324E-14	0.5360E-14	0.7033E-14
16	C2H	0.1000E-08	0.6916E-16	0.8449E-16	0.1091E-15	0.1533E-15
17	C3H	0.1000E-08	0.2759E-17	0.3422E-17	0.4499E-17	0.6540E-17
18	C4H	0.1000E-08	0.3247E-21	0.4201E-21	0.5797E-21	0.9319E-21
19	C3	0.1000E-08	0.6734E-27	0.9151E-27	0.1329E-26	0.2437E-26
20	C	0.7126E 01	0.1326E 01	0.1326E 01	0.1325E 01	0.1324E 01

INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0047	0.0047	0.0048	0.0048	0.0049
TEMPERATURE (OF)	1575.3	1588.3	1599.4	1614.9	1632.2
PRESSURE (LB/FT2)	2169.1	2169.0	2168.9	2168.8	2168.6
MASS FLUX(LB/FT2-SEC)	0.0264	0.0263	0.0263	0.0262	0.0261

	GAS COMPONENT	COMPOSITION (MOLE/MOLE GAS)				
1	H	0.4693E-07	0.5412E-07	0.6186E-07	0.7411E-07	0.9005E-07
2	H2	0.8921E 00	0.8935E 00	0.8946E 00	0.8960E 00	0.8975E 00
3	CH3	0.4682E-07	0.5109E-07	0.5529E-07	0.6153E-07	0.6912E-07
4	CH4	0.2231E-01	0.2103E-01	0.2003E-01	0.1873E-01	0.1737E-01
5	C2H2	0.2713E-07	0.3131E-07	0.3580E-07	0.4293E-07	0.5220E-07
6	C2H4	0.8312E-06	0.8552E-06	0.8765E-06	0.9060E-06	0.9395E-06
7	C2H6	0.2738E-06	0.2552E-06	0.2409E-06	0.2225E-06	0.2034E-06
8	N2	0.3529E-01	0.3524E-01	0.3520E-01	0.3515E-01	0.3510E-01
9	NH3	0.4340E-04	0.4183E-04	0.4057E-04	0.3890E-04	0.3710E-04
10	HCN	0.9392E-05	0.1021E-04	0.1101E-04	0.1219E-04	0.1363E-04
11	H2O	0.2581E-02	0.2361E-02	0.2197E-02	0.1989E-02	0.1777E-02
12	OH	0.7636E-12	0.8451E-12	0.9270E-12	0.1050E-11	0.1202E-11
13	CO2	0.1228E-03	0.1099E-03	0.1006E-03	0.8893E-04	0.7733E-04
14	CO	0.4753E-01	0.4770E-01	0.4782E-01	0.4798E-01	0.4814E-01
15	CN	0.9050E-14	0.1159E-13	0.1477E-13	0.2056E-13	0.2916E-13
16	C2H	0.2083E-15	0.2804E-15	0.3776E-15	0.5674E-15	0.8686E-15
17	C3H	0.9113E-17	0.1256E-16	0.1735E-16	0.2704E-16	0.4293E-16
18	C4H	0.1395E-20	0.2055E-20	0.3057E-20	0.5297E-20	0.9335E-20
19	C3	0.3976E-26	0.6346E-26	0.1033E-25	0.2042E-25	0.4091E-25
20	C	0.1323E 01	0.1322E 01	0.1321E 01	0.1320E 01	0.1319E 01

INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0049	0.0050	0.0050	0.0051	0.0051
TEMPERATURE (OF)	1651.6	1672.9	1690.8	1718.2	1749.7
PRESSURE (LB/FT2)	2168.5	2168.4	2168.3	2168.2	2168.0
MASS FLUX(LB/FT2-SEC)	0.0260	0.0259	0.0259	0.0258	0.0257

	GAS COMPONENT	COMPOSITION (MOLE/MOLE GAS)				
1	H	0.1103E-06	0.1391E-06	0.1690E-06	0.2226E-06	0.3076E-06
2	H2	0.8990E 00	0.9005E 00	0.9016E 00	0.9032E 00	0.9048E 00
3	CH3	0.7817E-07	0.8973E-07	0.1006E-06	0.1187E-06	0.1435E-06
4	CH4	0.1597E-01	0.1460E-01	0.1357E-01	0.1212E-01	0.1070E-01
5	C2H2	0.6394E-07	0.8072E-07	0.9807E-07	0.1292E-06	0.1785E-06
6	C2H4	0.9769E-06	0.1019E-05	0.1055E-05	0.1110E-05	0.1175E-05
7	C2H6	0.1839E-06	0.1654E-06	0.1515E-06	0.1324E-06	0.1141E-06
8	N2	0.3504E-01	0.3498E-01	0.3494E-01	0.3489E-01	0.3483E-01
9	NH3	0.3521E-04	0.3329E-04	0.3179E-04	0.2964E-04	0.2741E-04
10	HCN	0.1534E-04	0.1752E-04	0.1955E-04	0.2293E-04	0.2756E-04
11	H2O	0.1564E-02	0.1369E-02	0.1227E-02	0.1035E-02	0.8588E-03
12	OH	0.1386E-11	0.1626E-11	0.1857E-11	0.2247E-11	0.2801E-11
13	CO2	0.6591E-04	0.5590E-04	0.4880E-04	0.3947E-04	0.3133E-04
14	CO	0.4830E-01	0.4843E-01	0.4853E-01	0.4866E-01	0.4877E-01
15	CN	0.4139E-13	0.6286E-13	0.8968E-13	0.1452E-12	0.2614E-12
16	C2H	0.1322E-14	0.2198E-14	0.3401E-14	0.6073E-14	0.1247E-13
17	C3H	0.6748E-16	0.1171E-15	0.1884E-15	0.3522E-15	0.7705E-15
18	C4H	0.1607E-19	0.3149E-19	0.5682E-19	0.1208E-18	0.3177E-18
19	C3	0.7836E-25	0.1777E-24	0.3704E-24	0.9182E-24	0.3032E-23
20	C	0.1318E 01	0.1317E 01	0.1317E 01	0.1316E 01	0.1315E 01

INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0052	0.0052	0.0053	0.0053	0.0053
TEMPERATURE (OF)	1785.2	1824.9	1860.8	1913.7	1974.2
PRESSURE (LB/FT2)	2167.9	2167.8	2167.6	2167.5	2167.3
MASS FLUX(LB/FT2-SEC)	0.0256	0.0255	0.0255	0.0254	0.0253

	GAS COMPONENT	COMPOSITION (MOLE/MOLE GAS)				
1	H	0.4346E-06	0.6357E-06	0.8825E-06	0.1406E-05	0.2327E-05
2	H2	0.9063E 00	0.9077E 00	0.9087E 00	0.9100E 00	0.9112E 00
3	CH3	0.1760E-06	0.2200E-06	0.2667E-06	0.3503E-06	0.4706E-06
4	CH4	0.9310E-02	0.8021E-02	0.7032E-02	0.5831E-02	0.4746E-02
5	C2H2	0.2521E-06	0.3682E-06	0.5105E-06	0.8112E-06	0.1338E-05
6	C2H4	0.1250E-05	0.1335E-05	0.1414E-05	0.1532E-05	0.1671E-05
7	C2H6	0.9659E-07	0.8083E-07	0.6904E-07	0.5515E-07	0.4308E-07
8	N2	0.3477E-01	0.3472E-01	0.3468E-01	0.3463E-01	0.3458E-01
9	NH3	0.2514E-04	0.2291E-04	0.2110E-04	0.1878E-04	0.1652E-04
10	HCN	0.3359E-04	0.4169E-04	0.5028E-04	0.6558E-04	0.8749E-04
11	H2O	0.6975E-03	0.5585E-03	0.4588E-03	0.3470E-03	0.2552E-03
12	OH	0.3549E-11	0.4595E-11	0.5745E-11	0.7885E-11	0.1112E-10
13	CO2	0.2419E-04	0.1837E-04	0.1440E-04	0.1019E-04	0.6964E-05
14	CO	0.4887E-01	0.4895E-01	0.4901E-01	0.4906E-01	0.4910E-01
15	CN	0.4838E-12	0.9605E-12	0.1726E-11	0.3964E-11	0.9694E-11
16	C2H	0.2630E-13	0.6068E-13	0.1236E-12	0.3389E-12	0.9994E-12
17	C3H	0.1729E-14	0.4287E-14	0.9273E-14	0.2767E-13	0.8921E-13
18	C4H	0.8524E-18	0.2603E-17	0.6695E-17	0.2552E-16	0.1064E-15
19	C3	0.1011E-22	0.3991E-22	0.1269E-21	0.6517E-21	0.3708E-20
20	C	0.1314E 01	0.1313E 01	0.1313E 01	0.1312E 01	0.1312E 01

INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0054	0.0054	0.0055	0.0055	0.0056
TEMPERATURE (OF)	2042.4	2112.4	2197.7	2292.8	2397.8
PRESSURE (LB/FT2)	2167.2	2167.0	2166.8	2166.6	2166.4
MASS FLUX(LB/FT2-SEC)	0.0253	0.0252	0.0252	0.0252	0.0251

	GAS COMPONENT	COMPOSITION (MOLE/MOLE GAS)				
1	H	0.3734E-05	0.6813E-05	0.1164E-04	0.2371E-04	0.4163E-04
2	H2	0.9121E 00	0.9130E 00	0.9136E 00	0.9142E 00	0.9145E 00
3	CH3	0.6200E-06	0.8796E-06	0.1200E-05	0.1806E-05	0.2503E-05
4	CH4	0.3916E-02	0.3064E-02	0.2465E-02	0.1851E-02	0.1460E-02
5	C2H2	0.2138E-05	0.3878E-05	0.6586E-05	0.1328E-04	0.2311E-04
6	C2H4	0.1810E-05	0.2002E-05	0.2189E-05	0.2459E-05	0.2701E-05
7	C2H6	0.3420E-07	0.2547E-07	0.1962E-07	0.1391E-07	0.1046E-07
8	N2	0.3453E-01	0.3448E-01	0.3443E-01	0.3436E-01	0.3428E-01
9	NH3	0.1466E-04	0.1258E-04	0.1099E-04	0.9188E-05	0.7927E-05
10	HCN	0.1145E-03	0.1613E-03	0.2186E-03	0.3265E-03	0.4499E-03
11	H20	0.1917E-03	0.1332E-03	0.9657E-04	0.6331E-04	0.4454E-04
12	OH	0.1533E-10	0.2307E-10	0.3320E-10	0.5375E-10	0.7901E-10
13	CO2	0.4893E-05	0.3125E-05	0.2104E-05	0.1255E-05	0.8153E-06
14	CO	0.4913E-01	0.4914E-01	0.4915E-01	0.4915E-01	0.4915E-01
15	CN	0.2247E-10	0.6526E-10	0.1691E-09	0.6012E-09	0.1607E-08
16	C2H	0.2765E-11	0.1004E-10	0.3179E-10	0.1483E-09	0.4848E-09
17	C3H	0.2687E-12	0.1085E-11	0.3781E-11	0.2010E-10	0.7228E-10
18	C4H	0.4091E-15	0.2246E-14	0.1034E-13	0.8052E-13	0.3819E-12
19	C3	0.1921E-19	0.1529E-18	0.9847E-18	0.1226E-16	0.8116E-16
20	C	0.1311E 01	0.1311E 01	0.1310E 01	0.1310E 01	0.1310E 01

INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0056	0.0057	0.0057	0.0058	0.0058
TEMPERATURE (OF)	2512.8	2640.8	2773.8	2915.4	3064.1
PRESSURE (LB/FT2)	2166.2	2166.0	2165.7	2165.5	2165.2
MASS FLUX(LB/FT2-SEC)	0.0251	0.0251	0.0252	0.0252	0.0253

	GAS COMPONENT	COMPOSITION (MOLE/MOLE GAS)				
1	H	0.7908E-04	0.1569E-03	0.3278E-03	0.5949E-03	0.1055E-02
2	H2	0.9148E 00	0.9148E 00	0.9145E 00	0.9140E 00	0.9131E 00
3	CH3	0.3628E-05	0.5338E-05	0.8087E-05	0.1135E-04	0.1566E-04
4	CH4	0.1113E-02	0.8550E-03	0.6388E-03	0.4988E-03	0.3961E-03
5	C2H2	0.4340E-04	0.8490E-04	0.1743E-03	0.3115E-03	0.5433E-03
6	C2H4	0.3004E-05	0.3344E-05	0.3754E-05	0.4130E-05	0.4515E-05
7	C2H6	0.7545E-08	0.5509E-08	0.3887E-08	0.2890E-08	0.2194E-08
8	N2	0.3417E-01	0.3401E-01	0.3376E-01	0.3347E-01	0.3310E-01
9	NH3	0.6694E-05	0.5663E-05	0.4706E-05	0.4021E-05	0.3464E-05
10	HCN	0.6478E-03	0.9462E-03	0.1422E-02	0.1980E-02	0.2710E-02
11	H20	0.2981E-04	0.2034E-04	0.1329E-04	0.9246E-05	0.6610E-05
12	OH	0.1226E-09	0.1947E-09	0.3209E-09	0.4828E-09	0.7135E-09
13	C02	0.4985E-06	0.3146E-06	0.1883E-06	0.1215E-06	0.8125E-07
14	CO	0.4915E-01	0.4914E-01	0.4914E-01	0.4913E-01	0.4911E-01
15	CN	0.4914E-08	0.1681E-07	0.6230E-07	0.1754E-06	0.4790E-06
16	C2H	0.1861E-08	0.8344E-08	0.4114E-07	0.1439E-06	0.4886E-06
17	C3H	0.3090E-09	0.1578E-08	0.8920E-08	0.3456E-07	0.1301E-06
18	C4H	0.2231E-11	0.1672E-10	0.1414E-09	0.7406E-09	0.3790E-08
19	C3	0.6891E-15	0.8254E-14	0.1142E-12	0.8607E-12	0.6402E-11
20	C	0.1309E 01	0.1309E 01	0.1308E 01	0.1307E 01	0.1305E 01

INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0059	0.0059	0.0060	0.0060	0.0061
TEMPERATURE (OF)	3218.7	3379.1	3545.6	3719.7	3904.3
PRESSURE (LB/FT2)	2164.9	2164.5	2164.2	2163.8	2163.4
MASS FLUX(LB/FT2-SEC)	0.0254	0.0256	0.0260	0.0264	0.0270

	GAS COMPONENT	COMPOSITION (MOLE/MOLE GAS)				
1	H	0.1853E-02	0.3336E-02	0.6108E-02	0.9967E-02	0.1672E-01
2	H2	0.9115E 00	0.9087E 00	0.9039E 00	0.8974E 00	0.8865E 00
3	CH3	0.2142E-04	0.2968E-04	0.4135E-04	0.5383E-04	0.7068E-04
4	CH4	0.3164E-03	0.2489E-03	0.1938E-03	0.1575E-03	0.1253E-03
5	C2H2	0.9377E-03	0.1653E-02	0.2956E-02	0.4717E-02	0.7701E-02
6	C2H4	0.4917E-05	0.5367E-05	0.5846E-05	0.6231E-05	0.6606E-05
7	C2H6	0.1678E-08	0.1260E-08	0.9331E-09	0.7268E-09	0.5509E-09
8	N2	0.3260E-01	0.3189E-01	0.3089E-01	0.2983E-01	0.2839E-01
9	NH3	0.2989E-05	0.2545E-05	0.2142E-05	0.1848E-05	0.1560E-05
10	HCN	0.3674E-02	0.5033E-02	0.6918E-02	0.8893E-02	0.1151E-01
11	H2O	0.4776E-05	0.3377E-05	0.2362E-05	0.1763E-05	0.1287E-05
12	OH	0.1048E-08	0.1567E-08	0.2371E-08	0.3315E-08	0.4720E-08
13	CO2	0.5516E-07	0.3656E-07	0.2401E-07	0.1709E-07	0.1191E-07
14	CO	0.4909E-01	0.4905E-01	0.4898E-01	0.4888E-01	0.4871E-01
15	CN	0.1288E-05	0.3571E-05	0.1013E-04	0.2345E-04	0.5659E-04
16	C2H	0.1635E-05	0.5675E-05	0.2030E-04	0.5684E-04	0.1681E-03
17	C3H	0.4827E-06	0.1860E-05	0.7403E-05	0.2259E-04	0.7315E-04
18	C4H	0.1909E-07	0.1005E-06	0.5484E-06	0.2162E-05	0.9161E-05
19	C3	0.4683E-10	0.3599E-09	0.2876E-08	0.1545E-07	0.9072E-07
20	C	0.1303E 01	0.1299E 01	0.1293E 01	0.1284E 01	0.1271E 01

INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0061	0.0062	0.0062	0.0063	0.0063
TEMPERATURE (OF)	4104.5	4329.2	4595.6	4943.1	5505.7
PRESSURE (LB/FT2)	2162.9	2162.4	2161.8	2161.1	2160.0
MASS FLUX(LB/FT2-SEC)	0.0280	0.0296	0.0325	0.0399	0.0748

	GAS COMPONENT	COMPOSITION (MOLE/MOLE GAS)				
1	H	0.2724E-01	0.4460E-01	0.7484E-01	0.1323E 00	0.2530E 00
2	H2	0.8699E 00	0.8431E 00	0.7961E 00	0.7019E 00	0.4511E 00
3	CH3	0.9046E-04	0.1142E-03	0.1413E-03	0.1651E-03	0.1359E-03
4	CH4	0.9967E-04	0.7707E-04	0.5593E-04	0.3437E-04	0.1034E-04
5	C2H2	0.1217E-01	0.1916E-01	0.3043E-01	0.4885E-01	0.7125E-01
6	C2H4	0.6882E-05	0.7004E-05	0.6804E-05	0.5840E-05	0.2759E-05
7	C2H6	0.4155E-09	0.3010E-09	0.1991E-09	0.1037E-09	0.1901E-10
8	N2	0.2666E-01	0.2446E-01	0.2157E-01	0.1751E-01	0.1086E-01
9	NH3	0.1305E-05	0.1057E-05	0.8019E-06	0.5170E-06	0.1724E-06
10	HCN	0.1451E-01	0.1808E-01	0.2222E-01	0.2648E-01	0.2671E-01
11	H2O	0.9476E-06	0.6833E-06	0.4677E-06	0.2796E-06	0.9765E-07
12	OH	0.6569E-08	0.9137E-08	0.1278E-07	0.1800E-07	0.2325E-07
13	CO2	0.8452E-08	0.5926E-08	0.4007E-08	0.2464E-08	0.1081E-08
14	CO	0.4844E-01	0.4798E-01	0.4711E-01	0.4520E-01	0.3923E-01
15	CN	0.1295E-03	0.2981E-03	0.7154E-03	0.1902E-02	0.6594E-02
16	C2H	0.4686E-03	0.1323E-02	0.3964E-02	0.1361E-01	0.6391E-01
17	C3H	0.2222E-03	0.6844E-03	0.2253E-02	0.8608E-02	0.4680E-01
18	C4H	0.3598E-04	0.1439E-03	0.6270E-03	0.3308E-02	0.2795E-01
19	C3	0.4881E-06	0.2700E-05	0.1685E-04	0.1383E-03	0.2438E-02
20	C	0.1250E 01	0.1217E 01	0.1154E 01	0.1012E 01	0.4824E 00

TABLE B-4. Listing of ABLATIN2 Program

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C                                                                       ABL2   1
C                                                                       ABL2   2
C                                                                       ABL2   3
C-----INDEPTH RESPONSE OF AN ABLATIVE COMPOSITE                         ABL2   4
C     NON-EQUILIBRIUM FLOW ANALYSIS                                     ABL2   5
C     ALBLATIN2 SYSTEM                                                  ABL2   6
C                                                                       ABL2   7
C                                                                       ABL2   8
      REAL*8 Z22                                                        ABL2   9
      COMMON/KA/S1(6),S2(6),S3(6),S4(6),S5(6),A11(6),A22(6),            ABL2  10
     1       A33(6),A44(6),A55(6),FI(30),FII(30),GI(30),                ABL2  11
     2       GII(30),AA(30,6),S6(6),A66(6),JCODE(6),CPMX1               ABL2  12
      COMMON/KB/AI(30),BI(30),CI(30),DI(30),EI(30),AII(30),             ABL2  13
     1       BII(30),CII(30),DII(30),EII(30),TLOW(30)                   ABL2  14
      COMMON/KC/ICODE(30),Y(30),FW(30)                                  ABL2  15
      COMMON/KCC/SPCIE1(30),SPCIE2(30),TABLE(300,26),Z,INDPT            ABL2  16
      COMMON/KE/XTKE(100),ZOMGA(100),EK(100),SIG(100)                   ABL2  17
      COMMON/KEE/PL,RR,TZERO,EPS,KEY,NC,NS,MM,NQ                        ABL2  18
      COMMON/KF/CPS,CDO,DCDO,JCHAR,TC                                   ABL2  19
      COMMON/KI/KN,K7,DTC,REAC2,W,KMAX,AVGFW,N,Z2,DELZ,H                ABL2  20
      COMMON/KJ/DELTK,TVAR                                              ABL2  21
      COMMON/KK/WTOTAL,RHOII                                            ABL2  22
      COMMON/KM/XMOL(30)                                                ABL2  23
      COMMON/KQ/Z22                                                     ABL2  24
      DIMENSION T1(300),ZX(41),ZY(41),TP(41),P(41),WFLUX(41),           ABL2  25
     1          TT(21),YCOMP(30,41),PROD(21),PRODCP(21),CP(30),         ABL2  26
     2          PRODR(21),COND(30),CV(30),VIS(30),YI(30),Z1(300),       ABL2  27
     3          TOK(300),CHARDN(300)                                    ABL2  28
      DOUBLE PRECISION ZZ,HII,ZLL,TTTT,DTCC,REAC1,CPB1,CPB2             ABL2  29
      F(A)=+GROUP*A                                                     ABL2  30
      G(A)=A                                                            ABL2  31
C                                                                       ABL2  32
C     DELTEF=CHANGE IN DF FOR AN INCREMENT OF CHANGE IN H(FEET)         ABL2  33
      RHO=13.                                                           ABL2  34
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      WI=0.01                                                           ABL2  35
C                                                                       ABL2  36
C     RR=GAS CONSTANT(1.98726BTU/(LB-MOLE OR)                           ABL2  37
C     TZERO=REFERENCE TEMPERATURE                                       ABL2  38
C     TEMAX=MAXIMUM ALLOWABLE TEMPERATURE FOR THIS MODEL (OF)           ABL2  39
C                                                                       ABL2  40
      RR=1.98726                                                        ABL2  41
      TZERO=298.159                                                     ABL2  42
C                                                                       ABL2  43
C     HSIMPI=SIMPSON'S RULE INCREMENT SIZE(FT) USED                     ABL2  44
C            IN THE SOLUTION OF THE MOMENTUM EQUATION                   ABL2  45
      FR2=778.16/32.2                                                   ABL2  46
C                                                                       ABL2  47
C                                                                       ABL2  48
C     NC=NO. OF GAS SPECIES                                             ABL2  49
C     NNS=NO. OF LIQUID OR SOLID SPECIES                                ABL2  50
C     NS=NC+NNS(TOTAL NUMBER OF SPECIES)                                ABL2  51
C     MM=NO. OF ELEMENTS                                                ABL2  52
C     KODE=1 CONDUCTIVITY OF CHAR WITH GAS IN PORES                     ABL2  53
C     INDPT=0 COMPUTATIONS START AT THE BACK SURFACE OF THE CHAR        ABL2  54
C     INDPT=1 COMPUTATIONS START AT THE VIRGIN MATERIAL                 ABL2  55
C     PL=PRESSURE AT Z=L(LB/FT2)                                        ABL2  56
C     DELTK=TEMPERATURE INCREMENT                                       ABL2  57
C     TO=TEMPERATURE AT Z=0                                             ABL2  58
C     EPS=POROSITY                                                      ABL2  59
C     ZL=ABLATOR THICHKNESS(IN FEET)                                    ABL2  60
C     HI=INITIAL RUNGE-KUTTA INCREMENT SIZE(FT) USED                    ABL2  61
C        IN THE SOLUTION OF THE ENERGY EQUATION.                        ABL2  62
C     ALPHA=VISCOUS COEFFICIENT IN DARCY'S EQUATION(1/FT)               ABL2  63
C     BETA=INERTIAL COEFFICIENT IN DARCY'S EQUATION(1/FT2)              ABL2  64
C     SIGMA=STEPHAN-BOLTZMAN CONSTANT(0.481X10-12 BTU/FT2-SEC-OF4)      ABL2  65
C     EMIS=CHAR EMISIVITY.                                              ABL2  66
C     QFLUXI=INITIAL BACK SURFACE HEAT FLUX.                            ABL2  67
C     QINC=INCREMENT IN THE HEAT FLUX(FOR PARAMETER STUDIES)            ABL2  68
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C       QMAX=MAXIMUM BACK SURFACE HEAT FLUX.                            ABL2  69
C       TCHAR=BACK SURFACE TEMPERATURE OF CHAR                          ABL2  70
C                                                                       ABL2  71
C                                                                       ABL2  72
        FR=0.1666667                                                    ABL2  73
C                                                                       ABL2  74
C                                                                       ABL2  75
C-----READ INPUT PARAMETERS                                             ABL2  76
C                                                                       ABL2  77
C                                                                       ABL2  78
C                                                                       ABL2  79
 10     READ11,NC,NNS,MM,KODE,KEY,INDPT,TFMAX                           ABL2  80
 11     FORMAT(6I6,F10.1)                                               ABL2  81
        READ 12,PL,TO,FPS,ZL,HI                                         ABL2  82
 12     FORMAT(F10.3,10X,4F10.3)                                        ABL2  83
        READ21,ALPHA,BETA,SIGMA,EMIS                                    ABL2  84
        READ13,DTC,TCHAR,VR                                             ABL2  85
 13     FORMAT(7E10.3)                                                  ABL2  86
        NN=NC                                                           ABL2  87
        NS=NC+NNS                                                       ABL2  88
        NQ=NS                                                           ABL2  89
C                                                                       ABL2  90
C                                                                       ABL2  91
C                                                                       ABL2  92
C       S1...S6(APPLY BETWEEN 1000-6000 OK)                             ABL2  93
C       A11...A66(APPLY BETWEEN 300-1000 OK)                            ABL2  94
C       JCODE(J)=0 THE REFERENCE ELEMENT IS IN THE GAS STATE.           ABL2  95
C       JCODE(J)=1  THE REFERENCE ELEMENT IS IN THE SOLID STATE.        ABL2  96
C       AI...EI(HEAT CAPACITY CONSTANTS...1000-6000 OK)                 ABL2  97
C       FI,GI(NEEDED TO CALCULATE THE ENTHALPY,ENTROPY                  ABL2  98
C       AND FREE ENERGY....1000-6000 OK)                                ABL2  99
C       AII...GII(300-1000 OK)                                          ABL2 100
C       AA=FORMULA NUMBER. GIVES THE ATOMS OF ELEMENT J                 ABL2 101
C          IN SPECIE I.                                                 ABL2 102
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C     TLOW(I)=MINIMUM TEMPERATURE AT WHICH THE HIGH TEMPERATURE          ABL2 103
C             FIT IS APPLICABLE.                                         ABL2 104
C     FW(I)=MOLECULAR WEIGHT OF SPECIE I.                                ABL2 105
C     YI(I)=INITIAL MOLE FRACTION OF SPECIE I.                           ABL2 106
C     YI(I)=MOLE FRACTION OF SPECIE I.                                   ABL2 107
C     SPCIE1 AND SPCIE2 ARE THE SPECIES IDENTIFICATION                   ABL2 108
C     ICODE(I)=0 SPECIE IS A GAS                                         ABL2 109
C     ICODE(I)=1 SPECIE IS A SOLID                                       ABL2 110
C                                                                        ABL2 111
C                                                                        ABL2 112
C                                                                        ABL2 113
C                                                                        ABL2 114
C-----READ EMPIRICAL CONSTANTS TO CALCULATE THE SENSIBLE                 ABL2 115
C     ENTHALPY CHANGE OF THE CONSTITUENT ELEMENTS.                       ABL2 116
C                                                                        ABL2 117
C                                                                        ABL2 118
      DO 9 J=1,MM                                                        ABL2 119
      READ 18,S1(J),S2(J),S3(J),S4(J),S5(J),S6(J),JCODE(J)               ABL2 120
      READ 18,A11(J),A22(J),A33(J),A44(J),A55(J),A66(J)                  ABL2 121
 9    CONTINUE                                                           ABL2 122
      DO15I=1,NS                                                         ABL2 123
      READ 14,TLOW(I),FW(I),YI(I),SPCIE1(I),SPCIE2(I),ICODE(I)           ABL2 124
 14   FORMAT(10X,3E10.3,2X,2A3,I4)                                       ABL2 125
C                                                                        ABL2 126
C                                                                        ABL2 127
C-----READ EMPIRICAL CONSTANTS TO CALCULATE THE HEAT                     ABL2 128
C     CAPACITY OF THE SOLID PLUS TWO ADDITIONAL CONSTANTS                ABL2 129
C     TO CALCULATE THE ENTHALPY,THE ENTROPY AND THE FREE                 ABL2 130
C     ENERGY OF THE SYSTEM                                               ABL2 131
C                                                                        ABL2 132
C                                                                        ABL2 133
      READ13,AI(I),BI(I),CI(I),DI(I),EI(I),FI(I),GI(I)                   ABL2 134
      READ13,AII(I),BII(I),CII(I),DII(I),EII(I),FII(I),GII(I)             ABL2 135
C                                                                        ABL2 136
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C                                                                       ABL2 137
 15   READ13,(AA(I,J),J=1,MM)                                           ABL2 138
C                                                                       ABL2 139
C                                                                       ABL2 140
C                                                                       ABL2 141
C     EK=POTENTIAL PARAMETER/BOLTZMAN CONSTANT.                         ABL2 142
C     SIG=COLLISION DIAMETER(ANGSTRONG UNITS).                          ABL2 143
C     THESE CONSTANTS ARE USED TO DETERMINE THE                         ABL2 144
C     VISCOCITY AND THERMAL CONDUCTIVITY OF THE                         ABL2 145
C     REACTING GAS MIXTURE.                                             ABL2 146
C     NDATA=NO. OF XTKE VS. ZOMGA DATA POINTS                           ABL2 147
C     XTKE=PRODUCT OF TEMPERATURE AND 1/EK VALUE                        ABL2 148
C     ZOMGA=COLLISION INTEGRAL TABULATED VS XTKE                        ABL2 149
C                                                                       ABL2 150
C                                                                       ABL2 151
C                                                                       ABL2 152
      READ16,(EK(I),SIG(I),I=1,NC)                                      ABL2 153
 16   FORMAT(2F15.5)                                                    ABL2 154
      READ11,NDATA                                                      ABL2 155
      READ17,(XTKE(I),ZOMGA(I),I=1,NDATA)                               ABL2 156
 17   FORMAT(2F15.5)                                                    ABL2 157
 18   FORMAT(6E10.4,I3)                                                 ABL2 158
 21   FORMAT(3E15.5,F15.5)                                              ABL2 159
C                                                                       ABL2 160
C                                                                       ABL2 161
C-----INITIALIZATION OF PARAMETERS                                      ABL2 162
C                                                                       ABL2 163
C                                                                       ABL2 164
C     N=COUNTER OF RUNGE KUTTA STEPS                                    ABL2 165
      N=1                                                               ABL2 166
      K7=1                                                              ABL2 167
C     K7=1(CALL SUBPROGRAM INPUT)K7=2(BYPASS SUBPROGRAM                 ABL2 168
C                                                 INPUT)                ABL2 169
C                                                                       ABL2 170
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C       TO=INITIAL TEMPERATURE OF BACK SURFACE(OF)                      ABL2 171
C       IT IS A SPECIFIED BOUNDARY CONDITION.                           ABL2 172
C       TC=INSTANTANEOUS TEMPERATURE OF THE SYSTEM(OF)                  ABL2 173
        K1=1                                                            ABL2 174
C       K1=GIVES THE TOTAL NUMBER OF DATA POINTS STORED.                ABL2 175
C       SHOULD NOT EXCEED THE DIMENSION OF VARIABLES.                   ABL2 176
C                                                                       ABL2 177
        NN4=NC+4                                                        ABL2 178
        NN5=NN4+NNS                                                     ABL2 179
C                                                                       ABL2 180
C                                                                       ABL2 181
C       NN5 GIVES THE NUMBER OF VARIABLES STORED IN TABLE(I,J).         ABL2 182
C       THE FIRST FOUR VARIABLES ARE...                                 ABL2 183
C           1) THE TEMPERATURE(IN OK)                                   ABL2 184
C           2) THE HEAT ABSORBED BY REACTIONS(BTU/FT2-SEC)              ABL2 185
C           3) THE AVERAGE MOLECULAR WEIGHT                             ABL2 186
C           4) THE MASS FLUX(LBS/FT2-SEC)                               ABL2 187
C           5) THE REST OF THE VARIABLES ARE THE MOLE                   ABL2 188
C       FRACTIONS. FOR THE SOLIDS, THE TERM STORED                      ABL2 189
C       IS THE RATIO OF MOLES OF SOLID TO MOLE OF                       ABL2 190
C       GASES.                                                          ABL2 191
C                                                                       ABL2 192
C                                                                       ABL2 193
C                                                                       ABL2 194
C-----CONVERT INITIAL COMPOSITION OF THE GASES TO MOLE                  ABL2 195
C       FRACTION AND CALCULATE THE RATIO OF THE MOLES OF                ABL2 196
C       EACH SOLID SPECIE PER MOLE OF THE GAS MIXTURE. THIS             ABL2 197
C       IS DONE IN CASE THE YI(I) IS READ IN AS MOLES.                  ABL2 198
C                                                                       ABL2 199
C       ZL=THICKNESS OF CHAR IN INCHES                                  ABL2 200
        ZL=ZL/12.                                                       ABL2 201
        ZINC=ZL/98.                                                     ABL2 202
        ZINC=ZINC/5.                                                    ABL2 203
        IF(VR.GE.1.E-2)ZINC=ZINC/2.                                     ABL2 204
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      IF(VR.GE.2.E-2)ZINC=ZINC/2.                                       ABL2 205
 22   IND=0                                                             ABL2 206
      KMAX=0                                                            ABL2 207
      K10=0                                                             ABL2 208
      DELTFF=0.                                                         ABL2 209
      REAC1=0.                                                          ABL2 210
      CPB1=0.                                                           ABL2 211
      CPB2=0.                                                           ABL2 212
      Q1=0.                                                             ABL2 213
      DCDO=0.                                                           ABL2 214
      DCDOV=0.                                                          ABL2 215
      DELTK=0.                                                          ABL2 216
      K1=1                                                              ABL2 217
      TC=TO                                                             ABL2 218
      SUM=0.                                                            ABL2 219
      DO23I=1,NC                                                        ABL2 220
 23   SUM=SUM+YI(I)                                                     ABL2 221
      DO24I=1,NS                                                        ABL2 222
 24   YI(I)=YI(I)/SUM                                                   ABL2 223
C                                                                       ABL2 224
C                                                                       ABL2 225
C     HI=INITIAL RUNGE-KUTTA STEP SIZE                                  ABL2 226
C                                                                       ABL2 227
      H=HI                                                              ABL2 228
C                                                                       ABL2 229
C                                                                       ABL2 230
C-----CALCULATE THE INITIAL AVERAGE MOLECULAR WEIGHT OF THE GAS         ABL2 231
C                                                                       ABL2 232
C                                                                       ABL2 233
      AVGFW=0.                                                          ABL2 234
      DO31I=1,NS                                                        ABL2 235
      XMOL(I)=YI(I)                                                     ABL2 236
      Y(I)=YI(I)                                                        ABL2 237
      IF(ICODE(I).EQ.1)GOTO31                                           ABL2 238
```

```
      AVGFW=AVGFW+Y(I)*FW(I)                                            ABL2 239
 31   CONTINUE                                                          ABL2 240
C     W=MASS FLUX(LBS-FT2/SEC)                                          ABL2 241
      W=WI                                                              ABL2 242
      Z=0.                                                              ABL2 243
C     Z=DISTANCE IN FEET                                                ABL2 244
      Z2=0.                                                             ABL2 245
      Z22=Z2                                                            ABL2 246
      TVAR=(TC+459.69)/1.8                                              ABL2 247
C     TVAR=TEMPERATURE IN OK.                                           ABL2 248
      ZZ=0.                                                             ABL2 249
      ZLL=ZL                                                            ABL2 250
      PRINT 51,ZLL                                                      ABL2 251
   51 FORMAT(1X,'ZLL='D20.9)                                            ABL2 252
C                                                                       ABL2 253
C                                                                       ABL2 254
C                                                                       ABL2 255
C                                                                       ABL2 256
C-----INDEPTH RESPONSE OF ABLATIVE COMPOSITES.                          ABL2 257
C     FOR BACK SURFACE TEMPERATURE AND HEAT                             ABL2 258
C     FLUX SPECIFIED. THE EQUATION OF ENERGY                            ABL2 259
C     IS A SECOND ORDER, NON-LINEAR, ORDINARY DIFFERENTIAL              ABL2 260
C     EQUATION WITH VARIABLE COEFFICIENTS.                              ABL2 261
C                                                                       ABL2 262
C     THE NUMERICAL TEHCNIQUE USED IS A 4TH ORDER                       ABL2 263
C     VARIABLE STEP RUNGE-KUTTA ANALYSIS.                               ABL2 264
C                                                                       ABL2 265
C                                                                       ABL2 266
C     TCHAR=TEMPERATURE AT WHICH ALL OF THE VIRGIN                      ABL2 267
C     MATERIAL HAS DECOMPOSED.                                          ABL2 268
C                                                                       ABL2 269
      DELZ=H                                                            ABL2 270
      H11=H                                                             ABL2 271
      IF(TVAR.GT.TCHAR)GOTO32                                           ABL2 272
```

```
C
      CALL INDPTH(TC,CDOV,DCDOV,GASCP,Q,CPV,RHO,TVAR,DELTK,
     1N,DELZ,VR,W,H)
      H11=H
      DELZ=H
C
C     CDOV=THERMAL CONDUCTIVITY OF VIRGIN MATERIAL(
C     BTU/(FT-SEC-OF)
C     DCDOV=THE DERIVATIVE OF CDOV WITH TEMPERATURE(BTU/(FT-2EC))
C     GASCP=HEAT CAPACITY OF MIXTURE(BTU/LB-OF)
C     Q=HEAT ABSORBED BY DEPOLYMERIZATION OF THE
C     VIRGIN PLASTIC COMPOSITE(BTU/FT3-SEC)
C     CPV=HEAT CAPACITY OF VIRGIN COMPOSITE(BTU/LB-OF)
C     RHO=DENSITY OF VIRGIN COMPOSITE
C     DELTK=TEMPERATURE DIFFERENCE IN OK FOR A DISTANCE H.
C     N=NUMBER OF INTEGRATION STEPS
C     DELZ=INCREMENT OF DISTANCE(FT)
C     VR=SURFACE RECESSION VELOCITY(FT/SEC)
C     W=MASS FLUX(LBS/FT2-SEC)
C     H=RUNGE-KUTTA INTEGRATION STEP SIZE(FT)
C     DTC=QFLUX/CDOV
C
      WI=W
      DTCI=DTC
      QCZI=CDOV*DTC
      PRINT 1390,QCZI
 1390 FORMAT(1X,'QCZ='F15.5)
C
C
C-----CALCULATE THE HEAT CAPACITY OF THE PYROLYSIS GASES
C
C
      CALL CPMIX(TVAR,NN,CPMX)
      GASCP=CPMX/AVGEW
```

```
      GOTO113                                                           ABL2 307
C                                                                       ABL2 308
 32   CALL CHARPR                                                       ABL2 309
C                                                                       ABL2 310
C-----THIS SUBROUTINE CALCULATES THE THERMO-PHYSICAL                    ABL2 311
C     PROPERTIES IN THE CHAR                                            ABL2 312
C                                                                       ABL2 313
      DELZ=H                                                            ABL2 314
      Z1(1)=0.                                                          ABL2 315
      T1(1)=TO                                                          ABL2 316
      DTC=QFLUXI/CDO                                                    ABL2 317
      PRINT 36,CDO                                                      ABL2 318
   36 FORMAT(1X,'CDO='E15.6)                                            ABL2 319
      DTCI=DTC                                                          ABL2 320
      GOTO103                                                           ABL2 321
 101  TVAR=(TC+459.69)/1.8                                              ABL2 322
C                                                                       ABL2 323
C                                                                       ABL2 324
      IF(TVAR.GT.TCHAR)GOTO102                                          ABL2 325
C                                                                       ABL2 326
C                                                                       ABL2 327
C-----CALCULATE THE PHYSICO-CHEMICAL PROPERTIES AND DESCRIBE            ABL2 328
C     THE DECOMPOSITION OF THE VIRGIN MATERIAL USING INDPTH.            ABL2 329
C                                                                       ABL2 330
C                                                                       ABL2 331
      CALL INDPTH(TC,CDOV,DCDOV,GASCP,Q,CPV,RHO,TVAR,DELTK,             ABL2 332
     1N,DELZ,VR,W,H)                                                    ABL2 333
C                                                                       ABL2 334
C     FOR EXPLANATION OF THE VARIABLES IN THE ARGUMENT SEE              ABL2 335
C     PREVIOUS CALL INDPTH STATEMENT.                                   ABL2 336
C                                                                       ABL2 337
      H11=H                                                             ABL2 338
      WI=W                                                              ABL2 339
      ZLL=ZZ+0.0208333                                                  ABL2 340
```

```
      PRINT 139,TC,TVAR,DTC,GASCP,DCDOV,CPV,Q,CDOV,Z7                   ABL2 341
 139  FORMAT(1X,'T='F9.4,' TK='F9.4,' DT='E11.4,' CP='F6.3,' DKE='E11.4,ABL2 342
     1' CPP='E11.4,' Q='E11.4,' KE='E11.4,D15.7)                        ABL2 343
      QCZI=CDOV*DTC                                                     ABL2 344
      PRINT 1390,QCZI                                                   ABL2 345
C                                                                       ABL2 346
C                                                                       ABL2 347
C-----CALCULATE THE HEAT CAPACITY OF THE PYROLYSIS GASES                ABL2 348
C                                                                       ABL2 349
C                                                                       ABL2 350
      CALL CPMIX(TVAR,NN,CPMX)                                          ABL2 351
      GASCP=CPMX/AVGFW                                                  ABL2 352
      GOTO113                                                           ABL2 353
C                                                                       ABL2 354
C                                                                       ABL2 355
C-----USE SUBROUTINE CHARPR TO GENERATE NEEDED PHYSICAL PROPERTY        ABL2 356
C     DATA FOR THE CHAR ZONE(HEAT CAPACITY OF THE CHAR AND THE          ABL2 357
C     OVER ALL EFFECTIVE THERMAL CONDUCTIVITY OF THE GAS AND CHAR).     ABL2 358
C                                                                       ABL2 359
C                                                                       ABL2 360
 102  CALL CHARPR                                                       ABL2 361
      IF(IND.EQ.0)DTC=QCZI/CDO                                          ABL2 362
      IND=1                                                             ABL2 363
C                                                                       ABL2 364
C                                                                       ABL2 365
C-----CALCULATE THE BULK DENSITY OF THE CHAR                            ABL2 366
C                                                                       ABL2 367
C                                                                       ABL2 368
C                                                                       ABL2 369
C     ROCHAR=BULK DENSITY OF THE CHAR(LBS/FT**3)                        ABL2 370
      ROCHAR=(WTOTAL-W)/VR                                              ABL2 371
C                                                                       ABL2 372
      DELZ=H                                                            ABL2 373
C                                                                       ABL2 374
```

```
C                                                                       ABL2 375
C-----CALCULATE THE CHEMICAL KINETICS OF THE PYROLYSIS GASES            ABL2 376
C      AND CHAR ALONG WITH THE HEAT ABSORB BY THESE REACTING            ABL2 377
C      GASES USING KINET.                                               ABL2 378
C                                                                       ABL2 379
C                                                                       ABL2 380
 103   CALL KINET                                                       ABL2 381
       H11=H                                                            ABL2 382
       GASCP=CPMX1/AVGFW                                                ABL2 383
C                                                                       ABL2 384
C                                                                       ABL2 385
C----CALCULATE THE GROUP TERM                                           ABL2 386
C                                                                       ABL2 387
C                                                                       ABL2 388
 112   REACT=REAC2/DTC                                                  ABL2 389
       CONVEG=W*GASCP                                                   ABL2 390
       CPB1=CPB1+CONVEG*DELTFF                                          ABL2 391
       CONVES=CPS*ROCHAR*VR                                             ABL2 392
       CPB2=CPB2+CONVES*DELTFF                                          ABL2 393
       REAC1=REAC1+REACT*DELTFF                                         ABL2 394
       GROUP=(CONVEG+CONVES-DCDO*DTC+REACT)/CDO                         ABL2 395
C                                                                       ABL2 396
C                                                                       ABL2 397
C      DCDO=DERIVATIVE OF CDO WITH TEMPERATURE(BTU/FT-SEC-DF2)          ABL2 398
C      CDO=EFFECTIVE THERMAL CONDUCTIVITY(BTU/FT-SEC-DF)                ABL2 399
C      DTC=GRADIENT OF TEMPERATURE WITH DISTANCE(DF/FT)                 ABL2 400
C      VR=SURFACE RECESSION VELOCITY(FT/SEC)                            ABL2 401
C                                                                       ABL2 402
C                                                                       ABL2 403
       GOTO114                                                          ABL2 404
 113   Q2=Q/DTC                                                         ABL2 405
       IF(Q2.LT.0.)Q2=0.                                                ABL2 406
       CONVEG=W*GASCP                                                   ABL2 407
       CONVEV=CPV*RHO*VR                                                ABL2 408
```

```
      Q1=Q1+Q2*DELTFF                                                   ABL2 409
      GROUP=(CONVFG+CONVEV-DCDOV*DTC+Q2)/CDOV                           ABL2 410
C                                                                       ABL2 411
C                                                                       ABL2 412
C-----THE ABOVE GROUP TERM IS USED DURING THE DEPOLYMERIZATION OF       ABL2 413
C     THE VIRGIN PLASTIC COMPOSITE.                                     ABL2 414
C                                                                       ABL2 415
C                                                                       ABL2 416
  114 A=DTC                                                             ABL2 417
      DT=A                                                              ABL2 418
      ARK=H*DT                                                          ABL2 419
      A1=ARK                                                            ABL2 420
      DA1=ARK*GROUP                                                     ABL2 421
      DT=A+0.5*DA1                                                      ABL2 422
      ARK=H*DT                                                          ABL2 423
      A2=ARK                                                            ABL2 424
      DA2=ARK*GROUP                                                     ABL2 425
      DT=A+0.5*DA2                                                      ABL2 426
      ARK=H*DT                                                          ABL2 427
      A3=ARK                                                            ABL2 428
      DA3=ARK*GROUP                                                     ABL2 429
      DT=A+DA3                                                          ABL2 430
      ARK=H*DT                                                          ABL2 431
      A4=ARK                                                            ABL2 432
      DA4=ARK*GROUP                                                     ABL2 433
      DTC=DTC+(DA1+2.*(DA2+DA3)+DA4)/6.                                 ABL2 434
      IF(IND.EQ.0)GOTO115                                               ABL2 435
      QCZ=CDO*DTC                                                       ABL2 436
  115 TPREV=TC                                                          ABL2 437
      IF(H.LT.0.8E-8)GOTO117                                            ABL2 438
      TC=TC+(A1+2.*(A2+A3)+A4)/6.                                       ABL2 439
      GOTO118                                                           ABL2 440
  117 IF(K10.EQ.0)TTTT=TC                                               ABL2 441
      K10=1                                                             ABL2 442
```

```
      DTCC=DTC                                                          ABL2 443
      TTTT=TTTT+H11*DTCC                                                ABL2 444
      TC=TTTT                                                           ABL2 445
 118  DELTFF=TC-TPREV                                                   ABL2 446
      DELTK=DELTFF/1.8                                                  ABL2 447
C                                                                       ABL2 448
C                                                                       ABL2 449
C-----COMPARE THE TEMPERATURE CALCULATED WITH THE MAXIMUM VALUE.        ABL2 450
C                                                                       ABL2 451
C                                                                       ABL2 452
 138  ZPREV=ZZ                                                          ABL2 453
      ZZ=Z7+H11                                                         ABL2 454
      H11=H                                                             ABL2 455
      Z=ZZ                                                              ABL2 456
      IF(TC.GT.TFMAX)GOTO150                                            ABL2 457
      N=N+1                                                             ABL2 458
      IF(TVAR.LE.TCHAR)Z2=ZZ                                            ABL2 459
      IF(TVAR.LE.TCHAR)GOTO101                                          ABL2 460
      IF(Z2.GT.ZZ)GOTO101                                               ABL2 461
  140 PRINT 142,TC,H,DTC,GASCP,DCDO,GROUP,REACT,CDO                     ABL2 462
  142 FORMAT(1X,'TF='F9.4,' H='E14.6,  ' DT='E11.5,' CP='F6.4,' DKE='F11ABL2 463
     1.5,' GRP='E12.5,' Q='E11.4,' KE='E11.5)                           ABL2 464
      PRINT 1140,AVGFW,W,      TVAR,KMAX,CPS,GASCP,RHO,QCZ              ABL2 465
 1140 FORMAT(1X,'AVGFW='F 7.3,' W='F 7.5,  -            ' TVAR='F7.2,   ABL2 466
     1' KMAX='I5,' CPS='F 6.3,' GASCP='F 6.4,' RHO='F8.4,' QCZ='F7.2 )  ABL2 467
      Z2=Z2+ZINC                                                        ABL2 468
      Z1(K1)=ZPREV                                                      ABL2 469
      TOK(K1)=TVAR                                                      ABL2 470
      T1(K1)=TPREV                                                      ABL2 471
      CHARDN(K1)=ROCHAR                                                 ABL2 472
C                                                                       ABL2 473
C                                                                       ABL2 474
C-----STORE THE TEMPERATURE PROFILE FOR LATER USE IN THE SOLUTION       ABL2 475
C     OF THE MOMENTUM EQUATION.                                         ABL2 476
```

```
C                                                                       ABL2 477
C                                                                       ABL2 478
      PRINT 153,REAC1,CPB1,CPB2,ZPREV                                   ABL2 479
 153  FORMAT(1X,'REAC1='D15.7,' CPB1='D15.7,' CPB2='D15.7,              ABL2 480
     1' ZPREV='E15.7/)                                                  ABL2 481
      K1=K1+1                                                           ABL2 482
      IF(K1.GE.299)K1=299                                               ABL2 483
C                                                                       ABL2 484
C     THE NUMBER OF DIMENSIONES OF TABLE,T1 AND Z1.                     ABL2 485
C                                                                       ABL2 486
C-----K1 SHOULD NEVER BE GREATER THAN 299 TO AVOID VIOLANTING THE       ABL2 487
      GOTO101                                                           ABL2 488
C                                                                       ABL2 489
  150 TL=TC                                                             ABL2 490
      WFINAL=W                                                          ABL2 491
C     TL=FINAL TEMPERATURE                                              ABL2 492
      PRINT 1140,AVGFW,W,      TVAR,KMAX,CPS,GASCP,RHO,QCZ              ABL2 493
      PRINT 142,TC,H,DTC,GASCP,DCDO,GROUP,REACT,CDO                     ABL2 494
      PRINT 153,REAC1,CPB1,CPB2,ZPREV                                   ABL2 495
      TOK(K1)=(TC+459.69)/1.8                                           ABL2 496
      T1(K1)=TL                                                         ABL2 497
      CHARDN(K1)=ROCHAR                                                 ABL2 498
C                                                                       ABL2 499
C***********************************************************************ABL2 500
C***********************************************************************ABL2 501
C                                                                      * ABL2 502
C-----THE TEMPERATURE PROFILE HAS BEEN DEFINED                         * ABL2 503
C                                                                      * ABL2 504
C***********************************************************************ABL2 505
C***********************************************************************ABL2 506
C                                                                       ABL2 507
      DELTT=TL-T1(1)                                                    ABL2 508
C     DELTT=TEMPERATURE DROP ACROSS THE CHAR(DF)                        ABL2 509
      Z1(K1)=ZZ                                                         ABL2 510
```

```
C                                                                       ABL2 511
C                                                                       ABL2 512
C-----PRINT THE TEMPERATURE AND THE DENSITY PROFILE                     ABL2 513
C                                                                       ABL2 514
C                                                                       ABL2 515
      PRINT 154                                                         ABL2 516
 154  FORMAT(1H1, 7X,'T(OF)', 9X,'T(OK)', 11X,'Z')                      ABL2 517
      DO 156 I=1,K1                                                     ABL2 518
      PRINT 155,T1(I),TOK(I),Z1(I)                                      ABL2 519
 155  FORMAT(1X,4E15.7)                                                 ABL2 520
 156  CONTINUE                                                          ABL2 521
      DISTAN=Z1(K1)-Z1(1)                                               ABL2 522
C                                                                       ABL2 523
C     DISTAN IS THE THICKNESS OF THE CHAR.                              ABL2 524
C     CALCULATION OF THE PRESSURE PROFILE IN THE                        ABL2 525
C     CHAR USING SIMPSON'S RULE FOR THE INTEGRATION                     ABL2 526
C     OF THE MOMENTUM EQUATION FOLLOWS.                                 ABL2 527
C                                                                       ABL2 528
      JS=39                                                             ABL2 529
C                                                                       ABL2 530
C     JS=NUMBER OF SLICES IN THE CHAR                                   ABL2 531
C                                                                       ABL2 532
      HS=DISTAN/FLOAT(JS)                                               ABL2 533
C                                                                       ABL2 534
C     HS=INCREMENT OF GRID(IN FEET)                                     ABL2 535
C                                                                       ABL2 536
C                                                                       ABL2 537
C-----INITIALIZE                                                        ABL2 538
C                                                                       ABL2 539
C                                                                       ABL2 540
      SIMP1=0.                                                          ABL2 541
      SIMP2=0.                                                          ABL2 542
      ITEMP=K1                                                          ABL2 543
C                                                                       ABL2 544
```

```
C     ITEMP=TOTAL NUMBER OF TEMPERATURE POINTS STORED                   ABL2 545
C                                                                       ABL2 546
      LS=JS+1                                                           ABL2 547
      WFLUX(1)=WI                                                       ABL2 548
      ZX(LS)=Z1(K1)                                                     ABL2 549
      TP(LS)=TL                                                         ABL2 550
      P(LS)=PL                                                          ABL2 551
C                                                                       ABL2 552
C                                                                       ABL2 553
C-----THE INTEGRATION OF THE MOMENTUM EQUATION IS PERFORMED             ABL2 554
C                                                                       ABL2 555
C                                                                       ABL2 556
C                                                                       ABL2 557
C-----FROM THE FRONT SURFACE OF THE CHAR TO THE BACK SURFACE.           ABL2 558
C     THE INTEGRATION OF THE ENERGY EQUATION, ON THE OTHER              ABL2 559
C     HAND, WAS PERFORMED FROM THE VIRGIN MATERIAL TO THE FRONT         ABL2 560
C     SURFACE OF THE CHAR. BECAUSE THE DIRECTION OF INTEGRATION         ABL2 561
C     OF BOTH EQUATIONS ARE DIFFERENT IT IS NECESSARY TO RE-            ABL2 562
C     DEFINE Z=0. AT THE FRONT SURFACE OF THE CHAR.                     ABL2 563
C                                                                       ABL2 564
C                                                                       ABL2 565
      ACON1=2.6693E-3                                                   ABL2 566
      ACON5=2.42/3600.                                                  ABL2 567
      ACON7=778.16/32.2                                                 ABL2 568
      MS=20                                                             ABL2 569
      HSIMPI=HS/FLOAT(MS)                                               ABL2 570
      MP=MS+1                                                           ABL2 571
      DO260N=1,JS                                                       ABL2 572
      NBAR=N-1                                                          ABL2 573
      HN=NBAR                                                           ABL2 574
      LO=LS-NBAR                                                        ABL2 575
      ZX(LO)=ZX(LS)-HN*HS                                               ABL2 576
      ZY(MP)=ZX(LO)                                                     ABL2 577
C                                                                       ABL2 578
```

```
C-----DEFINE MP AS THE TOTAL NO. OF POINT OVER WHICH SIMPSONS'S
C     RULE IS TO BE APPLIED
C
      DO241M=1,MP
      MBAR=M-1
      HM=MBAR
      MO=MP-MBAR
      ZY(MO)=ZY(MP)-HM*HSIMP1
      ZVAR=ZY(MO)
      IF(ZVAR.LE.Z1(1))ZVAR=Z1(1)
C
C
C-----FOR A SPECIFIED CHAR DISTANCE OBTAIN THE
C     CORRESPONDING TEMPERATURE FROM THE TEMPE-
C     RATURE PROFILE
C
      CALL INTRPL(ZVAR,Z1,T1,ITEMP,TVIS)
C
C     TVIS IS THE INTERPOLATED TEMPERATURE IN OF
C     WHICH CORRESPONDS TO THE VALUE OF ZVAR
C
      TK=(459.69+TVIS)/1.8
C
C     TK=TEMPERATURE IN KELVIN
C
      DO225I=1,NC
      TKE=TK/EK(I)
C
C
C-----FOR THE VALUE OF INTERPOLATED TEMPERATURE FIND
C     THE CORRESPONDING COLLISION INTEGRAL TO CALCULATE
C     THE PURE GAS VISCOCITY USING THE METHOD OF WILKE-JOHNSON
C
C
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```
      CALL INTRPL(TKE,XTKE,ZOMGA,NDATA,OMGA)                            ABL2 613
C                                                                       ABL2 614
C     OMGA=COLLISION INTEGRAL                                           ABL2 615
C                                                                       ABL2 616
 205  VIS(I)=2.6693E-3*SQRT(FW(I)*TK)/(SIG(I)**2*OMGA)                 ABL2 617
 206  TVAR=TK                                                           ABL2 618
      DO218KL=3,NN5                                                     ABL2 619
C                                                                       ABL2 620
C                                                                       ABL2 621
C-----INTERPOLATE FOR THE DATA GENERATED IN KINET                       ABL2 622
C                                                                       ABL2 623
C                                                                       ABL2 624
      CALL INTRPL (TVAR,TABLE(1,1),TABLE(I,KL),KMAX,VARY)               ABL2 625
      IF(KL.GT.4)GOTO216                                                ABL2 626
C                                                                       ABL2 627
C     KMAX=NUMBER OF DATA POINTS STORED                                 ABL2 628
C                                                                       ABL2 629
      IF(KL.EQ.4)GOTO215                                                ABL2 630
      AVGFW=VARY                                                        ABL2 631
      GOTO218                                                           ABL2 632
 215  W=VARY                                                            ABL2 633
      GOTO218                                                           ABL2 634
 216  Y(KL-4)=VARY                                                      ABL2 635
      IF(VARY.GT.0.)GOTO217                                             ABL2 636
      Y(KL-4)=1.E-70                                                    ABL2 637
 217  IF(M.GT.1)GOTO218                                                 ABL2 638
      TP(LO)=TVIS                                                       ABL2 639
      WFLUX(LO)=W                                                       ABL2 640
      KYCOMP=KL-4                                                       ABL2 641
      YCOMP(KYCOMP,LO)=Y(KYCOMP)                                        ABL2 642
 218  CONTINUE                                                          ABL2 643
      VMIX=0.                                                           ABL2 644
      DO236J=1,NC                                                       ABL2 645
      TERM=1.                                                           ABL2 646
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```
      DO230L=1,NC                                                       ABL2 647
      IF(L.EQ.J)GOTO230                                                 ABL2 648
      TOPV=(1.+SQRT(VIS(J)/VIS(L))*SQRT(SQRT(FW(L)/FW(J))))**2          ABL2 649
      BOTV=  SQRT(2.)*SQRT(1.+FW(J)/FW(L))*2.                           ABL2 650
      PHIV=TOPV/BOTV                                                    ABL2 651
      TERM=TERM+PHIV*(Y(L)/Y(J))                                        ABL2 652
 230  CONTINUE                                                          ABL2 653
      VMIX=VMIX+VIS(J)/TERM                                             ABL2 654
 236  CONTINUE                                                          ABL2 655
C     ACON5=2.42/3600.                                                  ABL2 656
 238  VISCOS=VMIX*ACON5                                                 ABL2 657
 239  PROD(MO)=TVIS*VISCOS*W/AVGFW                                      ABL2 658
      TT(MO)=TVIS/AVGFW*(W**2)                                          ABL2 659
 241  CONTINUE                                                          ABL2 660
      ZX(LO-1)=ZX(LO)-HS                                                ABL2 661
C                                                                       ABL2 662
C-----COMMENCE SIMPSON'S RULE INTEGRATION                               ABL2 663
C                                                                       ABL2 664
      SUM1=0.                                                           ABL2 665
      SUM2=0.                                                           ABL2 666
      SUM3=0.                                                           ABL2 667
      SUM4=0.                                                           ABL2 668
      MODD=MP-2                                                         ABL2 669
      DO255KP=3,MODD,2                                                  ABL2 670
      SUM1=SUM1+2.*PROD(KP)                                             ABL2 671
 255  SUM3=SUM3+2.*TT(KP)                                               ABL2 672
      MEVEN=MP-1                                                        ABL2 673
      DO256KP=2,MEVEN,2                                                 ABL2 674
      SUM2=SUM2+4.*PROD(KP)                                             ABL2 675
 256  SUM4=SUM4+4.*TT(KP)                                               ABL2 676
      SIMP1=(HSIMPI/3.0)*(PROD(1)+SUM1+SUM2+PROD(MP))+SIMP1             ABL2 677
      SIMP2=(HSIMPI/3.0)*(TT(1)+SUM3+SUM4+TT(MP))+SIMP2                 ABL2 678
C     FR2=778.16/32.2                                                   ABL2 679
      P(LO-1)=SQRT(PL**2+(2.*RR)*FR2*(ALPHA*SIMP1+BETA*SIMP2))          ABL2 680
```

```
 260  CONTINUE                                                          ABL2 681
C                                                                       ABL2 682
C                                                                       ABL2 683
C-----CALCULATE THE SURFACE HEAT FLUX,QL,THE REBADIATION,QR,            ABL2 684
C     AND THE TOTAL AERODYNAMIC HEATING,QA.                             ABL2 685
C                                                                       ABL2 686
C                                                                       ABL2 687
 261  QL=QCZ                                                            ABL2 688
 262  QR=EMIS*SIGMA*(TL+459.69)**4                                      ABL2 689
      QA=QL+QR                                                          ABL2 690
C                                                                       ABL2 691
      TP(1)=T1(1)                                                       ABL2 692
C                                                                       ABL2 693
C-----PRINT OUTPUT                                                      ABL2 694
C                                                                       ABL2 695
 2603 PRINT 597                                                         ABL2 696
 597  FORMAT(1H1////////)                                               ABL2 697
 5982 PRINT 5984                                                        ABL2 698
 5984 FORMAT(35X,'INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)'//)       ABL2 699
 5986 PRINT 5990                                                        ABL2 700
 5990 FORMAT(12X,51H                                        THEORETICAL/ABL2 701
     1/)                                                                ABL2 702
      PRINT600,T1(1),NC                                                 ABL2 703
 600  FORMAT(18X,'CHAR BACK TEMPERATURE (OF)='F7.1,13X,'NUMBER OF GAS COABL2 704
     1MPONENTS='I3/)                                                    ABL2 705
      THICK=DISTAN*12.                                                  ABL2 706
      THICK1=Z1(1)*12.                                                  ABL2 707
      PRINT 602,THICK,THICK1                                            ABL2 708
 602  FORMAT(18X,'THICKNESS OF CHAR(INCHES)='F8.6,6X,'THICKNESS OF DECOMABL2 709
     1POSITION ZONE='F8.6/)                                             ABL2 710
      QCZZ=QCZ-QCZI                                                     ABL2 711
      PRINT 604,WTOTAL,WFLUX(LS)                                        ABL2 712
 604  FORMAT(18X,'TOTAL MASS FLUX(LBS/FT2-SEC)='F7.6,6X,29HGAS MASS FLUXABL2 713
     1 AT THE SURFACE=,1X,F7.6/)                                        ABL2 714
```

```
      PRINT 611,TFMAX,VR                                                ABL2 715
 611  FORMAT(18X,'FRONT SURFACE TEMPERATURE(OF)='F6.1,5X,'SURFACE RECESSABL2 716
     1ION VELOCITY(FT/SEC)='F7.5/)                                      ABL2 717
      PRINT 603,QCZZ,QCZI                                               ABL2 718
 603  FORMAT(25X,'RATE OF HEAT ABSORBED IN THE CHAR ZONE(BTU/FT2-SEC)=' ABL2 719
     1F9.4,//25X,'RATE OF HEAT ABSORBED IN THE DECOMPOSITION ZONE(BTU/FTABL2 720
     22-SEC)='F9.4/)                                                    ABL2 721
      HCHAR=QCZZ/QCZ*100.                                               ABL2 722
      HDECOM=QCZI/QCZ*100.                                              ABL2 723
      SUM=REAC1+CPB1+CPB2                                               ABL2 724
      HGAS=CPB1/SUM*100.                                                ABL2 725
      HSOLID=CPB2/SUM*100.                                              ABL2 726
      HREACT=REAC1/SUM*100.                                             ABL2 727
      PRINT 605,HCHAR                                                   ABL2 728
 605  FORMAT(25X,'PERCENT OF TOTAL HEAT ABSORBED IN THE CHAR ZONE='E15.7ABL2 729
     1/)                                                                ABL2 730
      PRINT 606,HDECOM                                                  ABL2 731
 606  FORMAT(25X,'PERCENT OF TOTAL HEAT ABSORBED IN DECOMP-ZONE='E15.7/)ABL2 732
      PRINT 607,HGAS                                                    ABL2 733
 607  FORMAT(25X,'PERCENT OF HEAT ABSORBED BY THE GAS IN THE CHAR ZONE='ABL2 734
     1E15.7/)                                                           ABL2 735
      PRINT 608,HSOLID                                                  ABL2 736
 608  FORMAT(25X,'PERCENT OF HEAT ABSORBED BY THE SOLIDS IN THE CHAR ZONABL2 737
     1E='E15.7/)                                                        ABL2 738
      PRINT 610,HREACT                                                  ABL2 739
 610  FORMAT(25X,'PERCENT OF HEAT ABSORBED BY REACTION IN THE CHAR ZONE=ABL2 740
     1'E15.7/)                                                          ABL2 741
      PRINT586                                                          ABL2 742
 586  FORMAT(1H1)                                                       ABL2 743
C                                                                       ABL2 744
C--------PRINT OUTPUT PARAMETERS CORRESPONDING TO JS, GRID SIZE         ABL2 745
C                                                                       ABL2 746
      IKE=1                                                             ABL2 747
      MIKE=5                                                            ABL2 748
```

```
      LIKE=1                                                            ABL2 749
 2602 PRINT 597                                                         ABL2 750
 2662 PRINT 5984                                                        ABL2 751
      IF(LIKE.GT.1)GO TO 265                                            ABL2 752
      PRINT2650,DELTT                                                   ABL2 753
 2650 FORMAT(35X,23HTEMPERATURE DROP (OF) =,1X,F20.1/)                  ABL2 754
      DELP=(P(1)-PL)                                                    ABL2 755
      PRINT2651,DELP                                                    ABL2 756
 2651 FORMAT(35X,24HPRESSURE DROP (LB/FT2) =,1X,F19.1/)                 ABL2 757
      PRINT2652,QL                                                      ABL2 758
 2652 FORMAT(35X,33HSURFACE HEAT FLUX (BTU/FT2-SEC) =,1X,F10.2/)        ABL2 759
      PRINT2653,QR                                                      ABL2 760
 2653 FORMAT(35X,32HRADIANT HEAT FLUX BTU/FT2-SEC)=,1X,F11.2/)          ABL2 761
      PRINT2654,QA                                                      ABL2 762
 2654 FORMAT(35X,35HAERODYNAMIC HEAT FLUX(BTU/FT2-SEC)=,1X,F8.2//)      ABL2 763
 265  PRINT2720,(ZX(KK),KK=IKE,MIKE)                                    ABL2 764
 2720 FORMAT(14X,15HCHAR DEPTH (FT),6X,5F13.4)                          ABL2 765
      PRINT2721,(TP(KK),KK=IKE,MIKE)                                    ABL2 766
 2721 FORMAT(14X,16HTEMPERATURE (OF),5X,5F13.1)                         ABL2 767
      PRINT2730,(P(KK),KK=IKE,MIKE)                                     ABL2 768
 2730 FORMAT(14X,17HPRESSURE (LB/FT2),4X,5F13.1)                        ABL2 769
      PRINT2723,(WFLUX(KK),KK=IKE,MIKE)                                 ABL2 770
 2723 FORMAT(14X,21HMASS FLUX(LB/FT2-SEC),5F13.4/)                      ABL2 771
      PRINT2724                                                         ABL2 772
 2724 FORMAT(14X,66H  GAS COMPONENT                          COMPOSITION (ABL2 773
     1MOLE/MOLE GAS)/)                                                  ABL2 774
      IF(KEY.GT.1)GOTO2727                                              ABL2 775
      DO 2728 KICK=1,LS                                                 ABL2 776
      DO2728LL=1,NS                                                     ABL2 777
      YCOMP(LL,KICK)=YI(LL)                                             ABL2 778
 2728 CONTINUE                                                          ABL2 779
 2727 DO2729LL=1,NS                                                     ABL2 780
      YCOMP(LL,1)=YI(LL)                                                ABL2 781
      PRINT 2725,LL,SPCIF1(LL),SPCIE2(LL),(YCOMP(LL,KK),KK=IKE,MIKE)    ABL2 782
```

```
2725 FORMAT(12X,I2,2X,2A3,11X,5E13.4)                                  ABL2 783
2729 CONTINUE                                                          ABL2 784
     IF(MIKE.GE.LS)GO TO 2800                                          ABL2 785
     LIKE=LIKE+1                                                       ABL2 786
     MIKE=MIKE+5                                                       ABL2 787
     IKE=IKE+5                                                         ABL2 788
     GO TO 2602                                                        ABL2 789
2800 PRINT586                                                          ABL2 790
 300 STOP                                                              ABL2 791
     END                                                               ABL2 792
```

```
      SUBROUTINE CPMIX(T,NN,CPMX)
C
C
C-----THIS SUBROUTINE COMPUTES THE MOLAL HEAT CAPACITY
C     OF A NON-REACTING GAS.  IT IS ONLY USE FOR THE
C     FROZEN FLOW CASE.
      COMMON/KB/AI(30),BI(30),CI(30),DI(30),EI(30),AII(30),
     1      BII(30),CII(30),DII(30),EII(30),TLOW(30)
      COMMON/KM/XMOL(30)
      DIMENSION CP(30)
      RR=1.98726
C
C     CPMX=HEAT CAPCITY(BTU/LB-MOLE-OF)
C
C
C
C-----CALCULATE THE HEAT CAPACITY OF EACH INDIVIDUAL SPECIE.
C
C
      CPMX=0.
      DO 3 I=1,NN
      IF(T.GT.TLOW(I))GOTO1
      CP(I)=(AII(I)+(((EII(I)*T+DII(I))*T+CII(I))*T+BII(I))*T)*RR
      GOTO2
 1    CP(I)=(AI(I)+(((EI(I)*T+DI(I))*T+CI(I))*T+BI(I))*T)*RR
 2    CPMX=CPMX+CP(I)*XMOL(I)
 3    CONTINUE
      RETURN
      END
```

```
      SUBROUTINE INDPTH(TC,CDOV,DCDOV,GASCP,Q,CPV,RHO,TVAR,
C
     1 DELTKK,N,DELZ,VR,W,H)
C
      DIMENSION DRHODT(5)
C
C     INDEPTH SUBROUTINE CALCULATES THE PHYSICAL PROPER-
C     TIES FOR THE VIRGIN MATERIAL AND PYROLYSIS GASES.
C
C     T=TEMPERATURE IN FARENHEIT.
      IF(N.GT.1)GOTO2
      DCDOV=.338983E-8
      READ 1,A,B,C,D,E
C     A THROUGH E ARE CONSTANT FOR THE HEAT CAPACITY OF THE
C     VIRGIN MATERIAL.
    1 FORMAT(5E12.6)
C     CDOV=THERMAL CONDUCTIVITY OF THE VIRGIN MATERIAL
C          (BTU/(FT-SEC-OF))
    2 CDOV=1.266102E-5+.338983E-8*TC
C     DCDOV=RATE OF CHANGE OF CDOV WITH THEMPERATURE.
      T=TC
      IF(T.GT.750.)GOTO3
      T2=TC*T
      T3=TC*T2
      T4=TC*T3
C
C     CPV=HEAT CAPACITY OF THE VIRGIN MATERIAL(BTU/LB-OF)
      CPV=A+B*T+C*T2+D*T3+E*T4
  3   IF(DELTKK.GT.2.)H=H*2./DELTKK
C
      CALL PHMCR(TVAR,DELTKK,QPHNLC,QMICRO,N)
C
      IF(TVAR.GE.789.)GOTO200
C
```

```
      CALL NYLON(TVAR,DELTKK,QNYLON)                                    INDP  35
        GOTO210                                                         INDP  36
  200 QNYLON=0.                                                         INDP  37
C                                                                       INDP  38
  210 CALL DNSITY(RHO,TVAR,DELZ,VR,N,DRHODT,W,H)                        INDP  39
      Q=(QNYLON*DRHODT(1)+QPHNLC*DRHODT(2)+QMICRO*DRHODT(3))*(-1.8)     INDP  40
      RETURN                                                            INDP  41
      END                                                               INDP  42
```

```
      SUBROUTINE CHARPR                                                 CHAR   1
C     CHARPR SUBROUTINE CALCULATES THE EFFECTIVE THERMAL                CHAR   2
C     CONDUCTIVITY AND HEAT CAPACITY OF THE CHAR.                       CHAR   3
C                                                                       CHAR   4
C                                                                       CHAR   5
      COMMON/KF/CPS,CDO,DCDO,JCHAR,TC                                   CHAR   6
C                                                                       CHAR   7
C     T=TEMPERATURE IN RANKINE                                          CHAR   8
C     TC=TEMPERATURE IN FARENHEIT                                       CHAR   9
C     CPS=HEAT CAPACITY OF CHAR(BTU/LB-OF)                              CHAR  10
C     CDO=EFFECTIVE THERMAL CONDUCTIVITY(BTU/FT-SEC-OF)                 CHAR  11
C     DCDO=RATE OF CHANGE OF CDO WITH TEMPERATURE                       CHAR  12
C                                                                       CHAR  13
      TC2=TC*TC                                                         CHAR  14
      TC3=TC2*TC                                                        CHAR  15
      IF(TC.GT.2500.)GOTO507                                            CHAR  16
      T=TC+459.7                                                        CHAR  17
      CPS=0.43+3.6E-5*T-87.2E3/(T*T)                                    CHAR  18
      IF(TC.LT.1000.)CPS=0.39                                           CHAR  19
  507 CPS=0.52                                                          CHAR  20
      CDO=11.57E-5+5.3E-15*TC3                                          CHAR  21
      DCDO=15.9E-15*TC2                                                 CHAR  22
      RETURN                                                            CHAR  23
      END                                                               CHAR  24
```

```
      SUBROUTINE PHMCR(T,DELT,QPHNLC,QMICRO,K6)                         PHMC   1
      DIMENSION A(4),B(4),C(4),D(4),E(4),A1(4),B1(4),C1(4),D1(4),E1(4)  PHMC   2
C     THIS SUBROUTINE COMPUTES THE HEAT OF PYROLYSIS OF PHENOLIC,       PHMC   3
C     BASED ON THE DATA OF SYKES AND NELSON(THERMOANALYSIS OF           PHMC   4
C     ABLATION MATERIALS)                                               PHMC   5
      IF(K6.GT.1)GOTO4                                                  PHMC   6
      NUMBER=4                                                          PHMC   7
      AREA=1350.                                                        PHMC   8
      AREA1=1464.                                                       PHMC   9
C     READ1,NUMBER,AREA,AREA1                                           PHMC  10
    1 FORMAT(I6,2F10.8)                                                 PHMC  11
      DO2I=1,NUMBER                                                     PHMC  12
      READ3,A(I),B(I),C(I),D(I),E(I)                                    PHMC  13
    2 READ3,A1(I),B1(I),C1(I),D1(I),E1(I)                               PHMC  14
    3 FORMAT(5E12.8)                                                    PHMC  15
    4 IF(T.LT.623.)GOTO5                                                PHMC  16
      IF(T.GT.1073.)GOTO5                                               PHMC  17
      I=1                                                               PHMC  18
      IF(T.GT.748..AND.T.LT.798.)I=2                                    PHMC  19
      IF(T.GT.798..AND.T.LT.898.)I=3                                    PHMC  20
      IF(T.GT.898.)I=4                                                  PHMC  21
      DT=(T-623.)                                                       PHMC  22
      DT2=DT*DT                                                         PHMC  23
      DT3=DT2*DT                                                        PHMC  24
      DT4=DT3*DT                                                        PHMC  25
C     CALCULATE THE HEAT OF PYROLYSIS OF PHENOLIC(QPHNOL)               PHMC  26
      H=A(I)+B(I)*DT+C(I)*DT2+D(I)*DT3+E(I)*DT4                         PHMC  27
      QPHNLC=H*DELT*69.312/AREA                                         PHMC  28
C                                                                       PHMC  29
C     69.312=TOTAL HEAT ABSORBED BY THE DECOMPOSITION OF                PHMC  30
C     PHENOLIC IN CAL/GRAM.                                             PHMC  31
C                                                                       PHMC  32
C     CALCULATE THE HEAT OF PYROLYSIS OF PHENOLIC MICRO-                PHMC  33
C     BALLOONS(QMICRO)                                                  PHMC  34
```

```
      I=1                                                               PHMC  35
      IF(T.GT.713..AND.T.LT.798.)I=2                                    PHMC  36
      IF(T.GT.798..AND.T.LT.913.)I=3                                    PHMC  37
      IF(T.GT.913.)I=4                                                  PHMC  38
      H=A1(I)+B1(I)*DT+C1(I)*DT2+D1(I)*DT3+E1(I)*DT4                    PHMC  39
      QMICRO=H*DELT*90.822/AREA1                                        PHMC  40
C     90.822=TOTAL HEAT ABSORBED BY THE DECOMPOSITION OF                PHMC  41
C     PHENOLIC MICRO-BALLOONS IN CAL/GRAM.                              PHMC  42
      RETURN                                                            PHMC  43
    5 QPHNLC=0.                                                         PHMC  44
      QMICRO=0.                                                         PHMC  45
    6 RETURN                                                            PHMC  46
      END                                                               PHMC  47
```

```
      SUBROUTINE NYLON(T,DELT,QNYLON)                                   NYLO   1
C     THIS SUBROUTINE COMPUTES THE HEAT OF PYROLYSIS OF NYLON           NYLO   2
C     BASED ON THE DATA OF SYKES AND NELSON(THERMOANALYSIS OF           NYLO   3
C     ABLATION MATERIALS)                                               NYLO   4
C                                                                       NYLO   5
C     SLOPE=SLOPE OF LINE OBTAIN FROM SYKES AND NELSON'S DATA.          NYLO   6
      QNYLON=0.                                                         NYLO   7
      SLOPE=0.6086957                                                   NYLO   8
C                                                                       NYLO   9
      AREA=1122.                                                        NYLO  10
C     AREA=AREA UNDER CURVE OF FIGURE-2(DIFFERENTIAL THERMAL            NYLO  11
C     ANALYSIS) BY SYKES AND NELSON                                     NYLO  12
      CONST=150.5738/AREA                                               NYLO  13
      IF(T.LT.647.)GOTO4                                                NYLO  14
      IF(T.GT.699.)GOTO2                                                NYLO  15
      IF(T.GE.689..AND.T.LE.699.)GOTO1                                  NYLO  16
      H=SLOPE*(T-647.)                                                  NYLO  17
      GOTO3                                                             NYLO  18
    1 H=24.4                                                            NYLO  19
      GOTO3                                                             NYLO  20
    2 DH=SLOPE*(T-693.)                                                 NYLO  21
      H=28.0-DH                                                         NYLO  22
      IF(T.GE.739.)H=0.                                                 NYLO  23
    3 QNYLON=DELT*H*CONST                                               NYLO  24
    4 RETURN                                                            NYLO  25
      END                                                               NYLO  26
```

```
      SUBROUTINE DNSITY(RHO,T,DELZ,VR,K6,DRHODT,W,H)
C
C
C-----THIS SUBROUTINE CALCULATES THE DENSITY OF PHENOLIC-NYLON
C     COMPOSITES AS A FUNCTION OF TEMPERATURE--BASED ON DATA
C     OF SYKES AND NELSON(THERMOANALYSIS OF ABLATION MATERIALS)
C
C
C
      COMMON/KK/WTOTAL,RHOII
      REAL*8 RHOT
C
      DIMENSION RHOI(5),RHOT(5),RHOC(5),A(7),E(7),RATER(7),
     1DRHODT(5),XN(5,7),FRAC(5),RHOVOL(5)
      DIMENSION MASFRC(5),MASFLX(5),VOLUME(5),VOLFRC(5),DELFLX(5)
      DIMENSION RHOCC(5),DRHO(5)
      INTEGER COMPST
      REAL MASFRC,MASFLX
C
C
      IF(K6.GT.1)GOTO7
C
C-----READ INPUT
C
      READ 1,COMPST,NREACT
    1 FORMAT(2I6)
C
C
C     COMPST=NUMBER OF COMPOSITE MATERIALS DEGRADING DURING
C     ABLATION.
C     NREACT=NUMBER OF PSEUDO-KINETIC REACTIONS USED TO DES-
C     CRIBE THE DEGRADATION OF THE ABLATIVE COMPOSITES.
C
C
```

```
C-----INITIALIZATION OF XN(I,J),WHICH IS THE ORDER OF THE
C      REACTION
C
C
      DO2J=1,NREACT
      DO2I=1,COMPST
    2 XN(I,J)=0.
C
C     A(J)=FREQUENCY FACTOR(SEC-1)
C     E(J)=ENERGY OF ACTIVATION(JOULE/(MOLE))
C
C
      R=8.314
C     R=8.314(JOULES/(MOLE-OK))
C     RHOI(1)=68.6(NYLON)
C     RHOI(2)=80.0(PHENOLIC RESIN)
C     RHOI(3)=17.8(PHENOLIC-MICROBALLOONS)
C     RHOC(1)=68.6*0.075=5.145
C     RHOC(2)=80.0*0.541=43.28
C     RHOC(3)=17.8*542=9.6476
C
C
C     MASFRC(1)=0.4
C     MASFRC(2)=0.25
C     MASFRC(3)=0.35
C
C
C
C-----INITIALIZE
C
C
C
C     XN(I,J)=ORDER OF THE KINETIC EXPRESSION.
C
```

```
      DO3J=1,NREACT                                                     DNSI  69
    3 READ 4,I,A(J),E(J),XN(I,J)                                        DNSI  70
    4 FORMAT(4X,I6,3E10.8)                                              DNSI  71
      READ 5,(RHOI(I),RHOC(I),MASFRC(I),I=1,COMPST)                     DNSI  72
    5 FORMAT(3E10.4)                                                    DNSI  73
C                                                                       DNSI  74
C                                                                       DNSI  75
C     RHOI(I)=INITIAL DENSITY OF COMPOSITE I                            DNSI  76
C     RHOC(I)=RESIDUAL DENSITY OF COMPOSITE I                           DNSI  77
C     RHOT(I)=DENSITY OF THE COMPOSITE I AT ANY TEMPERATURE             DNSI  78
C                                                                       DNSI  79
C                                                                       DNSI  80
C-----LET RHOT(I)=RHOI(I) AS INITIAL CONDITION                          DNSI  81
C                                                                       DNSI  82
C                                                                       DNSI  83
      DO 6 I=1,COMPST                                                   DNSI  84
      RHOCC(I)=RHOC(I)+0.001*RHOC(I)                                    DNSI  85
      MASFLX(I)=0.                                                      DNSI  86
    6 RHOT(I)=RHOI(I)                                                   DNSI  87
C                                                                       DNSI  88
C                                                                       DNSI  89
C-----CALCUALTE THE VOLUME FRACTION OF EACH COMPOSITE                   DNSI  90
C                                                                       DNSI  91
C                                                                       DNSI  92
      SUMVOL=0.                                                         DNSI  93
      DO 60 I=1,COMPST                                                  DNSI  94
      VOLUME(I)=MASFRC(I)/RHOT(I)                                       DNSI  95
   60 SUMVOL=SUMVOL+VOLUME(I)                                           DNSI  96
      DO 65 I=1,COMPST                                                  DNSI  97
C                                                                       DNSI  98
C     VOLFRC(I)=VOLUME FRACTION OF EACH COMPOSITE                       DNSI  99
C                                                                       DNSI 100
   65 VOLFRC(I)=VOLUME(I)/SUMVOL                                        DNSI 101
C                                                                       DNSI 102
```

```
C                                                                       DNSI 103
C-----COMPUTE THE DENSITY OF THE COMPOSITE                              DNSI 104
C                                                                       DNSI 105
C                                                                       DNSI 106
C                                                                       DNSI 107
C     RHO=DENSITY OF COMPOSITE                                          DNSI 108
      RHO=1./SUMVOL                                                     DNSI 109
C                                                                       DNSI 110
C                                                                       DNSI 111
C     RHOII=INITIAL DENSITY OF COMPOSITE                                DNSI 112
      RHOII=RHO                                                         DNSI 113
C                                                                       DNSI 114
C                                                                       DNSI 115
C                                                                       DNSI 116
C-----CALCULATE THE TOTAL MASS FLUX                                     DNSI 117
C                                                                       DNSI 118
C                                                                       DNSI 119
C                                                                       DNSI 120
C     WTOTAL=TOTAL MASS FLUX(LBS/FT**2-SEC)                             DNSI 121
C                                                                       DNSI 122
      WTOTAL=RHOII*VR                                                   DNSI 123
      PRINT 66,RHO,WTOTAL                                               DNSI 124
   66 FORMAT(1X,'INITIAL DENSITY OF COMPOSITE(LBS/FT**3)='F10.5,2X,     DNSI 125
     1'WTOTAL(LBS/FT**2-SEC)='E15.7/)                                   DNSI 126
    7 RRR=1000./(R*T)                                                   DNSI 127
      RHOPRV=RHO                                                        DNSI 128
      DO 9 I=1,COMPST                                                   DNSI 129
      SUM=0.                                                            DNSI 130
      DO 8 J=1,NREACT                                                   DNSI 131
      IF(XN(I,J).EQ.0.)GOTO8                                            DNSI 132
C                                                                       DNSI 133
C     RATER(J)=SPECIFIC REACTION VELOCITY                               DNSI 134
      IF(RHOT(I).LE.RHOC(I))RHOT(I)=RHOCC(I)                            DNSI 135
      RATER(J)=-RHOI(I)*((RHOT(I)-RHOC(I))/RHOI(I))**XN(I,J)*A(J)*EXP(- DNSI 136
```

```
     1E(J)*RRR)                                                         DNSI 137
      SUM=SUM+RATER(J)                                                  DNSI 138
 8    CONTINUE                                                          DNSI 139
      DRHODT(I)=SUM                                                     DNSI 140
      IF(RHOT(I).LE.RHOCC(I))DRHODT(I)=0.                               DNSI 141
    9 CONTINUE                                                          DNSI 142
C                                                                       DNSI 143
C-----CONTROLLING STEP SIZE FOR STABILITY                               DNSI 144
C                                                                       DNSI 145
      TEST=0.                                                           DNSI 146
      DO 90 I=1,COMPST                                                  DNSI 147
      DRHO(I)=-DELZ*DRHODT(I)/VR                                        DNSI 148
   90 TEST=AMAX1(TEST,DRHO(I))                                          DNSI 149
      IF(TEST.GT.0.1)H=H/2.                                             DNSI 150
      IF(TEST.LT..05)H=H*2                                              DNSI 151
      IF(H.GT.2.08E-4)H=2.08E-4                                         DNSI 152
C     DELZ=STEP SIZE IN FEET                                            DNSI 153
      IF(VR.GE.1.E-2.AND.H.GT.1.E-5)H=1.E-5                             DNSI 154
      DELZ=H                                                            DNSI 155
      RHO=0.                                                            DNSI 156
      W=0.                                                              DNSI 157
      DO10I=1,COMPST                                                    DNSI 158
      DELFLX(I)=-DELZ*DRHODT(I)                                         DNSI 159
C                                                                       DNSI 160
C     DELFLX(I)=CHANGE IN MASS FLUX DUE TO A CHANGE IN THE              DNSI 161
C     DENSITY OF THE COMPOSITES.                                        DNSI 162
C                                                                       DNSI 163
      RHOT(I)=RHOT(I)-DELFLX(I)/VR                                      DNSI 164
      RHOVOL(I)=RHOT(I)*VOLFRC(I)                                       DNSI 165
      RHO=RHO+RHOVOL(I)                                                 DNSI 166
C     RHO=BULK DENSITY OF THE COMPOSITE                                 DNSI 167
      MASFLX(I)=MASFLX(I)+DELFLX(I)                                     DNSI 168
   10 W=W+MASFLX(I)                                                     DNSI 169
      W1=(RHOII-RHO)*VR                                                 DNSI 170
```

```
      W=W1                                                              DNSI 171
      DO 100 I=1,COMPST                                                 DNSI 172
100   MASFRC(I)=RHOVOL(I)/RHO                                           DNSI 173
      PRINT 11,RHO,DELZ,VR,T,W                                          DNSI 174
11    FORMAT(1X,'RHO(OVERALL DENSITY OF ='F10.4,' DELZ='E10.4,'V='E10.4,DNSI 175
     1' T='E10.4,' W='E13.5)                                            DNSI 176
      PRINT 12                                                          DNSI 177
  12  FORMAT(8X,'VIRGIN MATERIAL)')                                     DNSI 178
      DO 14 I=1,COMPST                                                  DNSI 179
      PRINT 13,I,RHOT(I),I,DRHODT(I),I,DRHO(I),I,MASFRC(I)              DNSI 180
13    FORMAT(1X,'RHOT('I1,')='D12.6,' DRODT('I1,')='E12.6,' DRHO('I1,')=DNSI 181
     1'E12.6,' MASFRC('I1,')='E12.6)                                    DNSI 182
14    CONTINUE                                                          DNSI 183
      RETURN                                                            DNSI 184
      END                                                               DNSI 185
```

```
C     SUBROUTINE CHARPR CALCULATES THE EFFECTIVE THERMAL
C     CONDUCTIVITY AND HEAT CAPACITY OF THE CHAR.
C
C
      COMMON/KF/CPS,CDO,DCDO,JCHAR,TC
C
C     T=TEMPERATURE IN RANKINE
C     TC=TEMPERATURE IN FARENHEIT
C     CPS=HEAT CAPACITY OF CHAR(BTU/LB-OF)
C     CDO=EFFECTIVE THERMAL CONDUCTIVITY(BTU/FT-SEC-OF)
C     DCDO=RATE OF CHANGE OF CDO WITH TEMPERATURE
C
      TC2=TC*TC
      TC3=TC2*TC
      IF(TC.GT.2500.)GOTO507
      T=TC+459.7
      CPS=0.43+3.6E-5*T-87.2E3/(T*T)
      IF(TC.LT.1000.)CPS=0.39
  507 CPS=0.52
      CDO=11.57E-5+5.3E-15*TC3
      DCDO=15.9E-15*TC2
      RETURN
      END
```

```
      SUBROUTINE INTRPL(VAR,X,F,IMAX,SOM)                               INTR   1
C                                                                       INTR   2
C                                                                       INTR   3
C-----THIS PROGRAM PERFORMS LAGRANGIAN INTERPOLATION                    INTR   4
C     WITH NON-EQUAL STEP SIZE BETWEEN POINTS                           INTR   5
C     F=DEPENDANT VARIABLE                                              INTR   6
C     X=INDEPENDENT VARIABLE                                            INTR   7
C     VAR-VALUE OF X FOR WHICH CORRESPONDING VALUE OF                   INTR   8
C     F IS DESIRED BY INTERPOLATION                                     INTR   9
C     IMAX=NUMBER OF POINTS IN ARRAY X OR F                             INTR  10
C     SOM=VALUE OF INTERPOLATED DEPENDENT VARIABLE                      INTR  11
C     NPTS=NUMBER OF POINTS USED FOR INTERPOLATION                      INTR  12
C                                                                       INTR  13
      DIMENSION X(100),F(100),XN(300),FN(300)                           INTR  14
      NPTS=3                                                            INTR  15
  607 XUP=1.E30                                                         INTR  16
      DO611I=1,IMAX                                                     INTR  17
      T=VAR-X(I)                                                        INTR  18
      IF(T.GE.0.)GOTO609                                                INTR  19
  608 T=-T                                                              INTR  20
  609 IF(T.GE.XUP)GOTO611                                               INTR  21
  610 IP=I                                                              INTR  22
      XUP=T                                                             INTR  23
  611 CONTINUE                                                          INTR  24
      IN=1                                                              INTR  25
      NPP=NPTS+1                                                        INTR  26
      DO618I=1,NPP                                                      INTR  27
      FN(I)=F(IP)                                                       INTR  28
      XN(I)=X(IP)                                                       INTR  29
      IF(IN.GT.0)GOTO613                                                INTR  30
  612 IQ=IP-I                                                           INTR  31
      GOTO615                                                           INTR  32
  613 IQ=IP+I                                                           INTR  33
      IF(IMAX.GE.IQ)GOTO615                                             INTR  34
```

```
614   IP=IP-1                                                    INTR  35
      GOTO618                                                    INTR  36
615   IF(IQ.GT.0)GOTO617                                         INTR  37
616   IP=IP+1                                                    INTR  38
      GOTO618                                                    INTR  39
617   IP=IQ                                                      INTR  40
      IN=-IN                                                     INTR  41
618   CONTINUE                                                   INTR  42
      SOM=0.                                                     INTR  43
      FACT=1.                                                    INTR  44
      DO620J=1,NPTS                                              INTR  45
      SOM=SOM+FACT*FN(1)                                         INTR  46
      DO619I=J,NPTS                                              INTR  47
      IQ=I-J+1                                                   INTR  48
619   FN(IQ)=(FN(IQ+1)-FN(IQ))/(XN(I+1)-XN(IQ))                  INTR  49
620   FACT=FACT*(VAR-XN(J))                                      INTR  50
      RETURN                                                     INTR  51
      END                                                        INTR  52
```

```
      SUBROUTINE KINET                                                  KINE   1
C                                                                       KINE   2
C                                                                       KINE   3
C-----KINET CALCULATES THE COMPOSITION ,RATE,AND HEAT OF REACTION FOR   KINE   4
C     THE KINETICS MODEL                                                KINE   5
C                                                                       KINE   6
      REAL*8 C,FK,EK,RATER,Z22,H11                                      KINE   7
C     REAL*8 C,FK,EK,XMULTR,XMULTP                                      KINE   8
      COMMON/KC/ICODE(30),Y1(30),XFW(30)                                KINE   9
      COMMON/KCC/SPCIE1(30),SPCIE2(30),TABLE(300,26),Z,INDPT            KINE  10
      COMMON/KD/RSC(30,30),PSC(30,30),NREX(30,30),NPEX(30,30),          KINE  11
     1AF(30),AEF(30),SF(30),AK(30),BK(30),EKMAX(30),EKMIN(30),NCOEF(30) KINE  12
      COMMON/KEE/PL,RR,TZERO,EPS,KEY,NC,NS,MM,NQ                        KINE  13
      COMMON/KG/ENT(30),RATE(30),T,HEAT1,SUM7                           KINE  14
      COMMON/KH/KSP1,NEQ                                                KINE  15
      COMMON/KI/KN,K7,DTC,HEAT,WEPS,K2,AVGFW,K3,Z2,DELZ,H               KINE  16
      COMMON/KJ/DELTK,TVAR                                              KINE  17
      COMMON/KQ/Z22                                                     KINE  18
      DIMENSION RATIO(30),RATERR(30)                                    KINE  19
      DIMENSION TAU(30)                                                 KINE  20
      DIMENSION EKK(30),EK(30)                                          KINE  21
      DIMENSION FLUXMO(30),FLUXMA(30),C(30),PERCE(30),                  KINE  22
     1          TEST(30),FK(30),RK(30),RATER(30)                        KINE  23
      DIMENSION NSTORE(30),RATE1(30)                                    KINE  24
      DIMENSION DLFLUX(30)                                              KINE  25
C                                                                       KINE  26
C                                                                       KINE  27
C     KEY=3(NONEQUILIBRIUM FLOW)                                        KINE  28
C     DELZ=FINITE DIFFERENCE STEP SIZE IN CM.                           KINE  29
C                                                                       KINE  30
      IF(K7.GT.1)GOTO74                                                 KINE  31
      IPRINT=0                                                          KINE  32
C                                                                       KINE  33
C     KSP1=TOTAL NUMBER OF CHEMICAL SPECIES(SOLID + GASES)              KINE  34
```

```
C       KSP=NUMBER OF GASEOUS SPECIES                                   KINE  35
C       KSP2=KSP1+1(USED TO IDENTIFY THIRD BODY REACTIONS)              KINE  36
C                                                                       KINE  37
C-----INITIALIZATION OF PARAMENTERS                                     KINE  38
C                                                                       KINE  39
        KPASS=0                                                         KINE  40
        H=1.E-6                                                         KINE  41
        KSP1=NS                                                         KINE  42
        KSP=NC                                                          KINE  43
        KSP2=KSP1+1                                                     KINE  44
        KOS=NS+4                                                        KINE  45
        N=0                                                             KINE  46
        K2=0                                                            KINE  47
        Z22=Z2                                                          KINE  48
        K44=0                                                           KINE  49
C                                                                       KINE  50
C       Y1(I)=MOLE FRACTION OF THE CHEMICAL SPECIES                     KINE  51
C       KSP2=KSP1+1(USED TO IDENTIFY THIRD BODY REACTION)               KINE  52
C                                                                       KINE  53
        DO 83 I=1,KSP2                                                  KINE  54
        DO 83 J=1,KSP2                                                  KINE  55
        RSC(I,J)=0.                                                     KINE  56
        PSC(I,J)=0.                                                     KINE  57
        NREX(I,J)=0                                                     KINE  58
        NPEX(I,J)=0                                                     KINE  59
   83 CONTINUE                                                          KINE  60
C                                                                       KINE  61
C       RSC(I,J)=STOCHIOMETRIC COEFFICIENT OF THE REACTANT              KINE  62
C                J IN REACTION I.                                       KINE  63
C       PSC(I,J)=STOCHIOMETRIC COEFFICIENT OF THE PRODUCTS.             KINE  64
C       NPEX(I,J)=POWER ON THE CONCENTRATION OF THE PRODUCTS.           KINE  65
C       NREX(I,J)=POWER ON THE CONCENTRATION OF THE REACTANTS.          KINE  66
C                                                                       KINE  67
C                                                                       KINE  68
```

```
C-----CONVERT TO KINET UNITS                                            KINE  69
C                                                                       KINE  70
C                                                                       KINE  71
      ACON4=929.0304/453.59                                             KINE  72
      ACON41=ACON4*30.48                                                KINE  73
      ACON44=1./ACON4                                                   KINE  74
      ACON55=30.48**3/252.                                              KINE  75
      WNEW=WEPS/EPS                                                     KINE  76
      W=WNEW                                                            KINE  77
      WNEW1=WNEW                                                        KINE  78
C                                                                       KINE  79
C     XFW(I)=MOLECULAR WEIGHT OF SPECIE I                               KINE  80
C     INPUT SUBROUTINE READS IN THE KINETIC DATA                        KINE  81
C                                                                       KINE  82
      CALL INPUT1                                                       KINE  83
C                                                                       KINE  84
      K7=2                                                              KINE  85
C     IF K7 IS GREATER THAN 1 CALL INOUT IS BYPASSED                    KINE  86
C                                                                       KINE  87
      P=PL/2160.                                                        KINE  88
C                                                                       KINE  89
C     P=PRESSURE(IN ATMOSPHERES)                                        KINE  90
C                                                                       KINE  91
      R=82.06                                                           KINE  92
C                                                                       KINE  93
C     R AND RR ARE UNIVERSAL GAS CONSTANTS IN DIFFERENT UNITS.          KINE  94
C                                                                       KINE  95
C-----CALCULATE INITIAL AVERAGE MOLECULAR WEIGHT                        KINE  96
C                                                                       KINE  97
      SUM=0.                                                            KINE  98
      DO1J=1,KSP                                                        KINE  99
 1    SUM=SUM+XFW(J)*Y1(J)                                              KINE 100
      AVGFW=SUM                                                         KINE 101
      ACON1=W/AVGFW*ACON44                                              KINE 102
```

```
C       ACON1=TOTAL MOLAL FLUX IN GRAM-MOLES/(CM2-SEC)                    KINE 103
C                                                                         KINE 104
C                                                                         KINE 105
C                                                                         KINE 106
C-----CALCULATE INITIAL MOLAL FLUX(FLUXMO--GM-MOLES/CM2-SEC)              KINE 107
C                                                                         KINE 108
C                                                                         KINE 109
        DO2J=1,KSP1                                                       KINE 110
        FLUXMO(J)=ACON1*Y1(J)                                             KINE 111
C                                                                         KINE 112
C                                                                         KINE 113
C-----CALCULATE INITIAL MASS FLUX(FLUXMA)                                 KINE 114
C                                                                         KINE 115
C                                                                         KINE 116
 2      FLUXMA(J)=FLUXMO(J)*XFW(J)                                        KINE 117
        WNEW2=W                                                           KINE 118
        TPREV=TVAR-5.                                                     KINE 119
C                                                                         KINE 120
C-----CONVERT STEP SIZE TO CENTIMETERS                                    KINE 121
C                                                                         KINE 122
   74   DELZZ=DELZ*30.48                                                  KINE 123
        T=TVAR                                                            KINE 124
        XDELTT=TVAR-TPREV                                                 KINE 125
        SUM1=0.                                                           KINE 126
        RRR=1000./(RR*T)                                                  KINE 127
        ACON9=R*T/P                                                       KINE 128
        DO5J=1,KSP                                                        KINE 129
    5   SUM1=SUM1+FLUXMO(J)*ACON9                                         KINE 130
C                                                                         KINE 131
C                                                                         KINE 132
C-----CALCULATE THE CONCENTRATION C(J) OF THE SPECIES(GM-MOLES/CM3)       KINE 133
C                                                                         KINE 134
C                                                                         KINE 135
        SUM=0.                                                            KINE 136
```

```
      DO6J=1,KSP                                                        KINE 137
      C(J)=FLUXMO(J)/SUM1                                               KINE 138
    6 SUM=SUM+C(J)                                                      KINE 139
      C(KSP1)=SUM*Y1(KSP1)                                              KINE 140
      C(KSP2)=SUM                                                       KINE 141
C                                                                       KINE 142
C     C(KSP2)=CONCENTRATION USE FOR A THIRD BODY REACTION               KINE 143
C                                                                       KINE 144
C                                                                       KINE 145
C-----CALCULATE FK AND RK WHICH ARE THE FOWARD                          KINE 146
C     AND REVERSE REACTION RATE CONSTANTS.                              KINE 147
C                                                                       KINE 148
C                                                                       KINE 149
      RT=R*T                                                            KINE 150
C     EK=EQUILIBIRUM CONSTANT                                           KINE 151
      DO7I=1,NEQ                                                        KINE 152
      IF(SF(I).EQ.0.)GOTO900                                            KINE 153
      FK(I)=AF(I)*T**(-SF(I))*EXP(-AEF(I)*RRR)                          KINE 154
      GOTO902                                                           KINE 155
  900 FK(I)=AF(I)*EXP(-AEF(I)*RRR)                                      KINE 156
  902 A1=AK(I)                                                          KINE 157
      A2=BK(I)                                                          KINE 158
      EKK(I)=EXP(A1+A2/T)                                               KINE 159
      X12=EKMAX(I)                                                      KINE 160
      IF(EKK(I).GT.EKMAX(I))EKK(I)=EKMAX(I)                             KINE 161
      IF(EKK(I).LT.EKMIN(I))EKK(I)=EKMIN(I)                             KINE 162
      EK(I)=EKK(I)/(RT**NCOEF(I))                                       KINE 163
      RK(I)=FK(I)/EK(I)                                                 KINE 164
    7 CONTINUE                                                          KINE 165
C                                                                       KINE 166
C                                                                       KINE 167
C-----CALCULATION OF REACTION RATE OF SPECIE(J)                         KINE 168
C                                                                       KINE 169
C                                                                       KINE 170
```

```
C                                                                       KINE 171
      RATER(1)=FK(1)*(C(3)-C(1)*C(8)/EK(1))                             KINE 172
      RATER(2)=FK(2)*(C(3)-C(2)*C(9)/EK(2))                             KINE 173
      RATER(3)=FK(3)*(C(2)*C(2)-C(4)/EK(3))                             KINE 174
      RATER(4)=FK(4)*(C(4)-C(5)*C(8)/EK(4))                             KINE 175
      RATER(5)=FK(5)*(C(5)-C(6)*C(8)/EK(5))                             KINE 176
      RATER(6)=FK(6)*(C(6)-C(8)/EK(6))                                  KINE 177
      RATER(7)=FK(7)*(C(6)-C(7)*C(9)/EK(7))                             KINE 178
      RATER(8)=FK(8)*(C(16)-C(14)*C(8)/EK(8))                           KINE 179
      RATER(9)=FK(9)*(C(15)-C(14)*C(14)/EK(9))                          KINE 180
      RATER(10)=FK(10)*(C(8)-C(9)*C(9)/EK(10))                          KINE 181
      RATER(11)=FK(11)*(C(16)-C(17)*C(9)/EK(11))                        KINE 182
      RATER(12)=FK(12)*(C(9)*C(15)-C(14)*C(17)/EK(12))                  KINE 183
      RATER(13)=FK(13)*(C(15)-C(14)*C(18)/EK(13))                       KINE 184
      RATER(14)=FK(14)*(C(11)*C(8)-C(12)*C(16)/EK(14))                  KINE 185
      RATER(15)=FK(15)*(C(12)-C(6)*C(6)*C(6)/EK(15))                    KINE 186
      DO 121 I=1,KSP1                                                   KINE 187
      XJ=RATER(I)                                                       KINE 188
      IF(XJ.LT.0.)RATER(I)=0.                                           KINE 189
  121 CONTINUE                                                          KINE 190
      RATE(1)=RATER(1)                                                  KINE 191
      RATE(2)=RATER(2)-2.*RATER(3)                                      KINE 192
      RATE(3)=-RATER(1)-RATER(2)                                        KINE 193
      RATE(4)=RATER(3)-RATER(4)                                         KINE 194
      RATE(5)=RATER(4)-RATER(5)                                         KINE 195
      RATE(6)=RATER(5)-RATER(6)-RATER(7)+3.*RATER(15)                   KINE 196
      RATE(7)=RATER(7)                                                  KINE 197
      RATE(8)=RATER(1)+RATER(4)+RATER(5)+RATER(6)+RATER(8)-RATER(10)-   KINE 198
     1 RATER(14)                                                        KINE 199
      RATE(9)=RATER(2)+RATER(7)+2.*RATER(10)+RATER(11)-RATER(12)        KINE 200
      RATE(10)=0.                                                       KINE 201
      RATE(11)=-RATER(14)                                               KINE 202
      RATE(12)=RATER(14)-RATER(15)                                      KINE 203
      RATE(13)=0.                                                       KINE 204
```

```
      RATE(14)=RATER(8)+2.*RATER(9)+RATER(12)+RATER(13)                 KINE 205
      RATE(15)=-RATER(9)-RATER(12)-RATER(13)                            KINE 206
      RATE(16)=-RATER(8)-RATER(11)+RATER(14)                            KINE 207
      RATE(17)=RATER(11)+RATER(12)                                      KINE 208
      RATE(18)=RATER(13)                                                KINE 209
      RATE(19)=RATER(6)*2.-RATER(8)-RATER(9)                            KINE 210
C     RATE(J)= REACTION RATE(GRAM-M/LES/(CM3-SEC)) FOR SPECIE J.        KINE 211
C                                                                       KINE 212
      TPREV=TVAR                                                        KINE 213
      K44=K44+1                                                         KINE 214
      DSUM=0.                                                           KINE 215
      DSUMM=0.                                                          KINE 216
      TESS=0.                                                           KINE 217
      DO 130 I=1,KSP1                                                   KINE 218
      DLFLUX(I)=RATE(I)*XFW(I)*DELZZ                                    KINE 219
      RATIOO=DLFLUX(I)/FLUXMA(I)                                        KINE 220
      RATIO(I)=RATIOO                                                   KINE 221
      IF(RATIOO.GE.0.)GOTO129                                           KINE 222
      RATO=ABS(RATIOO)                                                  KINE 223
      IF(RATO.GT.0.1)KPASS=1                                            KINE 224
 129  ADFLUX=ABS(DLFLUX(I))                                             KINE 225
      TESS=AMAX1(TESS,ADFLUX)                                           KINE 226
      DSUM=DSUM+DLFLUX(I)                                               KINE 227
      IF(I.GT.KSP)GOTO130                                               KINE 228
      DSUMM=DSUM                                                        KINE 229
  130 CONTINUE                                                          KINE 230
C                                                                       KINE 231
C-----CHECK STEP SIZE FOR STABILITY                                     KINE 232
C                                                                       KINE 233
      IF(KPASS.EQ.1)H=H/4.                                              KINE 234
      IF(H.GT.1.08E-4)H=1.08E-4                                         KINE 235
      IF(RATO.LT.0.010)H=H*2                                            KINE 236
      IF(H.LT.2.5E-7)H=2.5E-7                                           KINE 237
      DELZZ=H*30.48                                                     KINE 238
```

```
      DO 13 J=1,KSP1                                                    KINE 239
      TEST(J)=FLUXMA(J)                                                 KINE 240
      FLUXMA(J)=FLUXMA(J)+RATE(J)*DELZZ*XFW(J)                          KINE 241
      IF(FLUXMA(J).GE.0.)GOTO13                                         KINE 242
      FLUXMA(J)=1.E-40                                                  KINE 243
   13 CONTINUE                                                          KINE 244
      KPASS=0                                                           KINE 245
      WNEW1=WNEW1-RATE(KSP1)*DELZZ*XFW(KSP1)*ACON4                      KINE 246
      WNEW=WNEW1                                                        KINE 247
      WEPS=WNEW*EPS                                                     KINE 248
      WNEW2=0.                                                          KINE 249
      SUM3=0.                                                           KINE 250
  132 DO 19 J=1,KSP1                                                    KINE 251
      FLUXMO(J)=FLUXMA(J)/XFW(J)                                        KINE 252
      IF(J.GT.KSP)GOTO19                                                KINE 253
      SUM3=SUM3+FLUXMO(J)                                               KINE 254
      WNEW2=WNEW2+FLUXMA(J)                                             KINE 255
   19 CONTINUE                                                          KINE 256
      WNEW2=WNEW2*ACON4                                                 KINE 257
      WNEW22=WNEW2                                                      KINE 258
      DO14J=1,KSP1                                                      KINE 259
      Y1(J)=FLUXMO(J)/SUM3                                              KINE 260
   14 PERCE(J)=Y1(J)*100.                                               KINE 261
      SUM=0.                                                            KINE 262
      DO 111 I=1,KSP                                                    KINE 263
      SUM=SUM+XFW(I)*Y1(I)                                              KINE 264
  111 CONTINUE                                                          KINE 265
      AVGFW=SUM                                                         KINE 266
      RHO=ACON41/ACON9*AVGFW                                            KINE 267
      VEL=WNEW/RHO                                                      KINE 268
C                                                                       KINE 269
C-----CONVERT THE UNITS OF THE HEAT OF REACTION                         KINE 270
C     TERM TO THOSE COMPATIBLE WITH GROUP                               KINE 271
C                                                                       KINE 272
```

```
C                                                                       KINE 273
      CALL THERM2                                                       KINE 274
C                                                                       KINE 275
C     HEAT=RATE OF HEAT ABSORBED OR RELEASE BY CHEMICAL                 KINE 276
C          REACTIONS(BTU/FT**3-SEC).                                    KINE 277
C                                                                       KINE 278
      HEAT=HEAT1*ACON55                                                 KINE 279
      HEAT3=HEAT/DTC                                                    KINE 280
      H11=H                                                             KINE 281
      Z22=Z22+H11                                                       KINE 282
      IF(Z2.LE.Z22)GOTO37                                               KINE 283
      RETURN                                                            KINE 284
   37 K2=K2+1                                                           KINE 285
      IF(K2.GE.299)K2=299                                               KINE 286
      DO17 I=5,KOS                                                      KINE 287
      TABLE(K2,I)=Y1(I-4)                                               KINE 288
   17 CONTINUE                                                          KINE 289
      TABLE(K2,1)=T                                                     KINE 290
      TABLE(K2,2)=HEAT                                                  KINE 291
      TABLE(K2,3)=AVGFW                                                 KINE 292
      TABLE(K2,4)=WNEW                                                  KINE 293
      PRINT 94, WNEW,WNEW2,DELZ,XDELTT                                  KINE 294
      PRINT 776                                                         KINE 295
  776 FORMAT(1H1,//11X,'HEAT OF FORMATION',3X,'MOLE FRACTION',          KINE 296
     1        5X,'RATE(I)',9X,'RATER(I)',8X,'FLUXMA(I)'///)             KINE 297
      DO 779 I=1,KSP1                                                   KINE 298
      PRINT 777,SPCIE1(I),SPCIE2(I),ENT(I),Y1(I),RATE(I),               KINE 299
     1          RATER(I),FLUXMA(I),DLFLUX(I),RATIO(I)                   KINE 300
  777 FORMAT(6X,2A3,7E16.7)                                             KINE 301
  779 CONTINUE                                                          KINE 302
      PRINT 780                                                         KINE 303
  780 FORMAT(1H0)                                                       KINE 304
      PRINT 781,Z,H,K2,K3,K44,Z22,DSUM,DSUMM                            KINE 305
  781 FORMAT(6X,'Z='1E12.6,3X,'H='E12.6,3X,'K2='I3,' K3='I8,1X,         KINE 306
```

```
     1'K44='I6,' Z22='D18.9,2E16.7)                                    KINE 307
      PRINT 6022,T                                                     KINE 308
 6022 FORMAT(7X,18HTEMPERATURE IN OK=,1F10.3)                          KINE 309
      TF=T*1.8-460.0                                                   KINE 310
      PRINT 6023,TF                                                    KINE 311
 6023 FORMAT(7X,18HTEMPERATURE IN OF=,1F10.3)                          KINE 312
 6024 FORMAT(7X,40HHEAT ABSORBED BY REACTIONS(BTU/FT2-SEC)=,1E14.5)    KINE 313
      PRINT 6024,HEAT3                                                 KINE 314
      PRINT 6025,WNEW                                                  KINE 315
 6025 FORMAT(7X,18HOVERALL MASS FLUX=,E14.7)                           KINE 316
      PRINT 6026,AVGFW                                                 KINE 317
 6026 FORMAT(7X,32HAVERAGE MOLECULAR WEIGHT OF GAS=,1F10.3///)         KINE 318
      PRINT 6032,SUM7                                                  KINE 319
 6032 FORMAT(//10X,36HENTHALPY OF THE REACTING GAS SYSTEM=,1E16.8)     KINE 320
   94 FORMAT(1X,5E20.8)                                                KINE 321
      PRINT 95,VEL,RHO                                                 KINE 322
 95   FORMAT(1X,'VEL(FT/SEC)='E15.7,' RHO(LBS/FT3)='E15.7/)            KINE 323
      RETURN                                                           KINE 324
      END                                                              KINE 325
```

```
      SUBROUTINE THERM2                                                 THER   1
C                                                                       THER   2
C                                                                       THER   3
C-----THERMO SUBROUTINE CALCULATES THE HEAT OF REACTION OF              THER   4
C     THE MIXTURE,THE HEAT OF FORMATION OF EACH INDIVIDUAL              THER   5
C     CHEMICAL SPECIE, AND THE HEAT CAPACITY OF THE MIXTURE             THER   6
C                                                                       THER   7
C                                                                       THER   8
      COMMON/KA/S1(6),S2(6),S3(6),S4(6),S5(6),A11(6),A22(6),            THER   9
     1       A33(6),A44(6),A55(6),FI(30),FII(30),GI(30),                THER  10
     2       GII(30),AA(30,6),S6(6),A66(6),JCODE(6),CPMX                THER  11
      COMMON/KB/AI(30),BI(30),CI(30),DI(30),EI(30),AII(30),             THER  12
     1       BII(30),CII(30),DII(30),EII(30),TLOW(30)                   THER  13
      COMMON/KC/ICODE(30),Y(30),FW(30)                                  THER  14
      COMMON/KG/ENT(30),RATE(30),T,HEAT1,SUM7                           THER  15
      COMMON/KEE/PL,RR,TZERO,EPS,KEY,NC,NS,MM,NQ                        THER  16
      DIMENSION CPDT1(6),ENT1(30),CP(30)                                THER  17
C                                                                       THER  18
C     TEMPERATURE IN OK.                                                THER  19
C                                                                       THER  20
      T1=T                                                              THER  21
      T2=T1*T                                                           THER  22
      T3=T2*T                                                           THER  23
      T4=T3*T                                                           THER  24
      T5=T4*T                                                           THER  25
      A1=T                                                              THER  26
      A2=T2/2.                                                          THER  27
      A3=T3/3.                                                          THER  28
      A4=T4/4.                                                          THER  29
      A5=T5/5.                                                          THER  30
      CPMX=0.                                                           THER  31
      SUM7=0.                                                           THER  32
      HEAT1=0.                                                          THER  33
      DO78I=1,NQ                                                        THER  34
```

```
      IF(T.LT.TLOW(I))GOTO6207                                          THER  35
C                                                                       THER  36
C     TLOW(I)=MINIMUM TEMPERATURE AT WHICH THE HIGH                     THER  37
C     TEMPERATURE FIT CAN BE USED.                                      THER  38
C                                                                       THER  39
C     ENT1=SENSIBLE ENTHALPY+CHEMICAL POTENTIAL                         THER  40
C                                                                       THER  41
      ENT1(I)=(AI(I)*A1+BI(I)*A2+CI(I)*A3+DI(I)*A4+EI(I)*A5             THER  42
     1+FI(I))*RR                                                        THER  43
C     CP=HEAT CAPACITY                                                  THER  44
      CP(I)=(AI(I)+BI(I)*T1+CI(I)*T2+DI(I)*T3+EI(I)*T4)*RR              THER  45
      IF(I.GT.1)GOTO6291                                                THER  46
C                                                                       THER  47
C                                                                       THER  48
C-----CALCULATE THE SENSIBLE ENTHALPY OF THE CONSTITUENT                THER  49
C     ELEMENTS.                                                         THER  50
C                                                                       THER  51
C                                                                       THER  52
      DO296J=1,MM                                                       THER  53
      CPDT1(J)=(S1(J)*A1+S2(J)*A2+S3(J)*A3+S4(J)*A4+S5(J)*A5            THER  54
     1        +S6(J))*RR                                                THER  55
  296 CONTINUE                                                          THER  56
      GOTO6291                                                          THER  57
C                                                                       THER  58
 6207 ENT1(I)=(AII(I)*A1+BII(I)*A2+CII(I)*A3+DII(I)*A4+EII(I)*A5        THER  59
     1+FII(I))*RR                                                       THER  60
      CP(I)=(AII(I)+BII(I)*T+CII(I)*T2+DII(I)*T3+EII(I)*T4)*RR          THER  61
      IF(I.GT.1)GOTO6291                                                THER  62
      DO297J=1,MM                                                       THER  63
      CPDT1(J)=(A11(J)*A1+A22(J)*A2+A33(J)*A3+A44(J)*A4                 THER  64
     1         +A55(J)*A5+A66(J))*RR                                    THER  65
  297 CONTINUE                                                          THER  66
C                                                                       THER  67
C                                                                       THER  68
```

```
C      JCODE(J)=0 THE REFERENCE ELEMENT IS IN THE GAS STATE.
C      JCODE(J)=1  THE REFERENCE ELEMENT IS IN THE SOLID STATE.
C
C-----RSUM IS THE SUM OF THE SENSIBLE ENTHALPY OF THE CONSTI-
C      TUENT ELEMENTS OF THE ITH SPECIE AT TEMPERATURE T(OK),
C      WITH RESPECT TO THE STANDARD STATE(P=1 ATM AND T=298 )
C
C
 6291 RSUM=0.
      DO398J=1,MM
      IF(JCODE(J).EQ.1)GOTO393
      RSUM=RSUM+0.5*AA(I,J)*CPDT1(J)
      GOTO398
 393  RSUM=RSUM+AA(I,J)*CPDT1(J)
 398  CONTINUE
C
C-----CALCULATE THE HEAT OF FORMATION ENT(I) FOR EACH SPECIE .
C
      ENT(I)=ENT1(I)-RSUM
      IF(ABS(ENT(I)).LT.3.)ENT(I)=0.
C
C-----CALCULATE HEAT1,WHICH IS THE HEAT ABSORBED BY THE CHEMICAL
C      REACTIONS(CALORIES/GM-MOLE)
C
      IF(I.GT.NC)GOTO8005
      HEAT1=HEAT1+RATE(I)*EPS*ENT(I)
      GO TO 787
 8005 HEAT1=HEAT1+RATE(I)*(1.-EPS)*ENT(I)
      GO TO 78
 787  SUM7=SUM7+Y(I)*ENT1(I)
      CPMX=CPMX+CP(I)*Y(I)
 78   CONTINUE
      RETURN
      END
```

```
      SUBROUTINE INPUT1                                                 INPU   1
      COMMON/KD/RSC(30,30),PSC(30,30),NREX(30,30),NPEX(30,30),          INPU   2
     1AF(30),AEF(30),SF(30),AK(30),BK(30),EKMAX(30),EKMIN(30),NCOEF(30) INPU   3
      COMMON/KH/KSP1,NEQ                                                INPU   4
      DIMENSION EQN(30,30)                                              INPU   5
C                                                                       INPU   6
C                                                                       INPU   7
C                                                                       INPU   8
C     RSC(I,J)=STOCHIOMETRIC COEFFICIENT OF REACTANT I IN REACTION J.   INPU   9
C     PSC(I,J)=STOCHIOMETRIC COEFFICIENT OF PRODUCT I IN REACTION J.    INPU  10
C     NREX(I,J)=POWER ON CONCENTRATION OF REACTANT I.                   INPU  11
C     NPEX(I,J)=POWER ON CONCENTRATION OF PRODUCT I.                    INPU  12
C     AF(J)=FREQUENCY FACTOR OF FORWARD REACTION.                       INPU  13
C     SF(J)=POWER DEPENDENCE ON TEMPERATURE FOR FORWARD REACTION.       INPU  14
C     AEF(J)=ACTIVATION ENERGY OF FORWARD REACTION.                     INPU  15
C     EQN=ALPHA-NUMERIC STORAGE OF TITLE OF CHEMICAL REACTION.          INPU  16
C     AK AND BK=EMPIRICAL CONSTANT FOR EQUILIBRIUM CONST. FIT.          INPU  17
C     AK AND BK ARE EMPIRICAL CONSTANTS FOR THE EQUILIBRIUM CONSTANT FITINPU  18
C     EKMAX AND EKMIN ARE THE MAX. AND MIN. VALUE OF THE EQUILIBRIUM    INPU  19
C     CONSTANTS.  THESE VALUES ARE USED TO AVOID EXTREME CASES.  THESE  INPU  20
C     ARE WHEN THE CONVERSION IS CLOSE TO ONE, OR CLOSE TO ZERO.        INPU  21
C     COEF(J)=SUM COEF. OF OF CONCENTRATION OF PROD. MINUS REACT.       INPU  22
C     KSP1=TOTAL NUMER OF GASES AND SOLIDS SPECIES.                     INPU  23
C     NEQ=NUMBER OF CHEMICAL REACTIONS.                                 INPU  24
C                                                                       INPU  25
C                                                                       INPU  26
C                                                                       INPU  27
C     READ INPUT                                                        INPU  28
C                                                                       INPU  29
C                                                                       INPU  30
 10   CONTINUE                                                          INPU  31
      READ 1,NEQ                                                        INPU  32
 1    FORMAT(I2)                                                        INPU  33
      PRINT 12                                                          INPU  34
```

```
      DO 6 J=1,NEQ                                                      INPU  35
      READ 7,(EQN(J,K),K=1,19)                                          INPU  36
7     FORMAT(19A4)                                                      INPU  37
      PRINT 13,(EQN(J,I),I=1,19)                                        INPU  38
      READ 2,I,RSC(J,I),I,RSC(J,I),I,RSC(J,I),I,PSC(J,I),I,PSC(J,I),    INPU  39
     1       I,PSC(J,I)                                                 INPU  40
      READ 3,I,NREX(J,I),I,NREX(J,I),I,NREX(J,I),I,NPEX(J,I),           INPU  41
     1       I,NPEX(J,I),I,NPEX(J,I)                                    INPU  42
      READ 4,AF(J),SF(J),AEF(J)                                         INPU  43
      READ 5,AK(J),BK(J),EKMAX(J),EKMIN(J),NCOEF(J)                     INPU  44
2     FORMAT(6(I3,F3.0))                                                INPU  45
3     FORMAT(12I3)                                                      INPU  46
4     FORMAT(E8.0,2X,2F10.1)                                            INPU  47
5     FORMAT(4E15.7,I5)                                                 INPU  48
    6 CONTINUE                                                          INPU  49
11    CONTINUE                                                          INPU  50
      PRINT 12                                                          INPU  51
12    FORMAT(1H1)                                                       INPU  52
13    FORMAT(1X,19A4/)                                                  INPU  53
      RETURN                                                            INPU  54
      END                                                               INPU  55
```

```
      SUBROUTINE INTRPL(VAR,X,F,IMAX,SOM)                               INTR   1
      DIMENSION X(1),F(1),XN(100),FN(100)                               INTR   2
C                                                                       INTR   3
C*****************************************************************     INTR   4
C*        THIS PROGRAM PERFORMS LAGRAGIAN INTERPOLATION          *     INTR   5
C*        WITH UNEQUAL STEP SIZE BETWEEN POINTS.                 *     INTR   6
C*****************************************************************     INTR   7
C                                                                       INTR   8
C         F=DEPENDENT VARIABLE                                          INTR   9
C         X=INDEPENDENT VARIABLE                                        INTR  10
C         VAR=VALUE OF X FOR WHICH CORRESPONDING VALUE OF               INTR  11
C             F IS DESIRED BY INTERPOLATION                             INTR  12
C         IMAX=NUMBER OF POINTS IN ARRAY X OR F.(MAX OF 100 )           INTR  13
C         SOM=VALUE OF INTERPOLATED DEPENDENT VARIABLE                  INTR  14
C         NPTS=NUMBER OF POINTS USED FOR INTERPOLATION                  INTR  15
      NPTS=3                                                            INTR  16
  607 XUP=1.E30                                                         INTR  17
      DO 611 I=1,IMAX                                                   INTR  18
      T=VAR-X(I)                                                        INTR  19
      IF(T.GE.0.)GO TO 609                                              INTR  20
  608 T=-T                                                              INTR  21
  609 IF (T .GE. XUP) GO TO 611                                         INTR  22
  610 IP=I                                                              INTR  23
      XUP=T                                                             INTR  24
  611 CONTINUE                                                          INTR  25
      IN=1                                                              INTR  26
      NPP=NPTS+1                                                        INTR  27
      DO 618 I=1,NPP                                                    INTR  28
      FN(I)=F(IP)                                                       INTR  29
      XN(I)=X(IP)                                                       INTR  30
      IF(IN .GT. 0.) GO TO 613                                          INTR  31
  612 IQ=IP-I                                                           INTR  32
      GO TO 615                                                         INTR  33
  613 IQ=IP+I                                                           INTR  34
```

```
      IF (IMAX .GE. IQ) GO TO 615                                       INTR   35
  614 IP=IP-1                                                           INTR   36
      GO TO 618                                                         INTR   37
  615 IF (IQ .GT. 0 ) GO TO 617                                         INTR   38
  616 IP=IP+1                                                           INTR   39
      GO TO 618                                                         INTR   40
  617 IP=IQ                                                             INTR   41
      IN =-IN                                                           INTR   42
  618 CONTINUE                                                          INTR   43
      SOM=0.                                                            INTR   44
      FACT=1.                                                           INTR   45
      DO 620 J=1,NPTS                                                   INTR   46
      SOM=SOM+FACT*FN(1)                                                INTR   47
      DO 619 I=J,NPTS                                                   INTR   48
      IQ=I-J+1                                                          INTR   49
  619 FN(IQ)=(FN(IQ+1)-FN(IQ)/XN(I+1)-XN(IQ))                           INTR   50
  620 FACT=FACT*(VAR-XN(J))                                             INTR   51
      RETURN                                                            INTR   52
      END                                                               INTR   53
```

ABLATIN2 ANALYSIS NOMENCLATURE

MAIN:

AA(I,J): Formula number. Gives the gram atoms of element J in species I.

AI...GI: These are the seven empirical constants for the high temperature fit (1000°-6000°K) for the free energy functions. The first five constants (AI through EI) are used in the heat capacity fit.

AII...GII: These are the seven empirical constants for the low temperature fit (300°K-1000°K) for the free energy function.

All...A66: These are the six empirical constants for the enthalpy fit of the constituent elements (300°K-1000°K).

ALPHA: Viscous coefficient in Darcy's equation (FT^{-1}).

AVGFW: Average molecular weight of the gas mixture.

BETA: Inertial coefficient in Darcy's equations ($1/FT^{2}$).

CDO: Thermal conductivity of the char (BTU/FT-sec-^{o}F).

CDOV: Thermal conductivity of the virgin material, (BTU/FT-sec-^{o}F).

CPB1: Total rate of heat absorbed by the gases in the char zone. (BTU/FT^{2}sec).

CPB2: Total rate of heat absorbed by the solids in the char zone. (BTU/FT^{2}sec).

CPS: Heat capacity of the char (BTU/lb-^{o}F).

CPV: Heat capacity of the virgin material (BTU/lb-^{o}F).

DCDO: Rate of change of the thermal conductivity of the char with temperature. (BTU/FT-sec-$^{o}F^{2}$).

DCDOV: Rate of change of the thermal conductivity of the virgin material with temperature. (BTU/FT-sec-$^{o}F^{2}$).

DELTF: Differential change in temperature in ^{o}F for an increment of distance H.

DELTK: Differential change in temperature in ^{o}K for an increment of distance H.

DELTP: Pressure drop across the char. (lbs./ft^{2}).

DELZ: Increment of distance (in feet).

DISTAN: Char thickness in feet.

DT: Temperature gradient (^{o}F/FT).

DTC: Temperature gradient in the char (^{o}F/FT).

DTCC: Temperature gradient in double precision arithmetic in the char (^{o}F/FT).

DTCI: Temperature gradient in the virgin material (^{o}F/FT).

EK: Potential parameter /Boltzman constant.

EMIS: Char emissivity.

EPS: Porosity of the char (FT^{2} voids/FT^{2} total).

FW(I): Molecular weight of species I.

GASCP: Is the heat capacity of the gas mixture in (BTU/lb-^{o}F).

GROUP: This is the bracketted term of Equation (3-36). (1/FT).

H: Runge-Kutta step size (in feet).

H11: Runge-Kutta step size in double precision arithmetic (in feet).

HCHAR: Percent of total heat absorbed in the char zone.

HDECOM: Percent of total heat absorbed in the decomposition zone.

HGAS: Percent of heat absorbed by the gas in the char zone.

HI: Initial value of Runge-Kutta step (in feet).

HREACT: Percent of heat absorbed by the reactions in the char zone.

HSOLID: Percent of heat absorbed in the solids in the char zone.

ICODE(I): Is a code to identify whether a species is a gas or a solid. If ICODE is zero, the species is a gas. If ICODE is one, the species is a solid.

IMAX: Number of data points for EK.

ITEMP: Total number of temperature points stored in temperature profile.

JCODE(J): Is a code used to determine whether the reference state of the constituent element J is in the gas or in the solid state.

JS: Total number of slices in which the char is divided for the solution of the momentum equation.

K1: Is a counter for the number of temperature points stored during the solution of the energy equation.

MM: Is the number of elements.

NC: Number of gas species read in.

NDATA: Number of collision integral points tabulated versus XTKE.

NN: Number of gas species in the system.

NN5: Is the total number of variables stored in TABLE (I,J).

NNS: Is the number of solid species in the system.

NQ: Is the total number of gas and solid species in the system.

NS: Is the total number of gas and solid species read in.

OMGA: Interpolated value of XTKE.

P: Pressure in lbs/ft^2.

PL: Pressure at the front surface of the char (lbs/ft^2).

Q: Is the rate of heat absorbed in the decomposition zone in (BTU/ft^3sec).

Q2: It equals Q/DTC (BTU/FT^2-sec-^oF).

QA: Aerodynamic heating rate (BTU/FT^2-sec). Equals QL+QR.

QCZ: Heat flux in the char zone (BTU/ft^2-sec).

QCZI: Heat flux in the decomposition zone (BTU/ft^2sec).

QL: Is the total heat flux at the surface (BTU/ft^2sec).

QR: Is the rate of re-radiation from the surface of the char (BTU/ft^2-sec).

REAC1: Is the total rate of heat absorbed by the che-

mical reactions. (BTU/ft^2-sec).

REAC2: Heat absorbed by the chemical reactions (BTU/ft^2-sec).

REACT: Equals REAC2/DTC (BTU/ft^2-sec-^{o}F).

RHO: Bulk density of the virgin material (lbs/ft^3).

ROCHAR: Bulk density of the char material (lbs/ft^3).

RR: Gas constant: 1.98726 (BTU/lb-mole ^{o}R).

S1...S6: These are six empirical constants for the enthalpy fit of the constituent elements (1000°K-6000°K).

SIG: Collision diameter (Angstrongs).

SIGMA: Stephan-Boltzman constant (4.81×10^{-13} BTU/ft^2-sec-^{o}F^4).

T1(K1): Variable in which the temperature profile is stored versus distance Z. K1 is a counter.

TC: Temperature in ^{o}F.

TCHAR: Temperature at which all the virgin material has degraded to gas and char (^{o}K).

TFMAX: Maximum specified temperature of the front surface of the char (^{o}F).

THICK: Is the thickness of the char zone, in inches.

THICK1: Is the thickness of the decomposition zone in inches.

TK: Interpolated value of the temperature (in^{o}K) at a distance Z in the char.

TL: Front surface temperature of the char (^{o}F) when the temperature profile has been defined.

TLOW(I): Maximum temperature of low temperature fit

for species I. (^{o}K)

TO: Initial temperature (in ^{o}F) at Z=0.

TPREV: Temperature (in ^{o}F) at the previous step.

TTTT: This is the temperature (in ^{o}F) in double precision arithmetic. A provision has been made in the program that if the step size is less than 8. x 10^{-9} ft., the Runge-Kutta analysis is calculated in double precision arithmetic to reduce round-off error.

TVAR: Temperature in ^{o}K.

TVIS: Interpolated value of the temperature profile (in ^{o}F) at a distance Z along the char.

VISCOS: Viscosity of the gas (in centipoise).

VR: Surface recession velocity (ft/sec).

W: Mass flux based on the total area (lbs/ft^2-sec).

WI: Mass flux of the gases entering the char based on the total area (lbs/ft^2-sec).

XTKE: Product of the temperature in ^{o}K and 1/EK.

YCOMP(I,J): Array to store the concentration profile.

Y(I): Mole fraction of species I.

YI(I): Initial mole fraction of species I.

Z: Distance along the decomposition zone or the char zone (ft).

ZINC: Increment of distance at which the temperature profile is stored (ft).

ZMAX: Maximum allowable thickness of the char zone. (Usually 0.25 inches).

ZZ: Distance of Z in double precision arithmetic (ft).

INDPTH:

This subroutine calculates the physical properties of the virgin material and the pyrolysis gases.

A...E: These are five empirical constants for the heat capacity of the virgin material.

DELTKK: Increment of temperature (^{o}K).

PHMCR:

This subroutine computes the heat absorbed by the decomposition of the phenolic resin and phenolic microballoons.

AREA: This is the area generated by a plot of calories versus temperature (^{o}K) by the decomposition of phenolic resin during a differential thermal analysis. (1350 cal/ ^{o}K).

AREA1: This is the area generated by a plot of calories versus temperature (^{o}K), by the decomposition of phenolic microballoons during a differential thermal analysis. (1464 calories / ^{o}K).

A(I)...E(I): These are five empirical constants used to fit a curve through a portion of the plot of calories versus temperature for the phenolic resin.

A1(I)...E1(I): These are five empirical constants used to fit a curve through a portion of the plot of calories versus temperature for the phenolic microballoons.

DT: Is the temperature difference in ^{o}K from a base temperature of 350 ^{o}C 9623°K). Below 350°C, decomposition of the virgin material has not been initiated.

DELT: Is the temperature increment (^{o}K) for an increment of the Runge-Kutta step.

H: Is the height (in calories) for the plot of calories versus temperature (^{o}K).

K6: Is a code used to bypass the read statements. When K6 is one, the data is read in. When K6 is two, the read statements are bypassed.

NUMBER: Is the number of fits used for the plots of calories versus temperature.

QMICRO: Heat absorbed by the decomposition of the phenolic microballoons (calories/gram).

QPHNLC: Heat absorbed by the decomposition of the phenolic resin (calories/gram).

NYLON:

This subroutine calculates the heat absorbed by the decomposition of nylon.

AREA: This is the area generated by a plot of calories versus temperature (^{o}K) for the decomposition of nylon (1122 calories / ^{o}K) during a differential thermal analysis.

QNYLON: Heat absorbed by the decomposition of nylon (calories/gram).

DNSITY:

This subroutine calculates the density change of phenolic nylon and the mass flux of the pyrolysis gas.

A(J): Frequency factor of reaction J (sec^{-1}).

COMPST: Is an integer variable giving the number of

composite in the ablator. In the case of phenolic nylon, it is three.

DELFLX(I): Is the change in mass flux of composite I due to degradation (lbs/ft^2-sec).

DRHO: Differential change in density due to degradation. This variable is used as a criteria for stability while the solution is marching through the decomposition zone (lbs/ft^3).

DRHODT(I): Rate of gas generation by the degradation of composite I (lbs/ft^3-sec).

E(J): Energy of activation of reaction J used to describe the degradation of the composite (Joules/gram-mole).

MASFLX(I): Rate of change of mass flux due to the degradation of composite I (lbs/ft^2-sec).

MASFRC(I): Mass fraction of each composite in the mixture of virgin material.

NREACT: Number of pseudo-order kinetic reactions used to describe the decomposition of the virgin material composite.

RATER(J): Specific reaction velocity of reaction J (lbs/ft^3-sec).

RHO: Bulk density of the composite (lbs/ft^3).

RHOC(I): Residual density of composite I (lbs/ft^3).

RHOCC(I): Lowest value of residual density of composite I (lbs/ft^3).

RHOI(I): Initial density of composite I (lbs/ft^3).

RHOII: Initial density of the virgin composite, (lbs/ft^3).

RHOT(I): Density of composite I at temperature T, (lbs/ft^3).

VOLFRC(I): Volume fraction of each composite I.

CHARPR:

This subroutine calculates the effective thermal conductivity and the heat capacity of the char.

T: Temperature in ^{o}R.

INTRPL:

This program performs Lagrangian interpolation with non-equal step size between points.

F: Dependent variable array.

IMAX: Number of points in array.

SOM: Value of the interpolated dependent variable.

VAR: Value of X for which corresponding value of F is derived by interpolation.

X: Independent variable array.

THERM2:

This subroutine calculates the heat of formation of each chemical species, the heat capacity of the mixture and the heat absorbed by chemical reactions.

CPDT1: Is the sensible enthalpy gain by the constituent elements from a reference temperature of 298.16^{o}K (cal/gram-mole).

CPMX: Heat capacity of the gas mixture (calories/gram-mole ^{o}K).

ENT1(I): Enthalpy of species I (caloreis/gram-mole).

ENT(I): Heat of formation of species I (cal/gram-mole).

HEAT1: Rate of heat generated, or absorbed, by the chemical reactions (calories/cm^3-sec).

KINET:

This program computes the rate of reaction of each chemical species.

AEF(J): Activation energy of reaction J (calories/gram-mole).

AF(J): Frequency factor of reaction J (sec^{-1}

DELZZ: Runge-Kutta step size (cm.).

DLFLUX(I): Differential change in molal flux due to the chemical reaction of species I. This variable is used for the purpose of controlling the step size (gram-mole/cm^2-sec).

FK(J): Forward reaction rate constant of reaction J.

FLUXMA(I): Mass flux of each chemical species I (gm/cm^2-sec).

FLUXMO(I): Molal flux of each chemical species I, (gram/moles/cm^2-sec).

HEAT: Rate of heat generated or absorbed by the chemical reactions (BTU/ft^3-sec).

K2: Is a counter to keep track of the number of temperature points stored in Table (I,J).

K7: When K7 is one, initialization occurs and subroutine INOUT is called. When it is 2, this is bypassed.

KOS: Total number of variables stored in the Table (I,J) array.

KSP: Number of gas components in the chemical system.

KSP1: Number of gas and solid species in the chemical system.

NPEX(I,J): Power on the concentration of product I in reaction J.

NREX(I,J): Power on the concentration of reactant I in reaction J.

P: Pressure of the system in atmosphere.

PERCE(J): Mole percent of specie J.

PSC(I,J): Stochiometric coefficient of the product I in reaction J.

R: Gas constant (82.06 cm^3-atm/gram-mole ^oK).

RATE(J): Rate of formation of species I (gram-moles/ cm^3-sec).

RATER(J): Specific reaction velocity of reaction J, (gram-moles/cm^3-sec).

RK(J): Reverse reaction rate constant of reaction J.

RR: Gas constant (1.98726 calories/gram-mole ^oK).

SF(J): Power on the temperature of the Arrhenius type kinetic expression.

SPCIE1(J): Species identification name.

T: Temperature (^oK).

TABLE(I,J): Is an array where I represents the number

of variables stored and J the number of temperature points. The variables stored are in the following order: T, HEAT, WNEW, AVGFW and KSP1 values of Y1(I).

TESS: Is the absolute maximum value of DLFLUX(I). This variable is used in controlling the step size for stability.

TF: Temperature (^{o}F).

TPREV: Is the previous value of the temperature (^{o}K).

WNEW: Total mass flux of the gases (lbs/ft^2-sec).

XMW (I): Molecular weight of species I.

Y1(I): Mole fraction of species I.

INPUT1:

This subroutine reads in the kinetic data.

AK(J): Empirical constant for the fit of the equilibrium constant with temperature.

BK(J): Empirical constant for the fit of the equilibrium constant with temperature.

EKMAX(J): Maximum allowable value for the equilibrium constant of reaction J.

EKMIN(J): Minimum allowable value for the equilibrium constant of reaction J.

NCOEF(J): Is the sum of the stochiometric coefficient of the products minus the reactants.

INPUT FORMAT: A Typical Input For Non-Equilibrium Flow*

CARD 1: FORMAT (6I6, F10.1)	COLUMNS
NC = 18	1-6
NNS = 1	7-12
MM = 4	13-18
KODE = 1	19-24
KEY = 3	25-30
INDPT = 0	31-36
TFMAX = 5500	37-46

CARD 2: FORMAT (F10.3, 10 x, 4F10.3)

PL = 2160	1-10
TO = 500	21-30
EPS = .30	31-40
ZL = .350000	41-50
HI = .0000001	51-60

CARD 3: FORMAT (3E15.5, F15.5)

ALPHA = .5E9	1-15
BETA = .5E5	16-30
SIGMA = .48E-12	31-45
EMIS = .90	46-60

*See Table B-2 for the complete Input data set.

CARD 4: FORMAT (4E10.3)	COLUMNS
DTC = 3000	1-10
TCHAR = 1073	11-20
VT = 5.E-4	21-30

CARD 5: FORMAT (6E10.3,I3)	
S1(1) = 1.363250E0	1-10
S2(1) = 1.85605E-3	11-20
S3(1) = -7.6675E-7	21-30
S4(1) = .151043E-9	31-40
S5(1) = -1.139E-14	41-50
S6(1) = -6.49672E2	51-60
JCODE(1) = 1	61-63

CARD 6: FORMAT (6E10.3)	
A11(1) = -.712442E0	1-10
A22(1) = 7.34065E-3	11-20
A33(1) = -5.526E-6	21-30
A44(1) = 1.51400E-9	31-40
A55(1) = -2.382E-14	41-50
A66(1) = -6.80533E1	51-60

CARDS 5 and 6 are read sequentially MM times as specified by CARD 1. In this example MM = 4. After CARDS 5 and 6 are read MM times, CARD 7 is read in.

CARD 7: FORMAT (10x, 3E10.3, 2x, 2A3, I4)	
TLOW(1) = 1000	11-20
FW(1) = 14.0	21-30

YI(1) = 1.0E-71	31-40
SPCIE1(1) = (Blank)	43-45
SPCIE2(1) = CH_2	46-48
ICODE(1) = 0	49-52

<u>CARD 8</u>: FORMAT (7E10.3)

AI(1) = 2.229698E0	1-10
BI(1) = 4.71092E-3	11-20
CI(1) = -1.7660E-6	21-30
DI(1) = 3.0649E-10	31-40
EI(1) = -2.017E-14	41-50
FI(1) = 3.383295E4	51-60
GI(1) = 7.707984E0	61-70

<u>CARD 9</u>:

AII(1) = 3.551365E0	1-10
BII(1) = -2.5070E-3	11-20
CII(1) = 1.23550E-5	21-30
DII(1) = 1.175E-08	31-40
EII(1) = 3.8124E-12	41-50
FII(1) = 3.366105E4	51-60
GII(1) = 1.796606E0	61-70

<u>CARD 10</u>: FORMAT (4E10.3)

AA(1,1) = 1.	1-10
AA(1,2) = 2.0	11-20
AA(1,3) = 0.0	21-30
AA(1,4) = 0.0	31-40

CARD 7, CARD 8, CARD 9 and CARD 10 are read sequentially as a group (NC+NNS) number of times. Only the data for the first species, in this case CH_2 is presented. The data for other species is given in Table B-2.

CARD 11: FORMAT (2F15.5)	COLUMNS
EK(1) = 136.5	1-15
SIG(1) = 3.822	16-30

CARD 11 is read NC number of times as specified in CARD 1.

CARD 12: FORMAT (I6)	
NDATA = 34	1-16

CARD 13: FORMAT (2F15.5)	
XTKE(1) = 0.30	1-15
ZOMGA(1) = 2.785	16-30

CARD 13 is repeated NDATA number of times as specified by CARD 12.

CARDS 1 through 13 are read in the MAIN program. These cards define the physical condition of the system.

In addition they provide the thermodynamic data and physical constants for the pyrolysis species. CARDS 14 through 19, below, provide the thermophysical information for the virgin material and also for the kinetic data for the degradation of the polymer.

CARD 14: FORMAT (5E12.6)	COLUMNS
A = 0.37000070E0	1-12
B = 0.7367133E-4	13-24
C = 0.1532518E-5	25-36
D = -.1962704E-4	37-48
E = .8857809E-12	49-60

CARD 14 is read in subroutine INDPTH.

CARD 15: FORMAT (5E12.8)	
A(1) = 0.10561790E0	1-12
B(1) = -1.836062E-2	13-24
C(1) = 1.7580490E-3	25-36
D(1) = -1.678598E-5	37-48
E(1) = 4.7310570E-8	49-60

CARD 16: FORMAT (5E12.8)	
A1(1) = -.35642660E-1	1-12
B1(1) = 4.5790730E-2	13-24
C1(1) = 1.2298170E-4	25-36
D1(1) = -.8277667E-7	37-48
E1(1) = -.2279748E-7	49-60

CARD 15 and CARD 16 are read sequentially four times in subroutine PHMCR. For a thorough explanation of the sources of data for the phenolic resin see Appendix C.

CARD 17: FORMAT (2I6)	
COMPST	1-6
NREACT	7-12

CARD 18: FORMAT (4x, I6, 3E10.8)	COLUMNS
I =	5-10
A(J) =	11-20
E(J) =	21-30
XN(I,J) =	31-40

CARD 18 is read NREACT number of times.

CARD 19: FORMAT (310.3)	
RHOI(1) =	1-10
RHOC(1) =	11-20
MASFRC(1) =	21-30

CARD 19 is read COMPST number of times. CARDS 17, 18 and 19 are read in subroutine DNSITY.

CARD 20: FORMAT (I2)	
NEQ =	1-2

CARD 21: FORMAT (19A4)	
EQN = Alphameric Reaction Expression	1-76

CARD 22: FORMAT (6(I2, F3.0))	
I =	1-2
RSC(1,I)	3-5
I =	6-7
RSC(1,I)	8-10
I =	11-12
RSC(1,I)	13-15
I =	16-17

	COLUMNS
PSC(1,I)	18-20
I =	21-22
PSC(1,I)	23-25
I =	26-27
PSC(1,I)	28-30

CARD 23:

I =	1-2
NREX(1,I)	3-5
I =	6-7
NREX(1,I)	8-10
I =	11-12
NREX(1,I)	13-15
I =	16-17
NPEX(1,I)	18-20
I =	21-22
NPEX(1,I)	23-25
I =	26-27
NPEX(1,I)	28-30

CARD 24: FORMAT (E8.0, 2x, 2F10.1)

AF(1) =	1-8
SF(1) =	11-20
AEF(1) =	21-30

CARD 25: FORMAT (4E15.7, I5)	COLUMNS
AK(1)	1-15
BK(1)	16-30
EKMAX(1)	31-45
NCOEF(1)	46-50

CARDS 21,22,23,24 and 25 are read sequentially NEQ number of times.

In CARD 22, J = 1 through 18 corresponds respectively to the following species: CH_2, CH_3, CH_4, C_2H_6, C_2H_4, C_2H_2, C_2H, H_2, H, N_2, C_6H_6O, C_6H_6, NH_3, CO, CO_2, H_2O, OH, O, C.

TABLE B-5. Listing of Typical Input Data for Non-Equilibrium Analysis

```
                                                                                DATA   1
    18     1     4     1     3     1     0                                      DATA   2
     2160.                 500.        .8 0.3500000 .00000001   5821.          DATA   3
       .50000E9       .50000E5       .481E-12   0.90                           DATA   4
1.363252E01.85605E-3-7.6675E-7.151043E-9-1.139E-14-6.49672E2  1                DATA   5
-.712442E07.34065E-3-5.5262E-61.51400E-9-2.382E-14-6.80533E1                    DATA   6
3.043690E06.11871E-4-7.3994E-9-2.033E-112.4594E-15-8.54910E2  0                 DATA   7
 1.00000E0 4.0000E00 0.0000E00 0.0000E00                                        DATA   8
             1000.E0  30.070E0     .0034    C2H6   0                            DATA   9
.1430799E1.188898E-1-.70440E-5.118720E-8-.7445E-13-.114311E5.1401321E2          DATA  10
.2882039E1.103219E-1.119142E-4-.14832E-7.44749E-11-.116209E5.7597900E1          DATA  11
 2.00000E0 6.00000E0 0.00000E0 0.00000E0                                        DATA  12
             1000.E0  28.054E0     .0218    C2H4   0                            DATA  13
 3.5023E00 1.159E-02-4.4745E-6 7.945E-10-5.323E-14 4.5439E03 2.4667E00          DATA  14
1.120244E0 1.3906E-2 2.6568E-6-1.1560E-85.2387E-125.332889E3 1.58378E1          DATA  15
 2.00000E0 4.00000E0 0.00000E0 0.00000E0                                        DATA  16
             1000.E0  26.038E0     .0233    C2H2   0                            DATA  17
 4.4966E00 5.2698E-3-1.840E-063.1054E-10-2.000E-142.5637E004-3.14481E0          DATA  18
7.90333E-1 2.3466E-2-3.5542E-5 2.7951E-8-8.448E-12 2.6255E04 1.4005E01          DATA  19
 2.00000E0 2.00000E0 0.00000E0 0.00000E0                                        DATA  20
             1000.E0  25.030E0  1.00E-71     C2H   0                            DATA  21
.3513479E1.358906E-2-.13231E-5.230520E-9-.1530E-13.5788759E5.4523285E1          DATA  22
.3006269E1.553788E-2-.35112E-5.124860E-8-.1896E-12.5796960E5.6920349E1          DATA  23
 2.00000E0 1.00000E0 0.00000E0 0.00000E0                                        DATA  24
             1000.E0   2.016E0     .2372      H2   0                            DATA  25
3.04369E00 6.1187E-4 -7.399E-9 -2.03E-11 2.459E-15-8.5491E02 -1.648E00          DATA  26
2.846085E04.1932E-03-9.6119E-69.5123E-09-3.309E-12-9.67254E2 -1.4118E0          DATA  27
0.000000E0 2.00000E0 0.00000E0 0.00000E0                                        DATA  28
             1000.E0   1.008E0 1.000E-71       H   0                            DATA  29
2.500000E0 0.00000E0 0.00000E0 0.00000E0 0.00000E02.547050E4-4.6001E-1          DATA  30
2.500000E0 0.00000E0 0.00000E0 0.00000E0 0.00000E02.547050E4-4.6001E-1          DATA  31
0.000000E0 1.00000E0 0.00000E0 0.00000E0                                        DATA  32
             1000.E0  28.016E0     .0277      N2   0                            DATA  33
2.854576E0 1.5976E-3-6.2566E-71.1316E-10-7.69E- 15-8.90174E2 6.39029E0          DATA  34
```

```
3.691615E0-1.3333E-32.65031E-6-9.769E-10-9.977E-14-1.06283E3 2.28750E0  DATA  35
0.000000E0 0.00000E0 2.00000E0 0.00000E0                                DATA  36
              1500.E0  94.114E0      .0385    C6H6O    0               DATA  37
-3.93169E06.93818E-2-5.2106E-51.24967E-82.0915E-12-1.33038E44.187817E1  DATA  38
-3.93169E06.93818E-2-5.2106E-51.24967E-82.0915E-12-1.33038E44.187817E1  DATA  39
 6.00000E0 6.00000E0 0.00000E0 1.00000E0                                DATA  40
              1500.E0  78.114E0      .0052     C6H6    0               DATA  41
.3511186E03.75399E-2-7.9473E-6-7.5092E-93.0385E-128.264418E31.986606E1 DATA  42
4.619872E02.88096E-2-1.1245E-51.95764E-9-1.257E-137.391621E4-1.78947E0 DATA  43
 6.00000E0 6.00000E0 0.00000E0 0.00000E0                                DATA  44
              1000.E0  17.032E0  1.00E-71      NH3    0                DATA  45
2.149399E06.49285E-3-2.2695E-63.7394E-10-2.361E-14-6.40196E3 9.23891E0 DATA  46
3.77162E00-4.8621E-49.8742E-06-9.5679E-93.1313E-12-6.72810E3 1.4654E00 DATA  47
0.00000E00 3.00000E0 1.00000E0 0.00000E0                                DATA  48
              1000.E0  28.011E0      .0233      CO    0                DATA  49
 2.9512E00 1.5526E-3-6.1911E-7 1.135E-10-7.788E-15-1.4232E04 6.5314E00 DATA  50
3.787133E0-2.171E-035.07573E-6-3.4738E-97.7217E-13-1.43635E4 2.63355E0 DATA  51
 1.00000E0 0.00000E0 0.00000E0 1.00000E0                                DATA  52
              1000.E0  44.011E0      .0164      CO2    0               DATA  53
 4.4129E003.1923E-03 -1.298E-6 2.415E-10-1.674E-14-4.8944E04-7.2876E-1 DATA  54
2.170100E0 1.0378E-2-1.0734E-56.34592E-9-1.628E-12-4.83526E4 1.06644E1 DATA  55
 1.00000E0 0.00000E0 0.00000E0 2.00000E0                                DATA  56
              1000.E0  18.016E0      .0492      H2O    0               DATA  57
 2.67075E0 3.0317E-3 -8.535E-7 1.179E-10-6.197E-15-2.9889E04 6.88383E0 DATA  58
4.15650E00-1.7244E-35.6982E-06-4.5930E-91.4234E-12-3.02888E4-6.8616E-1 DATA  59
0.000000E0 2.00000E0 0.00000E0 1.00000E0                                DATA  60
              1000.E0  17.008E0 1.000E-71       OH    0                DATA  61
2.889554E09.98350E-4-2.1880E-71.9803E-11-3.845E-163.881179E35.559701E0 DATA  62
3.823470E0-1.1187E-31.24668E-6-2.103E-10-5.254E-143.585278E35.8253E-01 DATA  63
0.000000E0 1.00000E0 0.00000E0 1.00000E0                                DATA  64
              1000.E0 16.000000  1.00E-71        O    0                DATA  65
2.537256E0-1.8422E-5-8.8018E-95.9643E-12-5.574E-162.92300E044.946794E0 DATA  66
3.021889E0-2.1737E-33.75422E-6-2.9947E-99.0777E-132.913719E42.646007E0 DATA  67
 0.0000E00 0.00000E0 0.0000E00 1.0000E00                                DATA  68
```

```
              1000.E0  12.011E0      .515       C   1                    DATA  69
1.36325E001.85605E-3-7.6675E-71.5104E-10-1.139E-14-6.4967E02-7.9890E00  DATA  70
-7.1244E-17.34065E-3-5.5262E-6 1.514E-09-2.382E-14-6.80533E1 2.79326E0  DATA  71
 1.0000E00 0.00000E0 0.0000E00 0.0000E00                                DATA  72
          136.5          3.822   CH2                                    DATA  73
          136.5          3.822   CH3                                    DATA  74
          136.5          3.822   CH4                                    DATA  75
          230.0          4.418  C2H6                                    DATA  76
          205.0          4.232  C2H4                                    DATA  77
          185.0          4.221  C2H2                                    DATA  78
          185.0          4.221   C2H                                    DATA  79
           33.3          2.986    H2                                    DATA  80
           33.3          2.986     H                                    DATA  81
           91.5          3.681    N2                                    DATA  82
          440.0          5.270  C6H6                                    DATA  83
         400.0           5.000  PHOH                                    DATA  84
          312.0          3.432   NH3                                    DATA  85
          110.0          3.590    CO                                    DATA  86
          190.0          3.996   CO2                                    DATA  87
          356.0          2.649   H2O                                    DATA  88
          113.0          3.433    OH                                    DATA  89
          113.0          3.433     O                                    DATA  90
    34                                                                  DATA  91
    0.30           2.785                                                DATA  92
    0.35           2.628                                                DATA  93
2.846085E04.19321E-3-9.6119E-69.51227E-9-3.309E-12-9.67253E2            DATA  94
3.691615E0-1.3333E-32.65031E-6-.97688E-9-9.977E-14-1.06283E3            DATA  95
3.597613E07.81456E-4-2.2387E-74.2490E-11-3.346E-15-1.19279E3  0         DATA  96
2.854576E01.59763E-3-6.2566E-7.113158E-9-7.690E-15-8.90174E2  0         DATA  97
3.718995E0-2.5167E-38.58374E-6-8.2999E-92.7082E-12-1.10577E3            DATA  98
              1000.E0   14.00E0 1.000E-71     CH2   0                    DATA  99
2.229698E04.71092E-3-1.7660E-63.0649E-10-2.017E-143.383295E47.707984E0  DATA 100
3.551365E0-2.5070E-31.23550E-5-1.175E-083.8124E-123.366105E41.796606E0  DATA 101
1.000000E0 2.00000E0 0.00000E0 0.00000E0                                DATA 102
```

```
                1000.E0  15.035E0 1.000E-71     CH3   0                    DATA 103
2.802766E06.25045E-3-2.2892E-63.8993E-10-2.528E-141.578749E45.684117E0  DATA 104
3.399505E04.26783E-32.03327E-7-1.1548E-94.1288E-131.564979E42.703747E0  DATA 105
1.000000E0 3.00000E0 0.00000E0 0.00000E0                                DATA 106
                1000.E0  16.043E0      .039     CH4   0                    DATA 107
 1.18000E0 1.0950E-2-4.0620E-6 7.137E-10-4.749E-14-9.8556E03 1.2506E01  DATA 108
4.249768E0-6.9127E-3 3.1602E-5-2.9715E-89.5103E-12-1.01866E4-9.1755E-1  DATA 109
    0.40            2.492                                               DATA 110
    0.45            2.368                                               DATA 111
    0.50            2.257                                               DATA 112
    0.55            2.156                                               DATA 113
    0.60            2.065                                               DATA 114
    0.65            1.982                                               DATA 115
    0.70            1.908                                               DATA 116
    0.75            1.841                                               DATA 117
    0.80            1.780                                               DATA 118
    0.85            1.725                                               DATA 119
    0.90            1.675                                               DATA 120
    0.95            1.629                                               DATA 121
    1.00            1.587                                               DATA 122
    1.10            1.514                                               DATA 123
    1.20            1.452                                               DATA 124
    1.30            1.399                                               DATA 125
    1.50            1.314                                               DATA 126
    1.70            1.248                                               DATA 127
    1.90            1.197                                               DATA 128
    2.2             1.138                                               DATA 129
    2.6             1.081                                               DATA 130
    3.2             1.022                                               DATA 131
    4.0             0.9700                                              DATA 132
    5.0             0.9269                                              DATA 133
    7.0             0.8727                                              DATA 134
   10.0             0.8242                                              DATA 135
   20.0             0.7432                                              DATA 136
```

```
   40.0              0.6718                                                  DATA 137
   70.0              0.6194                                                  DATA 138
  100.0              0.5882                                                  DATA 139
  200.0              0.5320                                                  DATA 140
  400.0              0.4811                                                  DATA 141
0.3700070E0 0.7367133E-4 .1532518E-5-.1962704E-8.8857809E-12                DATA 142
     3     7                                                                 DATA 143
         1 8.3000E14 232.000E0 1.00000E0                                     DATA 144
         2 5.10000E8 114.000E0 3.00000E0                                     DATA 145
         2 2.50000E5 100.000E0 1.30000E0                                     DATA 146
         2 2.00000E7 140.000E0 3.10000E0                                     DATA 147
         3 2.00000E5  70.000E0 2.00000E0                                     DATA 148
         3 9.70000E6 122.000E0 2.00000E0                                     DATA 149
         3 1.3000E10 172.000E0 3.00000E0                                     DATA 150
 68.6000E0 5.14500E0 0.4000E0                                                DATA 151
 80.0000E0 43.2800E0 0.2500E0                                                DATA 152
 17.8000E0 9.64760E0 0.3500E0                                                DATA 153
15  19                                                                       DATA 154
 CH4=CH2+H2(1670-2090 K)KO2LOV,RUSSIAN J.PHYS.CHEM.VOL37,SEP.1963,1-1-4 DATA 155
  3 1. 30 0. 30 0.  1 1.  8 1. 30 0.                                         DATA 156
  3  1 30  0 30  0  1  1  8  1 30  0                                         DATA 157
 4.5E+13          0.       91.                                              DATA 158
   0.1664396E+2  -0.4365610E+5          4.0E0          1.E-6    1           DATA 159
 CH4=CH3+H(1590-1750 K)                                                      DATA 160
  3 1. 30 0. 30 0.  2 1.  9 1. 30 0.                                         DATA 161
  3  1 30  0 30  0  2  1  9  1 30  0                                         DATA 162
 1.0E+15          0.      103.                                              DATA 163
   0.1725283E+2  -0.5315890E+5         10.0E0          1.E-6    1           DATA 164
 2CH3=C2H6                                                                   DATA 165
  2 2. 30 0. 30 0.  4 1. 30 0. 30 0.                                         DATA 166
  2  2 30  0 30  0  4  1 30  0 30  0                                         DATA 167
 1.5E+10          0.      28.2                                              DATA 168
  -0.2030537E+2   0.4381153E+5         1.E+10          5.2E-4   -1           DATA 169
 C2H6=C2H4+H2(1600-3700 K),G.V.GULYAEV, I-10                                 DATA 170
```

```
 4 1. 30 0. 30 0.  5 1.  8 1. 30 0.                                      DATA 171
 4  1 30  0 30  0  5  1  8  1 30  0                                      DATA 172
9.0E+13          0.      69.0                                           DATA 173
  0.1604147E+2  -0.1715366E+5          1.E+4          1.E-1    1        DATA 174
C2H4=C2H2+H2(1300-2000 K),RUSSIAN J.PHYS.CHEM.,P1128-1130,SEP1963 *     DATA 175
 5 1. 30 0. 30 0.  6 1.  8 1. 30 0.                                      DATA 176
 5  1 30  0 30  0  6  1  8  1 30  0                                      DATA 177
1.1E+13         0.0      72.0                                           DATA 178
  0.1538761E+2  -0.2100359E+5          2.1E4          1.E-8    1        DATA 179
C2H2=2C+H2(2000 K)GULYAEV,INST.OF PET SYNTHESIS,ACAD.OF SCI.,USSR,I-10 DATA 180
 6 1. 30 0. 30 0. 19 2.  8 1. 30 0.                                      DATA 181
 6  1 30  0 30  0 19  0  8  1 30  0                                      DATA 182
1.7E+06          0.       30.                                           DATA 183
 -0.5979611E+1   0.2595788E+5          2.E+8          4.17E0    0        DATA 184
C2H2=C2H+H (INVERTED ORDER)                                             DATA 185
 6 1. 30 0. 30 0.  7 1.  9 1. 30 0.                                      DATA 186
 6  1 30  0 30  0  7  1  9  1 30  0                                      DATA 187
4.5E+11          0.      35.5                                           DATA 188
  0.1603705E+2  -0.5805091E+5          1.E12          1.0E-2    1        DATA 189
C+H2O=CO+H2                                                             DATA 190
19 1. 16 1. 30 0. 14 1.  8 1. 30 0.                                      DATA 191
19  0 16  1 30  0 14  1  8  1 30  0                                      DATA 192
2.3E+11        -0.50      71.9                                           DATA 193
  0.1717660E+2  -0.1626795E+5         8.35E4         1.37E-7    1        DATA 194
C+CO2=2CO                                                               DATA 195
19 1. 15 1. 30 0. 14 2. 30 0. 30 0.                                      DATA 196
19  0 15  1 30  0 14  2 30  0 30  0                                      DATA 197
1.5E+10          0.       85.                                           DATA 198
  0.2068290E+2  -0.2015984E+5         1.57E5          1.E-06    1        DATA 199
H2+M=2H+M LWP-181 I-1, 2-1                                              DATA 200
 8 1. 20 1. 30 0.  9 2. 20 1. 30 0.                                      DATA 201
 8  1 20  1 30  0  9  2 20  1 30  0                                      DATA 202
3.6E+18         0.82     103.2                                           DATA 203
  0.1465827E+2  -0.5507806E+5          .3450          1.E-11    1        DATA 204
```

```
H2O+M=OH+H LWP(300-3250 K)                                              DATA 205
16 1. 20 1. 30 0. 17 1.  9 1. 30 0.                                      DATA 206
16  1 20  1 30  0 17  1  9  1 30  0                                     DATA 207
1.7E+22          1.31      118.0                                        DATA 208
  0.1575620E+2  -0.6166211E+5          0.35E0          1.E-14    1      DATA 209
H+CO2=CO+OH(1273-2273 K)                                                DATA 210
 9 1. 15 1. 30 0. 14 1. 17 1. 30 0.                                     DATA 211
 9  1 15  1 30  0 14  1 17  1 30  0                                     DATA 212
3.0E+12           0.        33.                                         DATA 213
  0.4460376E+1  -0.1056866E+5          3.85E0          1.E-9     0      DATA 214
CO2=CO+O(HARPER-BOEING) LWP 181 II-2                                    DATA 215
15 1. 30 0. 30 0. 14 1. 18 1. 30 0.                                     DATA 216
15  1 30  0 30  0 14  1 18  1 30  0                                     DATA 217
2.3E+11         -0.5       71.9                                         DATA 218
  0.1787079E+2  -0.6348669E+5         0.766E0       5.076E-14    1      DATA 219
C6H6O+H2=H2O+C6H6 APRIL ,PH.D. THESIS. MAY 1969                         DATA 220
11 1.  8 1. 30 0. 16 1. 12 1. 30 0.                                     DATA 221
11  1  8  1 30  0 16  1 12  1 30  0                                     DATA 222
2.0E+13           0.        45.                                         DATA 223
 -0.5793374E-1    0.8101410E+4        1.00E+7       1.000E-5     0      DATA 224
C6H6=3C2H2         APRIL ,PH.D. THESIS. MAY 1969                        DATA 225
12 1. 30 0. 30 0.  6 3. 30 0. 30 0.                                     DATA 226
12  1 30  0 30  0  6  3 30  0 30  0                                     DATA 227
1.4E+09           0.        52.                                         DATA 228
  0.3830254E+2  -0.6562874E+5         1.0E+10        1.0E-08     2      DATA 229
```

TABLE B-6. Typical Output for Non-Equilibrium

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INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)

THEORETICAL

CHAR BACK TEMPERATURE (OF)= 1471.7          NUMBER OF GAS COMPONENTS= 18
THICKNESS OF CHAR(INCHES)=0.020672      THICKNESS OF DECOMPOSITION ZONE=0.006869
TOTAL MASS FLUX(LBS/FT2-SEC)=.349420     GAS MASS FLUX AT THE SURFACE= .168964
FRONT SURFACE TEMPERATURE(OF)=5500.0     SURFACE RECESSION VELOCITY(FT/SEC)=0.01000
      RATE OF HEAT ABSORBED IN THE CHAR ZONE(BTU/FT2-SEC)=1711.8933
      RATE OF HEAT ABSORBED IN THE DECOMPOSITION ZONE(BTU/FT2-SEC)= 244.2668
      PERCENT OF TOTAL HEAT ABSORBED IN THE CHAR ZONE=  0.8751294E 02
      PERCENT OF TOTAL HEAT ABSORBED IN DECOMP-ZONE=  0.1248705E 02
      PERCENT OF HEAT ABSORBED BY THE GAS IN THE CHAR ZONE=  0.4130847E 02
      PERCENT OF HEAT ABSORBED BY THE SOLIDS IN THE CHAR ZONE=  0.2505246E 02
      PERCENT OF HEAT ABSORBED BY REACTION IN THE CHAR ZONE=  0.3363907E 02
```

INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)

TEMPERATURE DROP (OF) = 4028.4

PRESSURE DROP (LB/FT2) = 9.1

SURFACE HEAT FLUX (BTU/FT2-SEC) = 1956.16

RADIANT HEAT FLUX BTU/FT2-SEC)=, 546.15

AERODYNAMIC HEAT FLUX(BTU/FT2-SEC)= 2502.31

CHAR DEPTH (FT)	0.0006	0.0006	0.0007	0.0007	0.0007
TEMPERATURE (OF)	1471.7	1556.4	1648.1	1746.2	1848.7
PRESSURE (LB/FT2)	2169.1	2168.9	2168.6	2168.4	2168.2
MASS FLUX(LB/FT2-SEC)	0.1285	0.1606	0.1606	0.1606	0.1606

	GAS COMPONENT	COMPOSITION (MOLE/MOLE GAS)				
1	CH2	0.1000E-70	0.3100E-10	0.2112E-09	0.2614E-08	0.1767E-07
2	CH3	0.1000E-70	0.3152E-11	0.2733E-10	0.4766E-09	0.4591E-08
3	CH4	0.8250E-01	0.8141E-01	0.8098E-01	0.8100E-01	0.8100E-01
4	C2H6	0.7390E-02	0.7292E-02	0.7254E-02	0.7253E-02	0.7245E-02
5	C2H4	0.4739E-01	0.4676E-01	0.4651E-01	0.4652E-01	0.4654E-01
6	C2H2	0.5103E-01	0.3705E-01	0.3163E-01	0.3184E-01	0.3194E-01
7	C2H	0.1000E-70	0.1330E-01	0.1846E-01	0.1826E-01	0.1816E-01
8	H2	0.4400E 00	0.4342E 00	0.4319E 00	0.4320E 00	0.4320E 00
9	H	0.1000E-70	0.1330E-01	0.1846E-01	0.1826E-01	0.1816E-01
10	N2	0.4751E-01	0.4688E-01	0.4663E-01	0.4664E-01	0.4665E-01
11	C6H6D	0.8393E-01	0.8281E-01	0.8238E-01	0.8240E-01	0.8240E-01
12	C6H6	0.1128E-01	0.1113E-01	0.1107E-01	0.1108E-01	0.1108E-01
13	NH3	0.1000E-70	0.9867E-71	0.9815E-71	0.9817E-71	0.9818E-71
14	CO	0.5677E-01	0.5601E-01	0.5572E-01	0.5573E-01	0.5574E-01
15	CO2	0.3574E-01	0.3526E-01	0.3508E-01	0.3508E-01	0.3509E-01
16	H2O	0.1364E 00	0.1346E 00	0.1339E 00	0.1339E 00	0.1340E 00
17	OH	0.1000E-70	0.1085E-07	0.5764E-07	0.2389E-06	0.6032E-06
18	O	0.1000E-70	0.1109E-09	0.1103E-09	0.1104E-09	0.1104E-09
19	C	0.1110E 01	0.1095E 01	0.1089E 01	0.1089E 01	0.1090E 01

INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0008	0.0008	0.0009	0.0009	0.0010
TEMPERATURE (OF)	1953.8	2063.0	2172.5	2283.7	2396.5
PRESSURE (LB/FT2)	2168.0	2167.7	2167.5	2167.3	2167.1
MASS FLUX(LB/FT2-SEC)	0.1606	0.1606	0.1607	0.1607	0.1608

	GAS COMPONENT	COMPOSITION (MOLE/MOLE GAS)				
1	CH2	0.2192E-06	0.1000E-69	0.1734E-05	0.7617E-05	0.1632E-04
2	CH3	0.7686E-07	0.1000E-69	0.8569E-06	0.4981E-05	0.1114E-04
3	CH4	0.8099E-01	0.8101E-01	0.8093E-01	0.8079E-01	0.8060E-01
4	C2H6	0.7169E-02	0.7163E-02	0.6793E-02	0.6194E-02	0.5357E-02
5	C2H4	0.4659E-01	0.4662E-01	0.4682E-01	0.4713E-01	0.4757E-01
6	C2H2	0.3195E-01	0.3192E-01	0.3201E-01	0.3216E-01	0.3238E-01
7	C2H	0.1815E-01	0.1816E-01	0.1814E-01	0.1811E-01	0.1807E-01
8	H2	0.4321E 00	0.4321E 00	0.4325E 00	0.4332E 00	0.4341E 00
9	H	0.1815E-01	0.1812E-01	0.1815E-01	0.1822E-01	0.1832E-01
10	N2	0.4664E-01	0.4665E-01	0.4660E-01	0.4653E-01	0.4643E-01
11	C6H6O	0.8239E-01	0.8239E-01	0.8231E-01	0.8218E-01	0.8199E-01
12	C6H6	0.1108E-01	0.1109E-01	0.1108E-01	0.1107E-01	0.1105E-01
13	NH3	0.9816E-71	0.9818E-71	0.9809E-71	0.9794E-71	0.9772E-71
14	CO	0.5579E-01	0.5571E-01	0.5603E-01	0.5659E-01	0.5741E-01
15	CO2	0.3508E-01	0.3513E-01	0.3504E-01	0.3486E-01	0.3459E-01
16	H2O	0.1339E 00	0.1340E 00	0.1335E 00	0.1327E 00	0.1315E 00
17	OH	0.2018E-05	0.1000E-69	0.1804E-04	0.1105E-03	0.2490E-03
18	O	0.1103E-09	0.1000E-69	0.1449E-04	0.1392E-03	0.3274E-03
19	C	0.1089E 01	0.1090E 01	0.1088E 01	0.1086E 01	0.1083E 01

INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0010	0.0011	0.0011	0.0011	0.0012
TEMPERATURE (OF)	2513.6	2628.5	2744.1	2860.4	2976.0
PRESSURE (LB/FT2)	2166.9	2166.6	2166.4	2166.2	2166.0
MASS FLUX(LB/FT2-SEC)	0.1607	0.1609	0.1612	0.1616	0.1622

	GAS COMPONENT	COMPOSITION (MOLE/MOLE GAS)				
1	CH2	0.9922E-05	0.3263E-04	0.6520E-04	0.1081E-03	0.1730E-03
2	CH3	0.3257E-04	0.3727E-04	0.3926E-04	0.3988E-04	0.7375E-04
3	CH4	0.8058E-01	0.8016E-01	0.7958E-01	0.7885E-01	0.7782E-01
4	C2H6	0.3694E-02	0.2602E-02	0.1467E-02	0.3201E-03	0.9261E-04
5	C2H4	0.4981E-01	0.4975E-01	0.4918E-01	0.4805E-01	0.4501E-01
6	C2H2	0.3180E-01	0.3255E-01	0.3369E-01	0.3524E-01	0.3756E-01
7	C2H	0.1807E-01	0.1798E-01	0.1786E-01	0.1771E-01	0.1750E-01
8	H2	0.4340E 00	0.4361E 00	0.4388E 00	0.4423E 00	0.4463E 00
9	H	0.1771E-01	0.1823E-01	0.1906E-01	0.2025E-01	0.2257E-01
10	N2	0.4643E-01	0.4620E-01	0.4589E-01	0.4549E-01	0.4495E-01
11	C6H6O	0.8200E-01	0.8158E-01	0.8101E-01	0.8028E-01	0.7931E-01
12	C6H6	0.1105E-01	0.1100E-01	0.1094E-01	0.1085E-01	0.1074E-01
13	NH3	0.9773E-71	0.9725E-71	0.9659E-71	0.9575E-71	0.9462E-71
14	CO	0.5692E-01	0.5895E-01	0.6185E-01	0.6564E-01	0.7105E-01
15	CO2	0.3393E-01	0.3362E-01	0.3332E-01	0.3304E-01	0.3265E-01
16	H2O	0.1333E 00	0.1299E 00	0.1249E 00	0.1181E 00	0.1080E 00
17	OH	0.1000E-69	0.2156E-03	0.1173E-02	0.2516E-02	0.5017E-02
18	O	0.9881E-03	0.1132E-02	0.1193E-02	0.1172E-02	0.1159E-02
19	C	0.1084E 01	0.1077E 01	0.1066E 01	0.1053E 01	0.1034E 01

INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0012	0.0013	0.0013	0.0014	0.0014
TEMPERATURE (OF)	3092.2	3210.0	3329.7	3449.6	3567.1
PRESSURE (LB/FT2)	2165.7	2165.5	2165.3	2165.0	2164.8
MASS FLUX(LB/FT2-SEC)	0.1639	0.1660	0.1673	0.1682	0.1685

	GAS COMPONENT	COMPOSITION (MOLE/MOLE GAS)				
1	CH2	0.3888E-03	0.7688E-03	0.1362E-02	0.2495E-02	0.4413E-02
2	CH3	0.1436E-03	0.2467E-03	0.4062E-03	0.7837E-03	0.1526E-02
3	CH4	0.7485E-01	0.7101E-01	0.6788E-01	0.6487E-01	0.6145E-01
4	C2H6	0.1252E-04	0.5737E-05	0.2738E-05	0.8772E-06	0.1700E-06
5	C2H4	0.3584E-01	0.2418E-01	0.1454E-01	0.5890E-02	0.1482E-02
6	C2H2	0.4404E-01	0.5225E-01	0.5949E-01	0.6673E-01	0.7059E-01
7	C2H	0.1690E-01	0.1614E-01	0.1561E-01	0.1528E-01	0.1511E-01
8	H2	0.4558E 00	0.4656E 00	0.4724E 00	0.4795E 00	0.4842E 00
9	H	0.3114E-01	0.4408E-01	0.5338E-01	0.5617E-01	0.5636E-01
10	N2	0.4341E-01	0.4148E-01	0.4011E-01	0.3925E-01	0.3881E-01
11	C6H6O	0.7651E-01	0.7299E-01	0.7047E-01	0.6880E-01	0.6782E-01
12	C6H6	0.1040E-01	0.9979E-02	0.9688E-02	0.9529E-02	0.9475E-02
13	NH3	0.9137E-71	0.8730E-71	0.8442E-71	0.8260E-71	0.8168E-71
14	CO	0.8547E-01	0.1013E 00	0.1106E 00	0.1161E 00	0.1186E 00
15	CO2	0.3153E-01	0.3012E-01	0.2913E-01	0.2850E-01	0.2818E-01
16	H2O	0.7827E-01	0.4099E-01	0.1654E-01	0.4952E-02	0.1275E-02
17	OH	0.1412E-01	0.2770E-01	0.3737E-01	0.4012E-01	0.3974E-01
18	O	0.1119E-02	0.1069E-02	0.1034E-02	0.1012E-02	0.1000E-02
19	C	0.9818E 00	0.9185E 00	0.8758E 00	0.8494E 00	0.8366E 00

INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0015	0.0015	0.0015	0.0016	0.0016
TEMPERATURE (OF)	3681.8	3793.8	3903.2	4010.5	4115.6
PRESSURE (LB/FT2)	2164.6	2164.3	2164.1	2163.9	2163.6
MASS FLUX(LB/FT2-SEC)	0.1686	0.1686	0.1686	0.1686	0.1685

	GAS COMPONENT	COMPOSITION (MOLE/MOLE GAS)				
1	CH2	0.7336E-02	0.1115E-01	0.1608E-01	0.2132E-01	0.2673E-01
2	CH3	0.2718E-02	0.4308E-02	0.6392E-02	0.8602E-02	0.1089E-01
3	CH4	0.5686E-01	0.5102E-01	0.4345E-01	0.3540E-01	0.2708E-01
4	C2H6	0.2384E-07	0.4605E-08	0.3111E-08	0.1715E-08	0.1804E-08
5	C2H4	0.2476E-03	0.6069E-04	0.4416E-04	0.3552E-04	0.2901E-04
6	C2H2	0.7169E-01	0.7192E-01	0.7207E-01	0.7237E-01	0.7296E-01
7	C2H	0.1500E-01	0.1490E-01	0.1478E-01	0.1464E-01	0.1450E-01
8	H2	0.4862E 00	0.4875E 00	0.4888E 00	0.4902E 00	0.4914E 00
9	H	0.5716E-01	0.5839E-01	0.6003E-01	0.6176E-01	0.6353E-01
10	N2	0.3853E-01	0.3828E-01	0.3796E-01	0.3762E-01	0.3726E-01
11	C6H6O	0.6709E-01	0.6634E-01	0.6542E-01	0.6441E-01	0.6325E-01
12	C6H6	0.9459E-02	0.9437E-02	0.9387E-02	0.9308E-02	0.9190E-02
13	NH3	0.8110E-71	0.8057E-71	0.7990E-71	0.7919E-71	0.7842E-71
14	CO	0.1190E 00	0.1187E 00	0.1181E 00	0.1175E 00	0.1170E 00
15	CO2	0.2797E-01	0.2778E-01	0.2754E-01	0.2728E-01	0.2699E-01
16	H2O	0.2597E-03	0.1016E-03	0.7977E-04	0.6569E-04	0.5428E-04
17	OH	0.3946E-01	0.3920E-01	0.3888E-01	0.3853E-01	0.3816E-01
18	O	0.9932E-03	0.9866E-03	0.9784E-03	0.9697E-03	0.9603E-03
19	C	0.8299E 00	0.8245E 00	0.8179E 00	0.8108E 00	0.8031E 00

INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0017	0.0017	0.0018	0.0018	0.0019
TEMPERATURE (OF)	4218.6	4319.4	4418.2	4514.8	4609.5
PRESSURE (LB/FT2)	2163.4	2163.2	2162.9	2162.7	2162.5
MASS FLUX(LB/FT2-SEC)	0.1685	0.1685	0.1685	0.1685	0.1684

	GAS COMPONENT	COMPOSITION (MOLE/MOLE GAS)				
1	CH2	0.3083E-01	0.3420E-01	0.3648E-01	0.3788E-01	0.3868E-01
2	CH3	0.1268E-01	0.1430E-01	0.1562E-01	0.1672E-01	0.1767E-01
3	CH4	0.2068E-01	0.1519E-01	0.1119E-01	0.8278E-02	0.6150E-02
4	C2H6	0.1303E-09	0.3227E-08	0.3910E-08	0.3615E-08	0.5711E-08
5	C2H4	0.2462E-04	0.2100E-04	0.1825E-04	0.1608E-04	0.1428E-04
6	C2H2	0.7381E-01	0.7513E-01	0.7683E-01	0.7889E-01	0.8114E-01
7	C2H	0.1439E-01	0.1428E-01	0.1419E-01	0.1410E-01	0.1420E-01
8	H2	0.4922E 00	0.4926E 00	0.4923E 00	0.4914E 00	0.4900E 00
9	H	0.6490E-01	0.6612E-01	0.6711E-01	0.6788E-01	0.6871E-01
10	N2	0.3696E-01	0.3668E-01	0.3644E-01	0.3621E-01	0.3599E-01
11	C6H6O	0.6220E-01	0.6106E-01	0.5993E-01	0.5875E-01	0.5751E-01
12	C6H6	0.9056E-02	0.8875E-02	0.8656E-02	0.8385E-02	0.8060E-02
13	NH3	0.7780E-71	0.7720E-71	0.7670E-71	0.7622E-71	0.7576E-71
14	CO	0.1167E 00	0.1165E 00	0.1166E 00	0.1174E 00	0.1183E 00
15	CO2	0.2675E-01	0.2650E-01	0.2625E-01	0.2547E-01	0.2469E-01
16	H2O	0.4620E-04	0.3917E-04	0.3358E-04	0.2896E-04	0.2511E-04
17	OH	0.3785E-01	0.3756E-01	0.3732E-01	0.3709E-01	0.3686E-01
18	O	0.9526E-03	0.9454E-03	0.9530E-03	0.1486E-02	0.2002E-02
19	C	0.7969E 00	0.7911E 00	0.7861E 00	0.7813E 00	0.7767E 00

INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0019	0.0019	0.0020	0.0020	0.0021
TEMPERATURE (OF)	4702.4	4793.9	4884.4	4974.1	5063.1
PRESSURE (LB/FT2)	2162.2	2162.0	2161.7	2161.5	2161.2
MASS FLUX(LB/FT2-SEC)	0.1684	0.1684	0.1684	0.1685	0.1685

	GAS COMPONENT	COMPOSITION (MOLE/MOLE GAS)				
1	CH2	0.3901E-01	0.3870E-01	0.3812E-01	0.3749E-01	0.3681E-01
2	CH3	0.1797E-01	0.1835E-01	0.1856E-01	0.1868E-01	0.1872E-01
3	CH4	0.4816E-02	0.4053E-02	0.3505E-02	0.3020E-02	0.2594E-02
4	C2H6	0.3688E-09	0.2060E-08	0.1336E-08	0.2239E-08	0.1513E-08
5	C2H4	0.1196E-04	0.1053E-04	0.8926E-05	0.7524E-05	0.6251E-05
6	C2H2	0.7816E-01	0.7972E-01	0.7830E-01	0.7638E-01	0.7318E-01
7	C2H	0.1926E-01	0.2017E-01	0.2388E-01	0.2808E-01	0.3345E-01
8	H2	0.4853E 00	0.4760E 00	0.4645E 00	0.4514E 00	0.4378E 00
9	H	0.7459E-01	0.8450E-01	0.9776E-01	0.1129E 00	0.1290E 00
10	N2	0.3559E-01	0.3519E-01	0.3466E-01	0.3409E-01	0.3348E-01
11	C6H6O	0.5595E-01	0.5431E-01	0.5249E-01	0.5057E-01	0.4862E-01
12	C6H6	0.7654E-02	0.7190E-02	0.6664E-02	0.6100E-02	0.5522E-02
13	NH3	0.7490E-71	0.7406E-71	0.7296E-71	0.7175E-71	0.7046E-71
14	CO	0.1189E 00	0.1199E 00	0.1208E 00	0.1217E 00	0.1225E 00
15	CO2	0.2350E-01	0.2204E-01	0.2026E-01	0.1827E-01	0.1613E-01
16	H2O	0.2175E-04	0.1867E-04	0.1594E-04	0.1358E-04	0.1158E-04
17	OH	0.3645E-01	0.3603E-01	0.3551E-01	0.3494E-01	0.3433E-01
18	O	0.2774E-02	0.3794E-02	0.5010E-02	0.6379E-02	0.7841E-02
19	C	0.7680E 00	0.7593E 00	0.7480E 00	0.7354E 00	0.7219E 00

INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0021	0.0022	0.0022	0.0023	0.0023
TEMPERATURE (DF)	5151.5	5239.3	5326.6	5413.6	5500.1
PRESSURE (LB/FT2)	2161.0	2160.7	2160.5	2160.3	2160.0
MASS FLUX(LB/FT2-SEC)	0.1685	0.1686	0.1687	0.1688	0.1690

	GAS COMPONENT	COMPOSITION (MOLE/MOLE GAS)				
1	CH2	0.3614E-01	0.3542E-01	0.3476E-01	0.3404E-01	0.3321E-01
2	CH3	0.1869E-01	0.1859E-01	0.1847E-01	0.1828E-01	0.1797E-01
3	CH4	0.2231E-02	0.1917E-02	0.1646E-02	0.1419E-02	0.1253E-02
4	C2H6	0.2312E-08	0.1630E-08	0.2305E-08	0.1704E-08	0.1000E-69
5	C2H4	0.5228E-05	0.4313E-05	0.3641E-05	0.2994E-05	0.2438E-05
6	C2H2	0.7054E-01	0.6742E-01	0.6521E-01	0.6137E-01	0.5658E-01
7	C2H	0.3826E-01	0.4330E-01	0.4752E-01	0.5296E-01	0.5877E-01
8	H2	0.4235E 00	0.4074E 00	0.3924E 00	0.3753E 00	0.3540E 00
9	H	0.1457E 00	0.1649E 00	0.1824E 00	0.2032E 00	0.2300E 00
10	N2	0.3286E-01	0.3221E-01	0.3161E-01	0.3095E-01	0.3020E-01
11	C6H6O	0.4668E-01	0.4473E-01	0.4289E-01	0.4102E-01	0.3909E-01
12	C6H6	0.4949E-02	0.4394E-02	0.3876E-02	0.3391E-02	0.2943E-02
13	NH3	0.6917E-71	0.6779E-71	0.6653E-71	0.6514E-71	0.6356E-71
14	CO	0.1235E 00	0.1241E 00	0.1248E 00	0.1250E 00	0.1245E 00
15	CO2	0.1394E-01	0.1180E-01	0.9822E-02	0.8022E-02	0.6397E-02
16	H2O	0.9879E-05	0.8391E-05	0.7179E-05	0.6105E-05	0.5121E-05
17	OH	0.3373E-01	0.3310E-01	0.3251E-01	0.3186E-01	0.3111E-01
18	O	0.9345E-02	0.1076E-01	0.1207E-01	0.1317E-01	0.1405E-01
19	C	0.7082E 00	0.6936E 00	0.6800E 00	0.6650E 00	0.6478E 00

APPENDIX C

THERMOPHYSICAL PROPERTIES DATA

This appendix contains all the thermodynamic and physical property data used in this research along with the references and methods used to compute the heat capacity, enthalpy, free energy, thermal conductivity and viscosity of gases. In addition, the thermophysical properties required to characterize both the char and the virgin material are also presented. At the end of the chapter, a brief explanation and a typical input of the Thermochemical Generation Program (TGP) is presented. This program was written to develop a uniform thermodynamic data base for converting thermodynamic information from various sources to a convenient polynomial form.

Thermophysical Properties of Gases: The thermodynamic and physical properties data used by the ABLATIN1 and ABLATIN2 systems is presented. The thermodynamic data is presented in table form giving the values of empirical constants for polynomial fit. In this research it was convenient to use the thermodynamic data in functional form. This procedure not only reduced memory space, but in addition, it reduced the need for interpolation between tables of stored values. Coefficient for the polynomial fits have been obtained from numerous sources, mainly from the work of NASA at Lewis (1), Bauer and Duff at Los Alamos

(2), API Project 44 (8) and JANAF (6). The polynomial equations used for the heat capacity is of the form:

$$\frac{C^o_p}{R} = a+bT+cT^2+dT^3+eT^4 \qquad \text{(C-1)}$$

If we define the sensible enthalpy plus the heat of formation at a reference temperature as H^o_T, then:

$$H^o_T = \Delta H^o_{T_R} + \int_{T_R}^{T} C^o_p \, dT \qquad \text{(C-2)}$$

Where $\Delta H^o_{T_R}$ is the heat of formation at the reference temperature T_R. Substitution of Equation (C-1) into (C-2) and integrating results after some manipulation results in:

$$\frac{H^o_T}{RT} = a+\frac{b}{2}T+\frac{c}{3}T^2+\frac{d}{4}T^3+\frac{e}{5}T^4+\frac{f}{T} \qquad \text{(C-3)}$$

The definition of absolute entropy is:

$$S^o_T = \int_0^T \frac{C^o_p}{T} \, dT \qquad \text{(C-4)}$$

Hence, substituting Equation (C-1) into Equation (C-4) and integrating results after some manipulation:

$$\frac{S^o_T}{R} = a \ln T + bT + \frac{c}{2}T^2 + \frac{d}{3}T^3 + \frac{c}{4}T^4 \qquad \text{(C-5)}$$

The definition of Standard Molal Free Energy is

as follows:

$$\bar{F}_T^o = \bar{H}_T^o - TS_T^o \qquad \text{(C-6)}$$

Substituting the deffinitions for H_T^o and S_T^o in Equation (C-6) results in a polynomial expression for the free energy which is, after dividing by RT:

$$\frac{\bar{F}_T^o}{RT} = a(1-\ln T) - \frac{b}{2}T - \frac{c}{6}T^2 - \frac{dT^3}{12} - \frac{eT^4}{20} + \frac{f}{T} - g \qquad \text{(C-7)}$$

A set of coefficients is presented in Table C-1 for Equations (C-1), (C-3), (C-5) and (C-7). The coefficients presented in Table C-1 are two temperature intervals. A high temperature interval (1000°K-6000°K) denoted by the letter H and a low temperature interval (300°K-1000°K) denoted by the letter L. Most of the data used was from McBride et. al. (1) of NASA, covering the intervals 300°K to 1000°K and 1000°K to 6000°K. At 1000°K the low and high temperature fits were forced to match. The species for which data of McBride et. al. (1) was used were: C(Graphite), C(g), C_2, C_3, CH, CH_2, CH_3, CH_4, C_2H_2, C_2H_4, CN, C_2N_2, CO, CO_2, H, H_2, HCO, H_2O, N, N_2, NH, NH_3, NO, NO_2, N_2O, N_2O_4, O, O_2 and OH. The coefficients presented for the other species were obtained using the heat capacity coefficients of Duff et. al. (2) and the other two coefficients, f and g, were calculated from them.

TABLE C-1: Coefficients for the Empirical Fit of

C_p^o/R, S_T^o/R and $\overline{F}_T^o/RT$

		A	B	C	D	E	F	G
C(G)	H	.2579E1	-.1437E-3	.7225E-7	-.7417E-11	.1370E-16	.8543E5	.4321E1
	L	.2541E1	-.2210E-3	.4736E-6	-.4529E-9	.1602E-12	.8545E5	.4573E1
C_2	H	.4045E1	.1697E-3	.1585E-6	-.5527E-10	.4859E-14	.9961E5	.1281E1
	L.	.7509E1	-.1065E-1	.1007E-4	-.8621E-9	-.1752E-11	.9880E5	-.1607E2
C_3	H	.4713E1	.2903E-2	-.1214E-5	.2285E-9	-.1599E-13	.9375E5	-.2530E1
	L	.2633E1	.9419E-2	-.9593E-5	.5579E-8	-.1424E-11	.9431E5	.8079E1
C_4	H	.6077E1	.3443E-2	-.9479E-6	.9347E-10	-.1791E-14	.1195E6	-.5995E1
	L	.5670E1	.5883E-2	-.4751E-5	.2349E-8	-.4648E-12	.1195E6	-.4253E1
C_5	H	.7577E1	.4617E-2	-.1271E-5	.1187E-9	-.1123E-14	.1186E6	-.1431E2
	L	.7279E	.6762E-2	-.5027E-5	.2562E-8	-.5450E-12	.1186E6	-.1311E2
C_6	H	.9077E1	.5791E-2	-.1595E-5	.1441E-9	-.4628E-15	.1437E6	-.1904E2
	L	.8887E1	.7643E-2	-.5307E-5	.2779E-8	-.6265E-12	.1437E6	-.1837E2
C_7	H	.1057E2	.6963E-2	-.1917E-5	.1689E-9	.2555E-15	.1435E6	-.2736E2
	L	.1049E2	.8524E-2	-.5585E-5	.2995E-8	-.7075E-12	.1435E6	-.2722E2
C_8	H	.1207E2	.8133E-2	-.2238E-5	.1934E-9	.9903E-15	.1696E6	-.3209E2
	L	.1211E2	.9403E-2	-.5861E-5	.3207E-8	-.7885E-12	.1696E6	-.3249E2
C_9	H	.1357E2	.9308E-2	-.2562E-5	.2189E-9	.1641E-14	.1670E6	-.4041E2
	L	.1371E2	.1028E-1	-.6144E-5	.3427E-8	-.8705E-12	.1669E6	-.4134E2
C_{10}	H	.1508E2	.1048E-1	-.2885E-5	.2439E-9	.2339E-14	.1966E6	-.4514E2
	L	.1532E2	.1117E-1	-.6421E-5	.3641E-8	-.9510E-12	.1965E5	-.4661E2

		A	B	C	D	E	F	G
CH	H	.1961E1	.3312E-2	-.1469E-5	.2929E-9	-.2124E-13	.7105E5	.1021E2
	L	.3544E1	.8795E-4	-.1826E-5	.4455E-8	-.2186E-11	.7059E5	.1823E1
C_2H	H	.3513E1	.3589E-2	-.1323E-5	.2305E-9	-.1530E-13	.5789E5	.4523E1
	L	.3006E1	.5537E-2	-.3511E-5	.1249E-8	-.1896E-12	.5797E5	.6920E1
C_3H	H	.3965E1	.6200E-2	-.2265E-5	.3717E-9	-.2262E-13	.6283E5	.3467E1
	L	.2473E1	.1175E-1	-.8045E-5	.2729E-8	-.3544E-12	.6307E5	.1054E2
C_4H	H	.5873E1	.7403E-2	-.2729E-5	.4437E-9	-.2637E-13	.7605E5	-.4010E1
	L	.2695E1	.2267E-1	-.2451E-4	.1315E-7	-.2673E-11	.7649E5	.1039E2
C_5H	H	.5465E1	.1118E-1	-.4299E-5	.7241E-9	-.4441E-13	.9152E5	-.2843E1
	L	.1021E1	.3109E-1	-.3043E-7	.1481E-7	-.2783E-11	.9217E5	.1757E2
C_6H	H	.8361E1	.1164E-1	-.4637E-5	.8085E-9	-.5150E-13	.1053E6	-.1363E2
	L	.2717E1	.3941E-1	-.4505E-4	.2477E-7	-.5100E-11	.1050E6	.1184E2
C_7H	H	.9024E1	.1425E-1	-.5733E-5	.1009E-8	-.6475E-13	.1184E6	-.1733E2
	L	.1743E1	.4949E-1	-.5613E-4	.3040E-7	-.6175E-11	.1193E6	.1562E2
C_8H	H	.9773E1	.1663E-1	-.8198E5	.1181E-8	-.7600E-13	.1418E6	-.2083E2
	L	.1532E1	.5652E-1	-.6393E-4	.3473E-7	-.7085E-11	.1429E6	.1640E2
C_9H	H	.1113E2	.1843E-1	-.7453E-5	.1318E-8	-.8510E-13	.1435E6	-.2718E2
	L	.1099E1	.6769E-1	-.7887E-4	.4345E-7	-.8925E-11	.1448E6	.1813E2
$C_{10}H$	H	.1255E2	.2011E-2	-.8136E-5	.1440E-8	-.9305E-13	.1707E6	-.2677E2
	L	.2248E1	.7022E-1	-.8037E-4	.4395E-7	-.9005E-11	.1713E6	.1442E2
CH_2	H	.2229E1	.4711E-2	-.1766E-5	.3065E-9	-.2017E-13	.3383E5	.7708E1
	L	.3551E1	-.2507E-2	.1235E-4	-.1175E-7	.3812E-11	.3366E5	.1797E1
C_2H_2	H	.4497E1	.5269E-2	-.1840E-5	.3105E-9	-.2000E-13	.2563E5	-.3145E1
	L	.7903E0	.2347E-1	-.3554E-4	.2795E-7	-.8448E-11	.2625E5	.1401E2

		A	B	C	D	E	F	G
C_3H_2	H	.4501E1	.8696E-2	-.3155E-5	.5242E-9	-.3264E-13	.5191E5	.1827E0
	L	.1668E1	.2219E-1	-.2193E-4	.1110E-7	-.2153E-11	.5230E5	.1305E2
C_4H_2	H	.6375E1	.9648E-2	-.3706E-5	.6390E-9	-.4081E-13	.5391E5	-.9060E1
	L	.2071E1	.3115-1	-.3650E-4	.2047E-7	-.4277E-11	.5449E5	.1033E2
C_5H_2	H	.6655E1	.1325E-1	-.5105E-5	.8823E-9	-.5645E-13	.8063E5	-.8785E1
	L	.1006E1	.4108E-1	-.4555E-4	.2475E-7	-.5060E-11	.8139E5	.1669E2
C_6H_2	H	.8775E1	.1341E-1	-.5232E-5	.9113E-9	-.5860E-13	.8223E5	-.1805E2
	L	.2324E1	.4629E-1	-.5461E-4	.3087E-7	-.6480E-11	.8307E5	.1082E2
C_7H_2	H	.8139E1	.1757E-1	-.6763E-5	.1167E-8	-.7450E-13	.1079E6	-.1389E2
	L	.2029E1	.4775E-1	-.5111E-4	.2777E-7	-.5745E-11	.1088E6	.1366E2
C_8H_2	H	.1047E2	.1819E-1	-.7243E-5	.1277E-8	-.8285E-13	.1099E6	-.2657E2
	L	.1087E1	.6487E-1	-.7571E-4	.4207E-7	-.8700E-11	.1112E6	.1567E2
C_9H_2	H	.1006E2	.2185E-1	-.8502E-5	.1477E-8	-.9480E-13	.1331E6	-.2275E2
	L	.1691E1	.6335E-1	-.7042E-4	.3834E-7	-.7975E-11	.1342E6	.1499E2
$C_{10}H_2$	H	.1322E2	.2166E-1	-.8660E-5	.1532E-8	-.9955E-13	.1381E6	-.3773E2
	L	.1810E1	.7857E-4	-.9245E-4	.5162E-7	-.1072E-10	.1396E6	.1359E2
CH_3	H	.2803E1	.6250E-2	-.2289E-5	.3899E-9	-.2528E-13	.1579E5	.5684E1
	L	.3399E1	.4267E-2	.2033E-6	.1155E-8	.4129E-12	.1565E5	.2703E1
C_2H_3	H	.3481E1	.8497E-2	-.3113E-5	.5189E-9	-.3232E-13	.3179E5	.5172E1
	L	.3147E1	.8039E-2	.1453E-6	-.2569E-8	.7908E-12	.3189E5	.7097E1
C_3H_3	H	.4658E1	.1051E-1	-.3955E-5	.6723E-9	-.4248E-13	.3667E5	.6294E0
	L	.2588E1	.1891E-1	-.1393E-4	.5541E-8	-.9075E-12	.3699E5	.1031E2
C_4H_3	H	.5749E1	.1248E-1	-.4751E-5	.8136E-9	-.5170E-13	.4909E5	-.3429E1
	L	.2636E1	.2633E-1	-.2312E-4	.1093E-7	-.2068E-11	.4955E5	.1091E2
C_5H_3	H	.7099E1	.1455E-1	-.5664E-5	.9844E-9	-.6320E-13	.6543E5	-.9039E1
	L	.2649E1	.3462E-1	-.3266E-4	.1601E-7	-.3088E-11	.6608E5	.1139E2

		A	B	C	D	E	F	G
C_6H_3	H	.8312E1	.1640E-1	-.6416E-5	.1118E-8	-.7200E-13	.7660E5	-.1357E2
	L	.2926E1	.4064E-1	-.3886E-4	.1907E-7	-.3666E-11	.7738E5	.1117E2
CH_4	H	.1180E1	.1095E-1	-.4062E-5	.7137E-9	-.4749E-13	-.9855E4	.1250E2
	L	.4249E1	-.6912E-2	.3160E-4	-.2971E-7	.9510E-11	.1018E5	-.9175E0
C_2H_4	H	.3502E1	.1159E-1	-.4474E-5	.7945E-9	-.5323E-13	.4543E4	.2466E1
	L	.1120E1	.1390E-1	.2656E-5	-.1156E-7	.5238E-11	.5332E4	.1583E2
$C_3H_4^{-1}$	H	.4247E1	.1363E-1	-.5114E-5	.8668E-9	-.5465E-13	.2046E5	.1760E1
	L	.2745E1	.1792E-1	-.7243E-5	-.7208E-10	.5918E-12	.2074E5	.9139E1
$C_3H_4^{-2}$	H	.6126E1	.1306E-1	-.5210E-5	.9194E-9	-.5965E-13	.2072E5	-.9286E1
	L	.2496E1	.1839E-1	-.6755E-5	-.8296E-9	.8053E-12	.2159E5	.9894E1
$C_4H_4^{-1}$	H	.5392E1	.1576E-1	-.6028E-5	.1035E-8	-.6590E-13	.3484E5	-.1649E1
	L	.2231E1	.2772E-1	-.1885E-4	.6522E-8	-.8975E-12	.3535E5	.1331E2
$C_4H_4^{-2}$	H	.5088E1	.1614E-1	-.6192E-5	.1065E-8	-.6790E-13	.3289E5	-.1819E1
	L	.2598E1	.2399E-1	-.1215E-4	.2144E-8	.7127E-13	.3334E5	.1028E2
$C_5H_4^{-1}$	H	.7931E1	.1635E-1	-.6293E-5	.1086E-8	-.6935E-13	.4871E5	-.1361E2
	L	.2468E1	.4229E-1	-.4289E-4	.2225E-7	.4450E-11	.4947E5	.1121E2
$C_5H_4^{-2}$	H	.6560E1	.1792E-1	-.6963E-5	.1208E-8	-.7750E-13	.5111E5	-.6448E1
	L	.2010E1	.3603E-1	-.2778E-4	.1096E-7	-.1733E-11	.5183E5	.1491E2
$C_5H_4^{-3}$	H	.6258E1	.1823E-1	-.7078E-5	.1227E-8	-.7870E-13	.4816E5	-.1868E1
	L	.2211E1	.3393E-1	-.2470E-4	.9332E-8	-.1438E-11	.4881E5	.1722E2
$C_6H_4^{-1}$	H	.7080E1	.1962E-1	-.7668E-5	.1336E-8	-.8589E-13	.6279E5	-.1179E2
	L	.2522E1	.4236E-1	-.3545E-4	.1536E-7	-.2672E-11	.6363E5	.1369E2
$C_6H_4^{-2}$	H	.8014E1	.1965E-1	-.7685E-5	.1339E-8	-.8610E-13	.6326E5	-.1236E2
	L	.3073E1	.3951E-1	-.3103E-4	.1269E-7	-.2109E-11	.6403E5	.1080E2

		A	B	C	D	E	F	G
$C_6H_4^{-3}$	H	.5152E1	.2280E-1	-.8996E-5	.1577E-8	-.1018E-12	.5880E5	-.8328E0
	L	.8791E0	.3417E-1	-.1292E-4	-.2030E-8	.1584E-11	.5961E5	.2033E2
C_3H_5	H	.4163E1	.1670E-1	-.6328E-5	.1079E-8	-.6880E-13	.1439E5	.7926E1
	L	.3158E1	.1511E-1	.4407E-5	-.9188E-8	.2697E-11	.1468E5	.1374E2
$C_4H_5^{-1}$	H	.4650E1	.1925E-1	-.7335E-5	.1255E-8	-.7970E-13	.3071E5	.3784E1
	L	.3082E1	.2100E-1	-.2637E-5	-.4696E-8	.1634E-11	.3107E5	.1203E2
$C_4H_5^{-2}$	H	.4710E1	.1999E-1	-.7824E-5	.1364E-8	-.8775E-13	.3024E5	.9718E0
	L	.1593E1	.2699E-1	-.7206E-5	-.4060E-8	.1839E-11	.3086E5	.1666E2
C_2H_6	H	.1430E1	.1889E-1	-.7044E-5	.1187E-8	-.7445E-13	-.1143E5	.1401E2
	L	.1430E1	.1889E-1	-.7044E-5	.1187E-8	-.7445E-13	-.1143E5	.1401E2
$C_3H_6^{-1}$	H	.2530E1	.2103E-1	-.7953E-5	.1354E-8	-.8565E-13	.8170E3	.1171E2
	L	.3013E1	.1439E-1	.1195E-4	-.1763E-7	.5647E-11	.8268E3	.1022E2
$C_3H_6^{-2}$	H	.2927E1	.2041E-1	-.7676E-5	.9036E-9	-.8230E-13	.5054E4	.6002E1
	L	.1745E1	.1757E-1	.7810E-5	-.1324E-7	.3826E-11	.5422E4	.1302E2
$C_4H_6^{-1}$	H	.4007E1	.2255E-1	-.8552E-5	.1458E-8	-.9235E-13	.1546E5	.4838E1
	L	.3764E1	.1845E-1	.6784E-5	-.1369E-7	.4487E-11	.1560E5	.6898E1
$C_4H_6^{-2}$	H	.3971E1	.2259E-1	.8575E-5	.1464E-8	-.9285E-13	.1774E5	.5946E1
	L	.2437E1	.2913E-1	-.1298E-4	.6525E-9	.8151E-12	.1794E5	.1293E2
$C_4H_6^{-3}$	H	.3258E1	.2349E-1	-.8975E-5	.1539E-8	-.9780E-13	.1127E5	.8230E1
	L	.1310E1	.3537E-1	-.2098E-4	.4492E-8	.2204E-12	.1142E5	.1629E2
$C_4H_6^{-4}$	H	.2782E1	.2591E-1	-.5997E-5	-.4794E-8	.2247E-11	.1757E5	.1191E2
	L	.3991E1	.2286E-1	-.8745E-5	.1501E-8	-.9550E-13	.1736E5	.6002E1
C_5H_6	H	.3601E1	.2668E-1	-.1036E-4	.1799E-8	-.1155E-12	.8326E4	.4317E1
	L	.8735E0	.2770E-1	.4256E-5	-.1439E-7	.4465E-11	.8994E4	.1904E2

		A	B	C	D	E	F	G
C_6H_6	H	.4619E1	.2881E-1	-.1124E-4	.1957E-8	-.1257E-12	.7391E4	-.1789E1
	L	.3511E0	.3754E-1	-.7947E-5	-.7509E-8	.3038E-11	.8264E4	.1986E2
C_3H_8	H	.1291E1	.2775E-1	-.1047E-4	.1780E-8	-.1124E-12	-.1407E5	.1714E2
	L	.2055E1	.2528E-1	-.8879E-8	-.8879E-8	.3198E-11	-.1425E5	.1318E2
$C_4H_8^{-1}$	H	.2473E1	.2980E-1	-.1134E-4	.1940E-8	-.1231E-12	-.2852E4	.1359E2
	L	.3228E1	.1948E-1	.1816E-4	-.2582E-7	.8205E-11	-.2828E4	.1131E2
$C_4H_8^{-2}$	H	.2293E1	.3011E-1	-.1149E-4	.1971E-8	-.1252E-12	-.1973E4	.1510E2
	L	.2773E1	.2733E-1	.1802E-5	-.1306E-7	.4737E-11	-.2083E4	.1274E2
$C_4H_8^{-3}$	H	.2648E1	.2963E-1	-.1127E-4	.1929E-8	-.1224E-12	-.4064E4	.1182E2
	L	.2332E1	.3207E-1	-.9355E-5	-.3009E-8	.1738E-11	-.4086E4	.1285E2
$C_4H_8^{-4}$	H	.2647E1	.2959E-1	-.1125E-4	.1923E-8	-.1219E-12	-.3370E4	.1219E2
	L	.3218E1	.2521E-1	.3948E-5	-.1345E-7	.4555E-11	-.3452E4	.9706E1
$C_4H_8^{-5}$	H	.3216E1	.2940E-1	-.1127E-4	.1939E-8	-.1235E-12	.1076E4	.4977E1
	L	.1990E0	.3516E-1	-.9240E-5	-.3076E-8	.1213E-11	.1711E4	.2040E2
C_7H_8	L	-.5417E1	.7735E-1	-.5841E-4	.2372E-7	-.3986E-11	-.1258E4	.4924E2
	L	-.5417E1	.7735E-1	-.5841E-4	.2372E-7	-.3986E-11	-.1258E4	.4924E2
$C_4H_{10}^{-1}$	H	.4285E1	.2841E-1	-.1161E-4	.2081E-8	-.1363E-12	-.1765E5	.4799E1
	L	.3190E1	.2995E-1	.5455E-5	-.1707E-7	.5811E-11	-.1751E5	.9987E1
$C_4H_{10}^{-2}$	H	.4285E1	.2841E-1	-.1161E-4	.2081E-8	-.1363E-12	-.1799E5	.4816E1
	L	.1879E2	-.1312E0	.4290E-3	-.4265E-6	.1373E-9	-.1833E5	-.4601E2
C_6H_6O	L	-.3931E1	.6938E-1	-.5210E-4	.1249E-7	.2091E-11	-.1330E5	.4187E2
	L	-.3931E1	.6938E-1	-.5210E-4	.1249E-7	.2091E-11	-.1330E5	.4187E2
CN	H	.3602E1	.3408E-3	.9716E-7	-.1582E-10	-.4142E-15	.4731E5	.3552E1
	L	.3852E1	-.2763E-2	.6857E-5	-.5413E-8	.1490E-11	.4741E5	.2971E1
C_2N_2	H	.6502E1	.4053E-2	-.1664E-5	.3094E-9	-.2148E-13	.3490E5	-.9441E1
	L	.3402E1	.1775E-1	-.2686E-4	.2196E-7	-.7087E-11	.3555E5	.5412E1

		A	B	C	D	E	F	G
CO	H	.2951E1	.1552E-2	-.6191E-6	.1135E-9	-.7788E-14	-.1423E5	.6531E1
	L	.3787E1	-.2171E-2	.5075E-5	-.3473E-8	.7721E-12	-.1436E5	.2633E1
CO_2	H	.4412E1	.3192E-2	-.1298E-5	.2415E-9	-.1674E-13	-.4894E5	-.7287E0
	L	.2170E1	.1037E-1	-.1073E-4	.6345E-8	-.1628E-11	-.4835E5	.1066E2
H	H	.2500E1	.0000E0	.0000E0	.0000E0	.0000E0	.2547E5	-.4600E0
	L	.2500E1	.0000E0	.0000E0	.0000E0	.0000E0	.2547E5	-.4600E0
HCN	H	.3653E1	.3443E-2	-.1258E-5	.2169E-9	-.1430E-13	.1442E5	.2372E1
	L	.2168E1	.1072E-1	-.1508E-4	.1193E-7	-.3700E-11	.1468E5	.9281E1
HCO	H	.3270E1	.3519E-2	-.1377E-5	.2473E-9	-.1673E-13	-.2782E4	.7304E1
	L	.3864E1	-.5370E-3	.6903E-5	-.6645E-8	.2057E-11	-.2799E4	.4897E1
H_2	H	.3043E1	.6118E-3	-.7399E-8	-.2030E-10	.2459E-14	-.8549E3	-.1648E1
	L	.2846E1	.41932E-2	-.9611E-5	.9512E-8	-.3309E-11	-.9672E3	-.1411E1
H_2O	H	.2670E1	.3031E-2	-.8535E-6	.1179E-9	-.6197E-14	.2988E5	.6883E1
	L	.4156E1	-.1724E-2	.5698E-5	-.4593E-8	.1423E-11	-.3028E5	-.6861E0
N	H	.2442E1	.1227E-3	-.8499E-7	.2140E-10	-.1251E-14	.5614E5	.4492E1
	L	.2514E1	-.1124E-3	.2964E-6	-.3246E-9	.1259E-12	.5612E5	.4119E1
NH	H	.2727E1	.1419E-2	-.4582E-6	.7555E-10	-.4617E-14	.3892E5	.6044E1
	L	.3454E1	.5280E-3	-.1972E-5	.2957E-8	-.1208E-11	.3867E5	.2010E1
NH_3	H	.2149E1	.6492E-2	-.2269E-5	.3739E-9	-.2361E-13	-.6402E4	.9238E1
	L	.3771E1	-.4862E-3	.9874E-5	-.9567E-8	.3131E-11	-.6728E4	.1465E1
NO	H	.3152E1	.1406E-2	-.5707E-6	.1062E-9	-.7372E-14	.9852E4	.6944E1
	L	.4146E1	-.4119E-2	.9692E-5	-.7863E-8	.2230E-11	.9744E4	.2569E1
NO_2	H	.4612E1	.2638E-2	-.1094E-5	.2081E-9	-.1465E-13	.2340E4	.1367E1
	L	.3434E1	.2223E-2	.6714E-5	-.9742E-8	.3721E-11	.2864E4	.8408E1

		A	B	C	D	E	F	G
N_2	H	.2854E1	.1597E-2	-.6256E-6	.1131E-9	-.7690E-14	-.8901E3	.6390E1
	L	.3691E1	-.1333E-2	.2650E-5	-.9769E-9	-.9977E-13	-.1062E4	.2287E1
N_2O	H	.4626E1	.3021E-2	-.1215E-5	.2285E-9	-.1585E-13	.8135E4	-.1146E1
	L	.2382E1	.1035E-1	-.1116E-4	.6958E-8	-.1878E-11	.8723E4	.1022E2
N_2O_4	H	.1042E1	.6036E-2	-.2583E-5	.4928E-9	-.3478E-13	-.2741E4	-.2582E2
	L	.3165E1	.2719E-1	-.2535E-4	.1099E-7	-.1660E-11	-.7673E3	.1147E2
O	H	.2537E1	-.1842E-4	-.8801E-8	.5964E-11	-.5574E-15	.2923E5	.4946E1
	L	.3021E1	-.2173E-2	.3754E-5	-.2994E-8	.9077E-12	.2913E5	.2646E1
OH	H	.2889E1	.9983E-3	-.2188E-6	.1980E-10	-.3845E-15	.3881E4	.5559E1
	L	.3823E1	-.1118E-2	.1246E-5	-.2104E-9	-.5255E-13	.3585E4	.5825E0
O_2	H	.3597E1	.7814E-3	-.2238E-6	.4249E-10	-.3346E-14	-.1192E4	.3749E1
	L	.3719E1	-.2516E-2	.8583E-5	-.8299E-8	.2708E-11	-.1057E4	.3908E1

At the end of the appendix a general purpose program is presented that calculates the seven constants, "a" through "g", when the heat capacity at different temperature intervals, the heat of formation, and entropy at 298°K are supplied.

The first card specifies the order of the polynomial of the heat capacity and the number of data points. From the second card on, the heat capacity data with the corresponding temperature in °K are specified. The last card gives the temperature range over which the value of the heat capacity should be calculated and PRINTED out, and the heat of formation and entropy at 298°K which are necessary in the evaluation of the constants.

Gas Phase Physical Properties: The gas phase physical properties required for the solution of the equations of change are the thermal conductivity and the viscocity. The physical property equations are those presented by Sh rwood and Reid (3).

The thermal conductivity of a pure gas is calculated using the equation shown below:

$$k_{g_i} = \frac{2.66\ 13\times10^{-5}\ \left(\frac{T}{M_{w_i}}\right)\ \left(C_{v_i} + 4.47\right)}{\sigma^2\ \Omega_v} \qquad \text{(C-8)}$$

For an ideal gas the heat capacity at constant volume is C_{p_i} -R and the collision diameter, σ , and collision integral, Ω_v , are tabulated for individual gas components

in Table C-2 and Table C-3 respectively. The thermal conductivity of the gas mixture is calculated as:

$$\bar{k}_{g_i} = \sum_{i=1}^{n} x_i k_g \Big/ \sum_{i=1}^{n} x_i \qquad \text{(C-9)}$$

The viscocity of a pure gas is given by a similar equation:

$$\mu_{g_i} = \frac{(2.6693\text{x}10^{-3}) \cdot (M_{w_i} \; T)^{1/2}}{\sigma^2 \; \Omega_v} \qquad \text{(C-10)}$$

The viscocity of the gas mixture is calculated by the equation approximating the Chapman-Enskong Theory:

$$\bar{\mu} = \sum_{i=1}^{n} \mu_i \; \{ 1 + \sum_{\substack{j=1 \\ j \neq i}}^{n} \Phi_i \; (\eta_j / \eta_i) \}^{-1} \qquad \text{(C-11)}$$

where the parameter, Φ_{ij} , is calculated by Equation (C-12) below:

$$\Phi_{ij} = \{1 + (\mu_i / \mu_j)^{1/2} \; (M_{w_j}/M_{w_i})^{1/4}\}^2 \; \{\sqrt{8}(1+M_{w_i}/M_{w_j})^{1/2}\}^{-1} \qquad \text{(C-12)}$$

<u>Thermophysical Properties of the Virgin Material and Char</u>: The thermophysical properties used were those measured by Southern Research Institute (4). Figure C-1 shows the thermal conductivity plot with temperature for 40% nylon, 25% phenolic resin and 35% phenolic microballoon virgin composite. As is shown in the plot the thermal conductivity variation in the temperature range 200°F to 800°F

Table C-2 Lennard-Jones Potentials[a] and Enthalpy of Formation[b] for the Compounds

Component Name	Molecular Weight, M_{wi}	Collision Diameter, σ A°	Potential Parameter ÷ Boltzmann Constant $E°/\bar{k}$, °K	Enthalpy of Formation (290°K) cal/gram mole
CH_4	16	3.822	136.5	-17889.0
C_2H_6	30	4.418	230.0	-20316.6
C_2H_4	28	4.232	205.0	12496.0
C_2H_2	26	4.221	185.0	54194.0
C_6H_6	78	5.270	440.0	19778.8
C_6H_6O	94	5.000	400.0	-23500.0
CO_2	44	3.966	190.0	-94052.0
CO	28	3.590	110.0	-26416.0
H_2	2	2.986	33.3	0.0
H_2O	18	2.649	356.0	-57797.9
HCN	27	3.630	569.1	31100.0
NH_3	17	3.432	312.0	-11040.0
N_2	28	3.681	91.5	0.0
O_2	32	3.433	113.0	0.0

[a] Reid, Robert C. and Thomas K. Sherwood, The Properties of Gases and Liquids, 2nd ed., New York: McGraw-Hill, pp. 632-633. (1966).

[b] Perry, John H., ed., Chemical Engineers' Handbook, 3rd ed., New York: McGraw-Hill, 1950, pp. 236-243.

Table C-3 Values of the Collision Integral Based on Lennard-Jones Potential for Calculating Pure Component Conductivity and Viscosity

$\bar{k}T/E°$	Ω_v	$\bar{k}T/E°$	Ω_v
0.30	2.785	1.30	1.399
0.35	2.628	1.50	1.314
0.40	2.492	1.70	1.248
0.45	2.368	1.90	1.197
0.50	2.257	2.2	1.138
0.55	2.156	2.6	1.081
0.60	2.065	3.2	1.022
0.65	1.982	4.0	0.9700
0.70	1.908	5.0	0.9269
0.75	1.841	7.0	0.8727
0.80	1.780	10.0	0.8242
0.85	1.725	20.0	0.7432
0.90	1.675	40.0	0.6718
0.95	1.587	70.0	0.6194
1.00	1.629	100.0	0.5882
1.10	1.514	200.0	0.5320
1.20	1.452	400.0	0.4811

Reid, Robert C. and Thomas K. Sherwood, The Properties of Gases and Liquids, 2nd ed., New York: McGraw-Hill, 1966, p. 399.

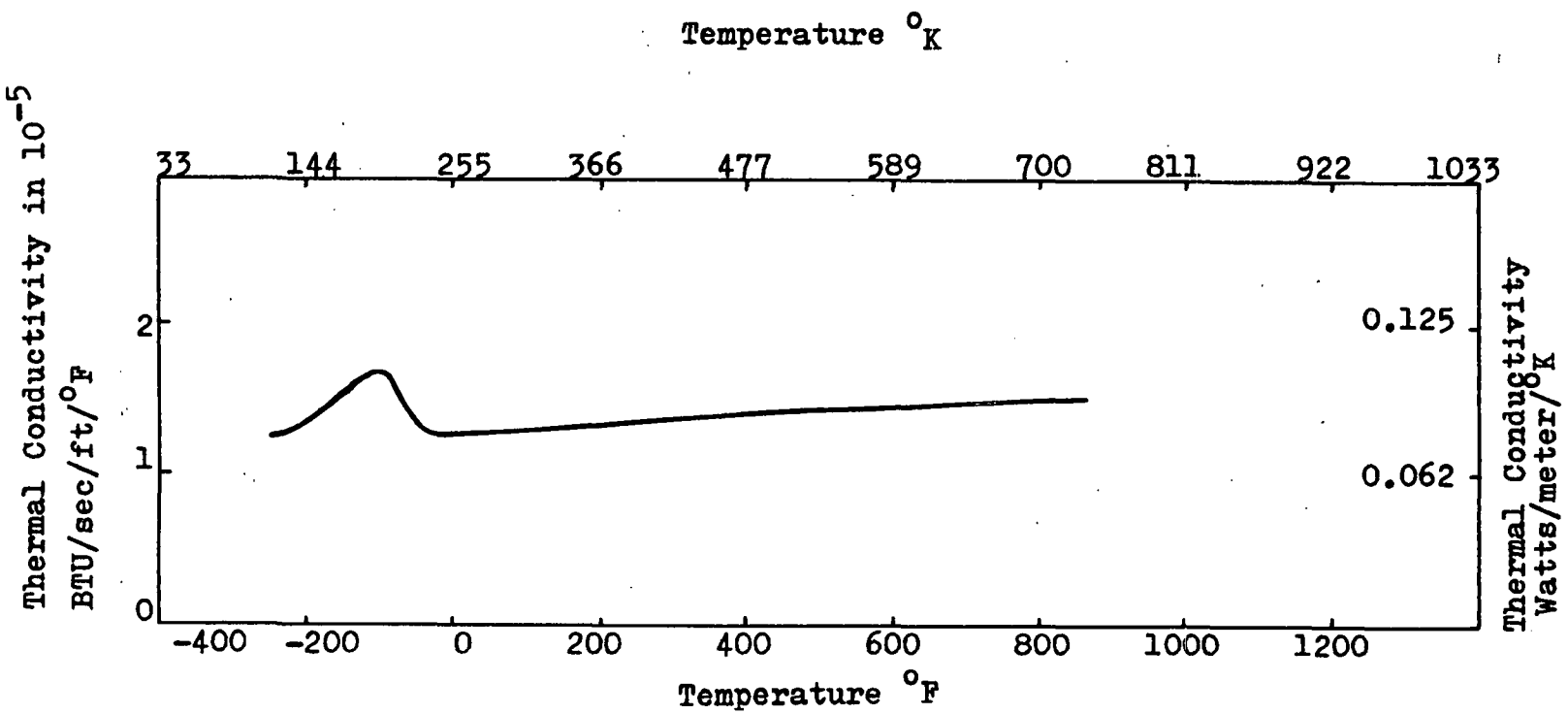

Figure C-1. Thermal Conductivity of Virgin Nylon Phenolic Resin Composite (4).

is small. No further measurements were made beyond 800°F as the degradation of the virgin material made the measurements impractical. However, for the purpose of the computer calculations these measurements were further extrapolated. Figure C-2 shows the thermal conductivity for the low density phenolic nylon char. The thermal conductivity data was fitted empirically by Engelke, et. al. (4) and shown to be:

$$k_e = 11.57 \times 10^{-5} + 5.3 \times 10^{-15} \; T^3 \qquad \text{(C-13)}$$

for the temperature range between 800° and 5000°F. The units of k_e are BTU-ft/sec/ft^2/°F.

In figure C-3 the heat capacity plot for the virgin material with temperature is shown. A least square fit of this data was performed by Engelke et. al. (4) and was shown to be:

$$C_{p_v} = 0.15 + 4.3 \times 10^{-4} \cdot T - 1114 \; T^{-2} \qquad \text{(C-14)}$$

where T is the temperature in degrees Rankin.

The heat capacity data for the char was that of Wilson (5) and is shown in Figure C-4.

Thermochemical Generation Program

Most of the thermodynamic data available today is usually reported in Table form; be it free energy data, enthalpy data, heat capacity data, entropy, etc. The major sources of such thermodynamic data are reported at the end of the Chapter (1,2,6,8). For an extensive review of other

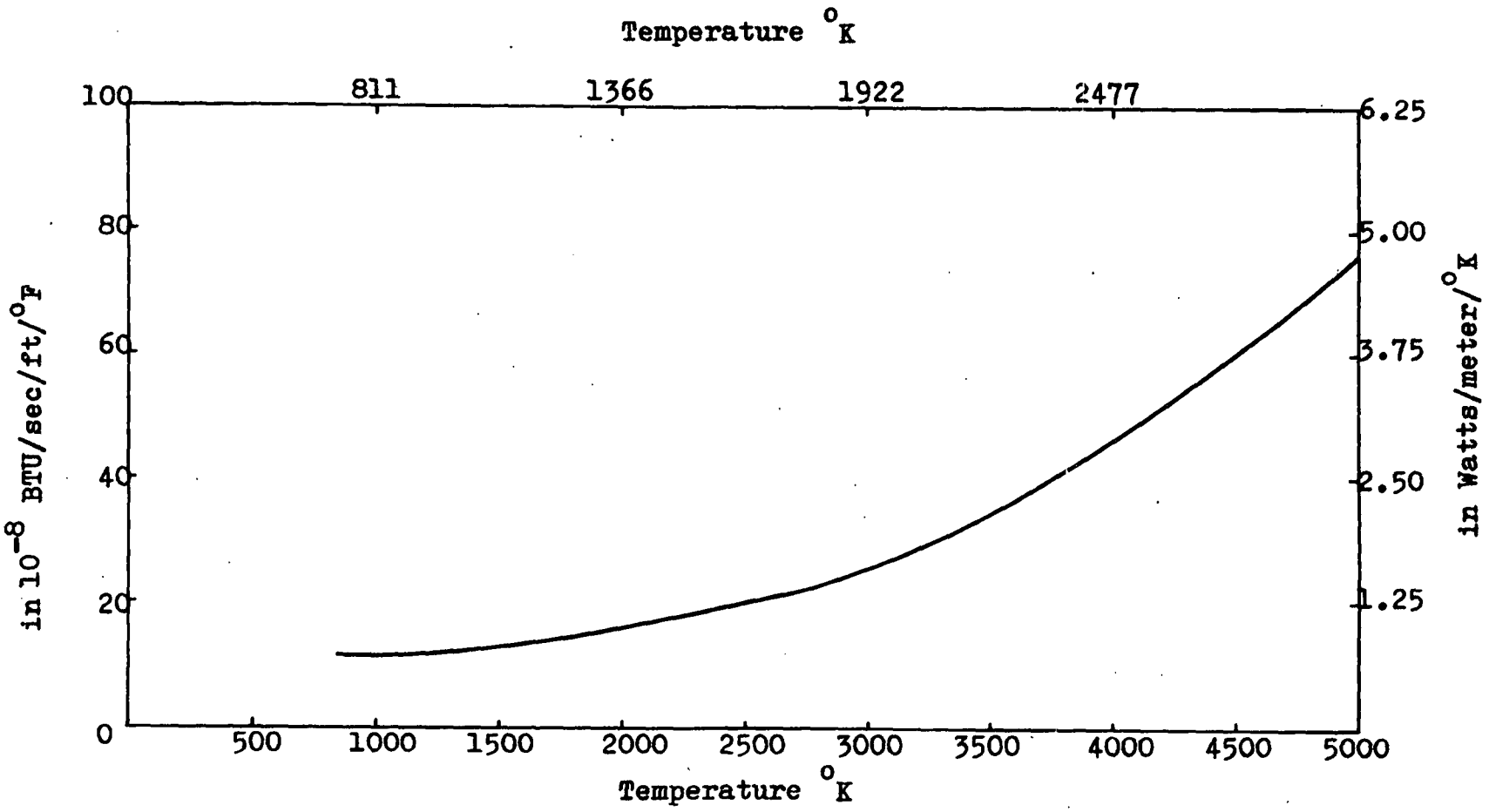

Figure C-2. Thermal Conductivity of Low Density Phenolic Nylon Char (4).

thermodynamic data sources see reference (7).

The thermodynamic data required in the development of both ablating analyses was voluminous. Therefore, to read-in the data in tabular form was ruled out. This would have implied more computer core, and tedious table look up during the computation, which in itself consumes precious computing time. The best alternative, therefore, was to preprocess all the thermodynamic data and reduce them to convenient polynomial forms.

The polynomial forms used for the heat capacity, enthalpy, entropy and free energy data were those published by NASA (1). This format was selected for its convenience and ease of programming. It constituted our initial data base on which we built as our work progressed.

Unfortunately, none of the other major sources of thermodynamic data had reduced them to the convenient polynomial forms of NASA (1). And in these cases where they did (2), the polynomial forms were incompatible with NASA's. It was therfore necessary to develop a Thermochemical Generation Program (TGP) to develop a uniform data base.

The Thermochemical Generation Program (TGP) is a double precision routine that requires heat capacity vs. temperature data, heat of formation at 298°K, and the standard molal entropy at 298°K. With this information TGP proceeds to fit a fourth order polynomial to the heat capacity data as shown in Equation C-1. Once the five constants (a through e) are calculated, the program proceeds

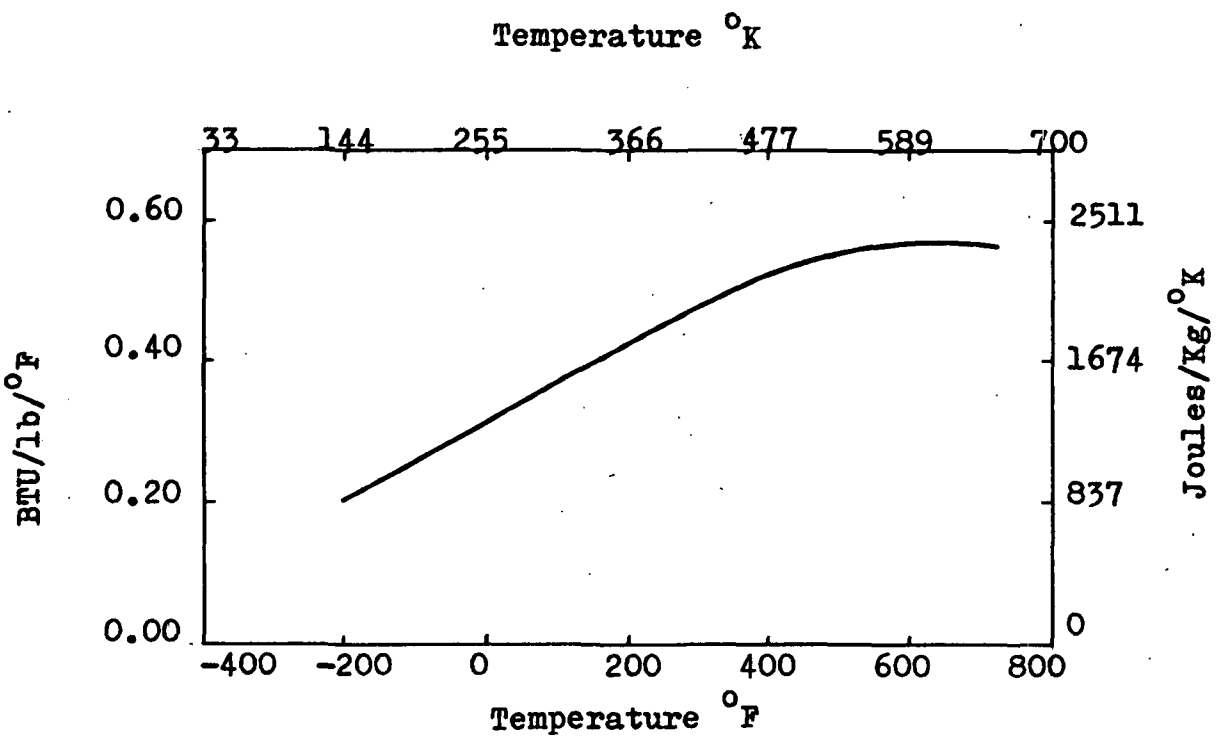

Figure C-3. Heat Capacity of Virgin Material.

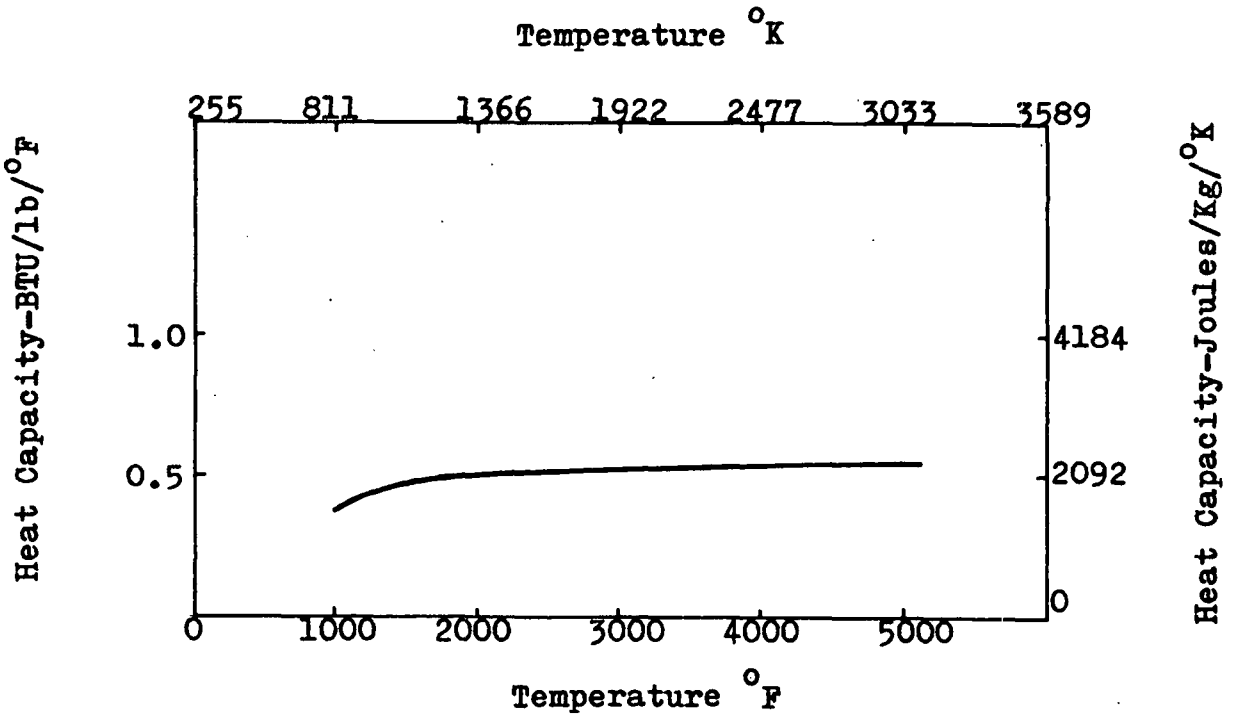

Figure C-4. Heat Capacity of Low Density Phenolic Nylon Char (4).

to compute the constant f using Equation (C-3) and the known value of the heat of formation at 298°K. Finally, the program calculates the constant g using Equation (C-5) and the value for the entropy at 298°K. With these seven constants the free energy function could, therefore, be calculated with the use of Equation (C-7). A FORTRAN listing of TGP is presented at the end of the chapter. It is identified by the symbol API44. This was done in honor of API project 44, which was the first concerted effort to develop a consistant set of thermodynamic data for hydrocarbons (8).

TABLE C-4. Listing of Thermochemical Generation Program

```
C
      DOUBLE PRECISION C(7)
      DIMENSION A(7),AP(7)
C     THIS PROGRAM FITS A POLYNOMIAL OF THE FORM A+BT+...+ET(5) TO HEAT
C     CAPACITY DATA USING A LEAST SQUARES DOUBLE PRECISION SUBROUTINE.
C     WITH THESE CONSTANTS IT EVALUATES THE TWO CONSTANTS OF INTEGRATION
C     AP(6) AND AP(7), THAT ARE NECESSARY IN THE EVALUATION OF THE FREE
C     ENERY FUNCTION FO/RT.THE FORMAT USED FOR THE FREE ENERGY CALCULA-
C     TION IS GIVEN IN NASA SP-3001--THERMODYNAMIC PROPERTIES TO 6000 K
C     FOR 210 SUBSTANCES INVOLVING THE FIRST 18 ELEMENTS--BY B.J.MCBRIDE
C     1963
C
C     DELH=HEAT OF FORMATION AT 298 OK
C     S=ABSOLUTE ENTROPY AT 298 OK
C     RR=1.987(UNIVERSAL GAS CONSTANT)
C     TZERO=298.15(BASE TEMPERATURE)
C     FORT=FREE ENERGY
C     CP=HEAT CAPACITY
C
RR=1.987
      TZERO=298.15
      TZERO1=TZERO
      TZERO2=TZERO*TZERO1
      TZERO3=TZERO2*TZERO
      TZERO4=TZERO3*TZERO
      TZERO5=TZERO4*TZERO
C
C     N=TOTAL NUMBER OF CONSTANTS FOR CP POLYNOMIAL
C
C     CALL THE LEAST SQUARES SUBROUTINE
C
  100 CALL LSQR(C,N)
C
```

```
      DO 1 I=1,N                                                        API   35
      AP(I)=C(I)                                                        API   36
      PRINT 101                                                         API   37
  101 FORMAT(1H0)                                                       API   38
      PRINT 102,AP(I),C(I),I                                            API   39
  102 FORMAT(1X,'AP(I)=',E20.8,3X,'HC(I)=',D20.9,I6)                    API   40
      CONTINUE                                                          API   41
      READ 2,TINITL,TFINAL,TINC,DELH,S,SNAME                            API   42
    2 FORMAT(5E10.6,6X,A4)                                              API   43
      PRINT 3, SNAME                                                    API   44
    3 FORMAT(//1X,'THE CONSTANTS ARE FOR=',A4//)                        API   45
C                                                                       API   46
C     C(I)=POLYNOMIAL CONSTANT                                          API   47
C                                                                       API   48
      PRINT 4,TINITL,TFINAL,SNAME,DELH                                  API   49
    4 FORMAT(//1X,9HTINITIAL=,E10.5,3X,'TFINAL='E10.5 ,3X,'HEAT OF FORMAAPI   50
     1TION OF',A4,1X,'AT 298 OK=',E16.5//)                              API   51
C     CALCULATE HEAT CAPACITY                                           API   52
      T=TINITL                                                          API   53
    5 T1=T                                                              API   54
      T2=T1*T                                                           API   55
      T3=T2*T                                                           API   56
      T4=T3*T                                                           API   57
      CP=AP(1)+AP(2)*T1+AP(3)*T2+AP(4)*T3+AP(5)*T4                      API   58
      PRINT6,CP,T                                                       API   59
    6 FORMAT(1X,'CP=',E18.5,3X,'T=',E18.5)                              API   60
      T=T+TINC                                                          API   61
      IF(T.LE.TFINAL) GO TO 5                                           API   62
C                                                                       API   63
C     PROCEED TO CALCULATE THE TWO CONSTANTS OF INTEGRATION AP(6)-AP(7) API   64
C                                                                       API   65
      AP(6)=-(AP(1)*TZERO+AP(2)*TZERO2/2.+AP(3)*TZERO3/3.+AP(4)*TZERO4/4API   66
     1.+AP(5)*TZERO5/5.)                                                API   67
      X=AP(6)                                                           API   68
```

```
      AP(7)=AP(1)*ALOG(TZERO)+AP(2)*TZERO+AP(3)*TZERO2/2.+AP(4)*TZERO3/3API    69
     1.+AP(5)*TZERO4/4.                                                 API    70
      X1=AP(7)                                                          API    71
      AP(7)=-X1+S                                                       API    72
      PRINT 7,AP(6),AP(7),S                                             API    73
    7 FORMAT (//1X,'AP(6)=',E15.5,2X,'AP(7)=',E15.5,'  S=',E15.51)      API    74
      AP(6)=X+DELH                                                      API    75
      MM=N+2                                                            API    76
      DO 8 I=1,MM                                                       API    77
    8 A(I)=AP(I)/RR                                                     API    78
      PRINT 9,(A(I),I=1,MM)                                             API    79
    9 FORMAT(/1X,7E17.7/)                                               API    80
C                                                                       API    81
C     CALCULATE THE FREE ENERGY                                         API    82
C                                                                       API    83
      T=TINITL                                                          API    84
   10 T1=T                                                              API    85
      T2=T1*T                                                           API    86
      T3=T2*T                                                           API    87
      T4=T3*T                                                           API    88
      A2=A(2)                                                           API    89
      A1=A(1)                                                           API    90
      FORT=A1*(1.-ALOG(T))-A2*T/2.-A(3)*T2/6.-A(4)*T3/12.-A(5)*T4/20.   API    91
     1+A(6)/T -A(7)                                                     API    92
      PRINT 11,FORT,T                                                   API    93
   11 FORMAT(1X,'FORT=',E15.5,'  T=',E15.5)                             API    94
      T=T + TINC                                                        API    95
      IF(T.LE.TFINAL)GO TO 10                                           API    96
      PRINT 13                                                          API    97
   13 FORMAT(1H1)                                                       API    98
      GO TO 100                                                         API    99
   12 STOP                                                              API   100
      END                                                               API   101
```

```
C     SUBROUTINE LSQR(CC,M,NUMBER,Y,X)                                  LSQR   1
C                                                                       LSQR   2
C                                                                       LSQR   3
C     LEAST SQUARE CURVE FITTING OF ANY ORDER POLYNOMIAL                LSQR   4
C     OF ORDER EQUAL TO OR LESS THAN 10                                 LSQR   5
C                                                                       LSQR   6
C                                                                       LSQR   7
C                                                                       LSQR   8
C     NUMBER   IS THE ACTUAL NUMBER OF X-Y DATA PAIRS.,MAXIMUM OF 200   LSQR   9
C     M IS THE DEGREE OF THE POLYNOMIAL.,MAXIMUM OF 10                  LSQR  10
C     N IS THE NUMBER OF EQUATIONS(=M+1)                                LSQR  11
C     X,Y IS THE ARRAY FOR THE DATA PAIRS                               LSQR  12
C     A IS THE ARRAY FOR THE SUM, WHICH BECOME THE COEFFICIENTS OF THE  LSQR  13
C     UNKNOWN IN THE SIMULTANEOUS EQUATIONS.                            LSQR  14
C     B IS THE ARRAY FOR THE CONSTANT TERMS IN THE SIMULTANEOUS EQUATIONLSQR  15
C     C IS THE ARRAY FOR THE UNKNOWNS, WHICH BECOME THE COEFFICIENS IN  LSQR  16
C     THE POLYNOMIAL.                                                   LSQR  17
C     P IS THE ARRAY FOR THE POWERS OF THE X(I),FROM 1 TO 2M.           LSQR  18
C                                                                       LSQR  19
      DOUBLE PRECISION X( 30),Y( 30),A(7,7),B(7),C(7),P(20),TEMP,FACTOR,LSQR  20
     1                 SUM                                              LSQR  21
      DIMENSION CC(3)                                                   LSQR  22
   17 READ 20,NUMBER,M                                                  LSQR  23
   20 FORMAT(2I6)                                                       LSQR  24
      DO 11 I=1,NUMBER                                                  LSQR  25
      READ 10,Y(I),X(I)                                                 LSQR  26
C     Y(I)=1./Y(I)                                                      LSQR  27
   10 FORMAT(2D10.0)                                                    LSQR  28
   11 CONTINUE                                                          LSQR  29
      MX2=M*2                                                           LSQR  30
      DO 13 I=1,MX2                                                     LSQR  31
      P(I)=0.0                                                          LSQR  32
      DO 13 J=1,NUMBER                                                  LSQR  33
      POWER=I                                                           LSQR  34
```

```
   13 P(I)=P(I)+X(J)**POWER                                          LSQR  35
C                                                                    LSQR  36
C                                                                    LSQR  37
C     DEVELOPING THE COEFFICIENTS AND THE CONSTANT TERMS OF THE NORMAL LSQR  38
C     EQUATIONS.                                                     LSQR  39
C                                                                    LSQR  40
C                                                                    LSQR  41
      N=M+1                                                          LSQR  42
      DO 30 I=1,N                                                    LSQR  43
      DO 30 J=1,N                                                    LSQR  44
      K=I+J-2                                                        LSQR  45
      IF(K)29,29,28                                                  LSQR  46
   28 A(I,J)=P(K)                                                    LSQR  47
      GO TO 30                                                       LSQR  48
   29 A(1,1)=NUMBER                                                  LSQR  49
   30 CONTINUE                                                       LSQR  50
      B(1)=0.                                                        LSQR  51
      DO 21 J=1,NUMBER                                               LSQR  52
   21 B(1)=B(1)+Y(J)                                                 LSQR  53
      DO 22 I=2,N                                                    LSQR  54
      B(I)=0.                                                        LSQR  55
      DO 22 J=1,NUMBER                                               LSQR  56
   22 B(I)=B(I)+Y(J)*X(J)**(I-1)                                     LSQR  57
C                                                                    LSQR  58
C     PIVOTAL CONDENSATION                                           LSQR  59
C                                                                    LSQR  60
      NM1=N-1                                                        LSQR  61
      DO 300 K=1,NM1                                                 LSQR  62
      KP1=K+1                                                        LSQR  63
      L=K                                                            LSQR  64
      DO 400 I=KP1,N                                                 LSQR  65
      IF(DABS(A(I,K))-DABS(A(L,K)))400,400,401                       LSQR  66
  401 L=I                                                            LSQR  67
  400 CONTINUE                                                       LSQR  68
```

```
      IF(L-K)500,500,405                                                LSQR  69
  405 DO 410 J=K,N                                                      LSQR  70
      TEMP=A(K,J)                                                       LSQR  71
      A(K,J)=A(L,J)                                                     LSQR  72
  410 A(L,J)=TEMP                                                       LSQR  73
      TEMP=B(K)                                                         LSQR  74
      B(K)=B(L)                                                         LSQR  75
      B(L)=TEMP                                                         LSQR  76
C                                                                       LSQR  77
C     ELIMINATION,BACK SOLUTION, AND PRINTING RESULTS                   LSQR  78
C                                                                       LSQR  79
  500 DO 300 I=KP1,N                                                    LSQR  80
      FACTOR=A(I,K)/A(K,K)                                              LSQR  81
      A(I,K)=0.0                                                        LSQR  82
      DO 301 J=KP1,N                                                    LSQR  83
  301 A(I,J)=A(I,J)-FACTOR*A(K,J)                                       LSQR  84
  300 B(I)=B(I)-FACTOR*B(K)                                             LSQR  85
      C(N)=B(N)/A(N,N)                                                  LSQR  86
      I=NM1                                                             LSQR  87
  710 IP1=I+1                                                           LSQR  88
      SUM=0.0                                                           LSQR  89
      DO 700 J= IP1,N                                                   LSQR  90
  700 SUM=SUM+A(I,J)*C(J)                                               LSQR  91
      C(I)=(B(I)-SUM)/A(I,I)                                            LSQR  92
      I=I-1                                                             LSQR  93
      IF(I)800,800,710                                                  LSQR  94
  800 DO 900 I=1,N                                                      LSQR  95
      CC(I)=C(I)                                                        LSQR  96
  900 PRINT 901, I,C(I)                                                 LSQR  97
  901 FORMAT(1X,I6,5X,D17.8)                                            LSQR  98
      PRINT 9143                                                        LSQR  99
 9143 FORMAT(//T46,   'LINEAR INTERPOLATION' , ///T5,'OBSERVATION',     LSQR 100
     1 T27, 'CALCULATION', T49, 'RESIDUAL', T67,'READING NO.'///)       LSQR 101
      DO 905 I=1,NUMBER                                                 LSQR 102
```

```
C     XKK=C(1)+C(2)*X(I)+C(3)*X(I)**2                                  LSQR 103
      XKK=C(1)+C(2)*X(I)                                               LSQR 104
      RESID = Y(I)- XKK                                                LSQR 105
C     PRINT 904,XK,X(I)                                                LSQR 106
      XK=XKK                                                           LSQR 107
      YY = Y(I)                                                        LSQR 108
      XX = X(I)                                                        LSQR 109
      PRINT 904,YY,XK,RESID,XX                                         LSQR 110
  904 FORMAT(4E20.6)                                                   LSQR 111
  905 CONTINUE                                                         LSQR 112
  902 FORMAT(1H1)                                                      LSQR 113
      RETURN                                                           LSQR 114
      END                                                              LSQR 115
```

INPUT FORMAT FOR T G P

CARD 1: FORMAT (2I6)	COLUMNS
NUMBER = Number of heat capacity data points.	1-6
M = Order of polynomial fit.	7-12

CARD 2: FORMAT (2D10.1)	
X(I) = Heat Capacity data (cal/gm-mole-^{o}K).	1-10
Y(I) = Temperature (^{o}K).	11-20

CARD 3: FORMAT (5E10.6, 6x, A4)	
TINITL = Initial temperature of fit.	1-10
TFINAL = Final temperature of fit	11-20
TINC = Increment at which data is to be printed.	21-30
DELH = Heat of formation of the species at 298°K.	31-40
S = Entropy at 298°K.	41-50
SNAME = Species name.	55-60

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APPENDIX D

ISOTHERMAL ANALYSIS PROGRAM

This program was developed to study hundreds of possible chemical reactions that could occur in the C-H-O-N system. With this program we were able to determine if reactions were important between the temperature range of 500°K to 3500°K.

The procedure was to use stochiometric amounts of reactants and calculate the conversion at a given temperature through a char one quarter of an inch thick. This procedure was repeated at higher temperatures and the behavior of the reaction was recorded for later analysis. Those reactions for which the conversions at 3500°K were less than 5 percent were eliminated. It was felt that since the actual char would have an average temperature much less than 3500°K, it was a conservative criteria to select the reaction on this basis.

As it turned out many reactions which had a conversion greater than 5 percent were later eliminated since many of the reactants were present in trace amounts, and therefore, even if their conversion at 3500°K was 100 percent, their contribution to heat absorption was considered negligible. These decisions were based on the composition of gases entering the char. How these compositions were estimated

is explained in Appendix F.

It should be pointed out that the isothermal analysis approach used in this research was different from that used by April (1). April only considered the reactions to be irreversible. In this research, reverse reaction rate constants were used. The reverse reaction rate constants were computed from the known equilibrium constant calculated from the chemical equilibrium program. Table D-1 lists the isothermal analysis program.

TABLE D-1. Listing of the Isothermal Analysis Program

```
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 OK-3500 OK
C
      DIMENSION EQN(18)
      DOUBLE PRECISION R22,R33,P11,P22,P33,FR1,FR2,FR3,FP1,FP2,FP3,
     A   Z,DELZ,RA,FKK,RKK,FKKK,RKKK,CR1,CR2,CR3,CP1,CP2,CP3,HH,RADELZ,
     B   FT,R44,R55,R66,P44,P55,P66,HMIN,HI,ZZ,ZINC
      DOUBLE PRECISION TTT
C
C     READ THE EQUATION R1+R2+R3=P1+P2+P3
 1111 READ729,(EQN(I),I=1,18)
 729  FORMAT(18A4)
C
C     READ THE STOCHIOMETRIC COEFFICIENTS OF THE RATE EQUATION
 1112 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                              ISOT  35
      READ733,AF,SF,AEF                                                 ISOT  36
 733  FORMAT(E8.0,2F6.0)                                                ISOT  37
C                                                                       ISOT  38
      READ (5,734 ) A1,A2                                               ISOT  39
 734  FORMAT(1X,2E14.7)                                                 ISOT  40
      READ 735,TINIT,TINC,TFINAL,HI,HMIN                                ISOT  41
 735  FORMAT(3F10.1,2D10.4)                                             ISOT  42
      T=TINIT                                                           ISOT  43
C                                                                       ISOT  44
 828  PRINT829,(EQN(I),I=1,18)                                          ISOT  45
 829  FORMAT(1H1,18A4)                                                  ISOT  46
      PRINT 830                                                         ISOT  47
 830  FORMAT( 1X,35HINITIAL COMPOSITION (MOLE FRACTION))                ISOT  48
      PRINT 833,XR1,XR2,XR3,XP1,XP2,XP3                                 ISOT  49
C                                                                       ISOT  50
      PRINT 831                                                         ISOT  51
 831  FORMAT(1H0,   'FINAL COMPOSITION (MOLE FRACTION)                  ISOT  52
     1 TEMP  FRACTIONAL     Z         DELZ     REACTION RATE     EK°)   ISOT  53
      PRINT 8311                                                        ISOT  54
 8311 FORMAT(1H ,109H    R1        R2       R3       P1       P2       P3  ISOT  55
     1 (OF)  CONVERSION                        (MOL/CC-SEC)        )    ISOT  56
C                                                                       ISOT  57
C     MASS FLUX OF DECOMPOSITION PRODUCTS, W, IN LB/FT2-SEC             ISOT  58
      W=0.01                                                            ISOT  59
C                                                                       ISOT  60
C     INITIAL VALUE OF TEMPERATURE,T,IS 500-OK                          ISOT  61
      R22=R2/R1                                                         ISOT  62
      R33=R3/R1                                                         ISOT  63
      P11=P1/R1                                                         ISOT  64
      P22=P2/R1                                                         ISOT  65
      P33=P3/R1                                                         ISOT  66
      ZINC=1.D-3                                                        ISOT  67
      R44=R4                                                            ISOT  68
```

```
      R55=R5                                                            ISOT  69
      R66=R6                                                            ISOT  70
      P44=P4                                                            ISOT  71
      P55=P5                                                            ISOT  72
      P66=P6                                                            ISOT  73
      DELZ=HI                                                           ISOT  74
C     INITIAL VALUE OF THE PRESSURE ,P, IS 1.0 ATMS                     ISOT  75
      P=1.0                                                             ISOT  76
C     GAS CONSTANT,R,IN CALORIES/GMMOLE-OK                              ISOT  77
      R=1.987                                                           ISOT  78
C                                                                       ISOT  79
C     CALCULATION OF THE AVERAGE MOL WGT OF THE GAS,FWA                 ISOT  80
C     ENTERING THE CHAR ZONE                                            ISOT  81
      FWAR=FWR1*XR1+FWR2*XR2+FWR3*XR3                                   ISOT  82
      FWAP=FWP1*XP1+FWP2*XP2+FWP3*XP3                                   ISOT  83
      FWA=FWAR+FWAP                                                     ISOT  84
C                                                                       ISOT  85
C     CALCULATION OF THE MOLAL FLOW RATE OF THE GAS,FTO                 ISOT  86
C     FTO HAS UNITS OF GMMOLES PER CM2-SEC                              ISOT  87
      ACON4=453.59/929.0304                                             ISOT  88
      FTO=W/FWA*ACON4                                                   ISOT  89
C                                                                       ISOT  90
C     CALCULATION OF MOLAL FLUX OF THE INDIVIDUAL COMPONENTS            ISOT  91
C     MOLAL FLUX UNITS ARE GMMOLES PER FT-FT SEC                        ISOT  92
      FR10=XR1*FTO                                                      ISOT  93
      FR20=XR2*FTO                                                      ISOT  94
      FR30=XR3*FTO                                                      ISOT  95
      FP10=XP1*FTO                                                      ISOT  96
      FP20=XP2*FTO                                                      ISOT  97
      FP30=XP3*FTO                                                      ISOT  98
C                                                                       ISOT  99
C     CALCULATION OF THF SPACE TIME,ST,IN CUBIC-CM SEC/GMMOLES          ISOT 100
      ST=(0.25*144.0)/(FTO*0.06103)                                     ISOT 101
C                                                                       ISOT 102
```

```
C     FT HAS UNITS OF GM-MOLES/CM2-SEC                                  ISOT 103
      FT=FTO                                                            ISOT 104
 2221 FR1=FR10                                                          ISOT 105
      FR2=FR20                                                          ISOT 106
      FR3=FR30                                                          ISOT 107
      FP1=FP10                                                          ISOT 108
      FP2=FP20                                                          ISOT 109
      FP3=FP30                                                          ISOT 110
      ZZ=0.                                                             ISOT 111
      Z=0.                                                              ISOT 112
C                                                                       ISOT 113
C     CALCULATION OF THE COMPOSITION OF THE REACTING MIXTURE            ISOT 114
C     C/S ARE CONCENTRATIONS IN GMMOLES/CUBIC-CM                        ISOT 115
      RR=82.054                                                         ISOT 116
      TOK=T                                                             ISOT 117
C                                                                       ISOT 118
C     CALCULATION OF RATE CONSTANTS FOR FORWARD AND REVERSE REACTIONS   ISOT 119
C     RATE CONSTANT UNITS ARE IN CUBIC CM,GMMOLES AND SEC               ISOT 120
C                                                                       ISOT 121
C     FORWARD REACTION RATE CONSTANT, FK                                ISOT 122
      FK=AF*TOK**(-SF)*EXP((-AEF*1000.0)/(R*TOK))                       ISOT 123
C     REVERSE REACTION RATE CONSTANT, RK                                ISOT 124
C                                                                       ISOT 125
      EK=EXP(A1+A2/T)                                                   ISOT 126
      COEF=P4+P5+P6-R4-R5-R6                                            ISOT 127
      EKK=EK/((RR*T)**COEF)                                             ISOT 128
      RK=FK/EKK                                                         ISOT 129
      FKK=FK                                                            ISOT 130
      RKK=RK                                                            ISOT 131
 2222 H=P/(RR*TOK*FT)                                                   ISOT 132
      HH=H                                                              ISOT 133
      CR1=FR1*HH                                                        ISOT 134
      CR2=FR2*HH                                                        ISOT 135
      CR3=FR3*HH                                                        ISOT 136
```

```
      CP1=FP1*HH                                                        ISOT 137
      CP2=FP2*HH                                                        ISOT 138
      CP3=FP3*HH                                                        ISOT 139
      FKKK=FKK*CR1**R44                                                 ISOT 140
      IF(R55.LE.0.) GO TO 520                                           ISOT 141
      FKKK=FKKK*CR2**R55                                                ISOT 142
      IF(R66.LE.0.) GO TO 520                                           ISOT 143
      FKKK=FKKK*CR3**R66                                                ISOT 144
  520 RKKK=RKK*CP1**P44                                                 ISOT 145
      IF(P55.LE.0.) GO TO 521                                           ISOT 146
      RKKK=RKKK*CP2**P55                                                ISOT 147
      IF(P66.LE.0.) GO TO 521                                           ISOT 148
      RKKK=RKKK*CP3**P66                                                ISOT 149
      IF(SF.EQ.0.)GOTO521                                               ISOT 150
      TTT=T**(-SF)                                                      ISOT 151
      FKKK=FKKK*TTT                                                     ISOT 152
  521 RA=FKKK-RKKK                                                      ISOT 153
      IF(RA.LT.0.)RA=0.                                                 ISOT 154
      IF(RA.LE.0.)GOTO5211                                              ISOT 155
C                                                                       ISOT 156
C                                                                       ISOT 157
      RADELZ=RA*DELZ                                                    ISOT 158
 5210 RADELZ=RA*DELZ                                                    ISOT 159
      RATIO=RADELZ/FR1                                                  ISOT 160
      IF(RATIO.GT.1.E-7)DELZ=DELZ/4.                                    ISOT 161
      IF(RATIO.GT.1.E-7)GOTO5210                                        ISOT 162
      IF(RATIO.LT.1.E-11)DELZ=DELZ*2.                                   ISOT 163
      IF(DELZ.LE.5.D-7)GOTO5211                                         ISOT 164
      IF(RATIO.LT.1.E-11)GOTO5210                                       ISOT 165
 5211 IF(DELZ.LT.HMIN)DELZ=HMIN                                         ISOT 166
      IF(DELZ.GT.1.E-4)DELZ=1.E-4                                       ISOT 167
      RADELZ=RA*DELZ                                                    ISOT 168
      FR1=FR1-RADELZ                                                    ISOT 169
      FR2=FR2-RADELZ*R22                                                ISOT 170
```

```
      FR3=FR3-RADELZ*R33                                                ISOT 171
      FP1=FP1+RADELZ*P11                                                ISOT 172
      FP2=FP2+RADELZ*P22                                                ISOT 173
      FP3=FP3+RADELZ*P33                                                ISOT 174
      FT=FR1+FR2+FR3+FP1+FP2+FP3                                        ISOT 175
      FTT=FR1*FWR1+FR2*FWR2+FR3*FWR3+FP1*FWP1+FP2*FWP2+FP3*FWP3         ISOT 176
      FTT=FTT*2.048172                                                  ISOT 177
      Z=Z+DELZ                                                          ISOT 178
      IF(FR1.LE.0.)GOTO5240                                             ISOT 179
      IF(ZZ.GT.Z)GOTO2222                                               ISOT 180
      RAA=RA                                                            ISOT 181
      FR11=FR1                                                          ISOT 182
      XCA=1.-FR11/FR10                                                  ISOT 183
      YR1=FR1/FT                                                        ISOT 184
      YR2=FR2/FT                                                        ISOT 185
      YR3=FR3/FT                                                        ISOT 186
      YP1=FP1/FT                                                        ISOT 187
      YP2=FP2/FT                                                        ISOT 188
      YP3=FP3/FT                                                        ISOT 189
      Z2=Z                                                              ISOT 190
      DZZZ=DELZ                                                         ISOT 191
      PRINT 833,YR1,YR2,YR3,YP1,YP2,YP3,T,XCA,Z2,DZZZ,RAA,EK            ISOT 192
      PRINT 522,FKKK,RKKK,FTT                                           ISOT 193
  522 FORMAT(1X'FKKK='D25.16,' RKKK='D25.16,' W='F10.7/)                ISOT 194
      ZZ=ZZ+ZINC                                                        ISOT 195
      IF(RA.LE.0.)GOTO5240                                              ISOT 196
      IF(Z.LT.0.100)GOTO2222                                            ISOT 197
C     CALCULATION OF FINAL COMPOSITION (MOLE FRACTION)                  ISOT 198
 5240 YR1=FR1/FT                                                        ISOT 199
      YR2=FR2/FT                                                        ISOT 200
      YR3=FR3/FT                                                        ISOT 201
      YP1=FP1/FT                                                        ISOT 202
      YP2=FP2/FT                                                        ISOT 203
      YP3=FP3/FT                                                        ISOT 204
```

```
      RAA=RA                                                            ISOT 205
      FR11=FR1                                                          ISOT 206
      Z2=Z                                                              ISOT 207
      DZZZ=DELZ                                                         ISOT 208
  123 PRINT 833,YR1,YR2,YR3,YP1,YP2,YP3,T,XCA,Z2,DZZZ,RAA,EK            ISOT 209
      PRINT 522,FKKK,RKKK,FTT                                           ISOT 210
 5220 CONTINUE                                                          ISOT 211
      XCA=1.-FR11/FR10                                                  ISOT 212
  833 FORMAT(1H0,6F8.4,F9.1,F8.4,2X,4E12.5)                             ISOT 213
C                                                                       ISOT 214
C     READ NEW DATA IF THE CONVERSION IS 100 PERCENT                    ISOT 215
C     CONVERSION WILL BE 100 PERCENT FOR ALL HIGHER TEMPERATURES        ISOT 216
C                                                                       ISOT 217
C     THEN REPEAT THE CALCULATIONS AT THE NEW TEMPERATURE               ISOT 218
C                                                                       ISOT 219
      IF(FR1.LE.0.)GOTO2208                                             ISOT 220
      IF(XCA.LT.0.2)T=T+TINC                                            ISOT 221
      T=T+TINC                                                          ISOT 222
      IF(XCA.GT.0.97)GOTO2208                                           ISOT 223
      IF(TINC.GT.0.)GOTO2207                                            ISOT 224
      IF(T.GE.TFINAL)GOTO2221                                           ISOT 225
      GOTO2208                                                          ISOT 226
 2207 IF(T.LE.TFINAL)GOTO2221                                           ISOT 227
C                                                                       ISOT 228
C     RE-INITIALIZE                                                     ISOT 229
C                                                                       ISOT 230
C                                                                       ISOT 231
 2208 PRINT 833,YR1,YR2,YR3,YP1,YP2,YP3,T,XCA,Z2,DZZZ,RAA,EK            ISOT 232
C     PRINT DATA                                                        ISOT 233
      PRINT 2209,FTT                                                    ISOT 234
 2209 FORMAT(1H0,25H MASS FLUX(LB/FT2-SEC) = , F8.4)                    ISOT 235
      PRINT2210,AF,SF,AEF                                               ISOT 236
 2210 FORMAT(1H0,3HAF=,E9.2,5H  SF=,F6.2,6H  AEF=,F6.1)                 ISOT 237
      PRINT2211,AR,SR,AER                                               ISOT 238
```

```
 2211 FORMAT(1H0,3HAR=,E9.2,5H  SR=,F6.2,6H  AER=,F6.1)                ISOT 239
      PRINT2212                                                        ISOT 240
 2212 FORMAT(1H0,29HFWR1 FWR2 FWR3 FWP1 FWP2 FWP3)                     ISOT 241
      PRINT2213,FWR1,FWR2,FWR3,FWP1,FWP2,FWP3                          ISOT 242
 2213 FORMAT(1X,6F6.1)                                                 ISOT 243
      PRINT 2218                                                       ISOT 244
 2218 FORMAT(1H0,28H  STOCHIOMETRIC COEFFICIENTS)                      ISOT 245
      PRINT2214                                                        ISOT 246
 2214 FORMAT(1H0,24H  R1  R2  R3  P1  P2  P3)                          ISOT 247
      PRINT2215,R1,R2,R3,P1,P2,P3                                      ISOT 248
 2215 FORMAT(1X,6F4.1)                                                 ISOT 249
      PRINT 2219                                                       ISOT 250
 2219 FORMAT(1H0,45H  EXPONENTS ON THE COMP. OF THE RATE EQUATION)     ISOT 251
      PRINT 2216                                                       ISOT 252
 2216 FORMAT(1H0,24H  R4  R5  R6  P4  P5  P6)                          ISOT 253
      PRINT 2217,R4,R5,R6,P4,P5,P6                                     ISOT 254
 2217 FORMAT(1X,6F4.1)                                                 ISOT 255
C     READ IN NEW DATA FOR CALCULATIONS OF NEXT EQUATION               ISOT 256
      GOTO1111                                                         ISOT 257
   24 STOP                                                             ISOT 258
      END                                                              ISOT 259
```

INPUT FORMAT FOR THE ISOTHERMAL ANALYSIS PROGRAM

CARD 1: FORMAT (18A4)	COLUMNS
EQN(I) = Alphameric Reaction Expression	1-72

CARD 2: FORMAT (6F4.0)	
R1 = Stochiometric coefficient of Reactant 1	1-4
R2 = Stochiometric Coefficient of Reactant 2	5-8
R3 = Stochiometric Coefficient of Reactant 3	9-12
P1 = Stochiometric Coefficient of Product 1	13-16
P2 = Stochiometric Coefficient of Product 2	17-20
P3 = Stochiometric Coefficient of Product 3	21-24

CARD 3: FORMAT (6F4.0)	
R4 = Exponent of Reactant 1	1-4
R5 = Exponent of Reactant 2	5-8
R6 = Exponent of Reactant 3	9-12
P4 = Exponent of Product 1	13-16
P5 = Exponent of Product 2	17-20
P6 = Exponent of Product 3	21-24

CARD 4: FORMAT (6F5.0)	
FWR1 = Molecular Weight of Reactant 1	1-5
FWR2 = Molecular Weight of Reactant 2	6-10
FWR3 = Molecular Weight of Reactant 3	11-15

	COLUMNS
FWP1 = Molecular Weight of Product 1	16-20
FWP2 = Molecular Weight of Product 2	21-25
FWP3 = Molecular Weight of Product 3	26-30

CARD 5: FORMAT (3E10.0)

XR1 = Mole Fraction of Reactant 1	1-10
XR2 = Mole Fraction of Reactant 2	11-20
XR3 = Mole Fraction of Reactant 3	21-30

CARD 6: FORMAT (E8.0, 2F6.0)

AF = Frequency Factor (cm^3/gm-mole/sec)	1-8
SF = Exponent on Temperature	9-14
AEF = Activation Energy (Kcal/gm-mole)	15-20

CARD 7: FORMAT (1X, 2E 14.7)

A1 = 1st Constant of Equilibrium Constant	2-15
A2 = 2nd Constant of Equilibrium Constant	16-29

CARD 7 read the constants for the equilibrium constant fit of the form EXP(A1+A2/T).

CARD 8: FORMAT (3F10.1, 2010.4)

TINIT = Initial Temperature (^oK)	1-10
TINC = Temperature Increment (^oK)	11-20
TFINAL = Final Temperature (^oK)	21-30
HI = Initial Step Size (FT)	31-40
HMIN = Minimum Step Size (FT)	41-50

APPENDIX E

A DESCRIPTION OF THE CHEMICAL EQUILIBRIUM ANALYSIS PROGRAM

The chemical equilibrium analysis program is based on the free energy minimization method that is described in detail in Chapter IV. This analysis is a general method to calculate the equilibrium composition of a multi-component, polyphase system.

As input, the program requires that the user specify the temperature, pressure and an estimate of the composition of the chemical species of interest which are consistent with the elemental composition. In its present form the program reads in the thermodynamic data as seven constants for a polynomial of the form of Equation (C-7). This method of reading the data into the program is compact and flexible. A brief description of the program follows:

The Chemical Equilibrium Analysis Program

The Chemical Equilibrium Program consists of a MAIN executive program and four subroutines. These subroutines are THERMO, HOLD1, TRACE, and MATINV, and a description of each is given in this section.

MAIN: This is the executive routine of the chemical equilibrium program. This program generates the matrix necessary to solve the set of algebraic equations.

These coefficients are calculated following the same procedure described in Chapter IV. The coefficients are those shown in Table 4-1. The MAIN program calls THERMO to get the free energy function, and MATINV to invert the matrix and calculate the Lagrange multipliers. These multipliers are used to re-estimate the values of the composition of the gases for the next iteration as is shown in Equation (4-32). It should be noted, however, that values of χ_i are re-adjusted using the convergence procedure described in Chapter IV. This is to avoid possible divergence of the solution. It should be noted also that the composition of the solid species are explicitly solved in the matrix inversion subroutine and are also corrected by the same technique.

THERMO: This subroutine provides the main program with the values of the free energy function for each of the species being calculated. In addition, the program calculates the heat of formation of each species along with the sinsible enthalpy change per mole.

The THERMO subroutine uses a polynomial expression similar to the one shown in Equation (C-7) of Appendix C to calculate the free energy function. This polynomial form is a very convenient and efficient way for repetitive calculation. It is certainly more accurate and less time consuming than a table look-up and requires less storage than the table form.

MATINV: This subroutine is a standard method for solving a set of linear equations by inverting a non-singular nxn matrix. The inversion is performed iteratively by reducing the original matrix by a series of row operations. The method is then repeated with the resulting identity matrix. This subroutine is the same as used in the ABLATIN2 analysis that is described in Appendix A.

HOLD1: One of the major numerical drawbacks of the free energy minimization technique is that its convergence speed is reduced quite drastically by the presence of trace species during the numerical calculations. These trace species are those whose composition are less than 10^{-8} and therefore their contribution to the total free energy of the system is computationally negligible.

This subroutine checks for the presence of trace species. This is done if the procedure has not converged within a preset number of iterations. In our case, this number is ten. After checking for trace species, the subroutine re-orders the species in descending order of compositions and eliminates those less than 10^{-8}. However, the program holds the species in storage for a final check at the end of the minimization procedure. This check is performed by subroutine TRACE which is described below.

TRACE: If species have been eliminated during the computational procedure, subroutine TRACE is called to recompute their value at the end of the convergence procedure. The technique used is thoroughly explained in

Chapter IV. The equation used to calculate the trace species is Equation (4-46). A listing of the program follows.

At the end of the Appendix, an example illustrates how to use the program. The example selected is for silicone elastomers, and typical results are presented.

TABLE E-1. Listing of the Chemical Equilibrium Program

```
C
C
C-----THIS PROGRAM COMPUTES COMPLEX CHEMICAL EQUILIBRIUM FOR
C     A MULTICOMPONENT,POLYPHASE SYSTEM BY FREE ENERGY MINI-
C     MIZATION.(J.CHEM.PHYS.,VOL28,NO.5,1958)
C
C
C
      COMMON/KA/ICODE(40),SPCIE1(40),SPCIE2(40),AA(40,5),
     1          ENT1(40),ENT(40)
      COMMON/KB/AI(40),BI(40),CI(40),DI(40),EI(40),FI(40),
     1       GI(40),AII(40),BII(40),CII(40),DII(40),EII(40),
     2       FII(40),GII(40),DELH(40),FORT(40),C(40),TLOW(40),
     3       Y(40),XMW(40),MLFRC(40)
      COMMON/KBB/CPDT1(5),PERC(40),PERC1(40)
      COMMON/KC/IICODE(40),XPCIE1(40),XPCIE2(40),XAA(40,5),
     1           XENT(40),XENT1(40)
      COMMON/KD/XAI(40),XBI(40),XCI(40),XDI(40),XEI(40),
     1       XFI(40),XGI(40),XAII(40),XBII(40),XCII(40),
     2       XDII(40),XEII(40),XFII(40),XGII(40),XMLFR(40)
      COMMON/KDD/XDELH(40),XCPDT(40),XCPDT1(05),XFORT(40),
     1XY(40),XC(40),XTLOW(40),XXMW(40),XPERC(40),XPERC1(40)
      COMMON/KE/S1(5),S2(5),S3(5),S4(5),S5(5),A11(5),A22(5),
     1       A33(5),A44(5),A55(5),S6(5),A66(5),JCODE(5),S(40)
      COMMON/KF/NC,NS,MM,RR,MM1,NQ,NN,KW,IN,KOUT,KCODE,KSOLID
      COMMON/KG/T,TZERO,TZERO1,TZERO2,TZERO3,TZERO4,TZERO5,P
      DIMENSION YSUM(40),XMASS(40),DELT(40),X(40),XLAM(40),
     1          FY(40),R(7,7),B(7,1),PI(7),BB(7),FSUM(40),
     2          XMFR(40),YX(40)
      DIMENSION AAA(40)
      DIMENSION XMOL(40)
      DIMENSION XMAS1(20)
      DIMENSION XMASSS(30)
      REAL MLFRC
```

```
    5 MAXNT=100                                                         CHEM  35
      KX=0                                                              CHEM  36
      KPASSS=0                                                          CHEM  37
      MA=1                                                              CHEM  38
C                                                                       CHEM  39
      KSOLID=0                                                          CHEM  40
C                                                                       CHEM  41
C-----READ INITIAL,FINAL,INCREMENTAL AND BASE TEMPERATURE. ALSO READ CRICHEM  42
C     FOR CONVERGENCE,NUMBER OF GAS AND SOLID SPECIES,AND NUMBER OF ELEMCHEM  43
C                                                                       CHEM  44
C                                                                       CHEM  45
C--------READ INPUT PARAMETERS                                          CHEM  46
C                                                                       CHEM  47
C                                                                       CHEM  48
      READ1,XT,TMAX,TINC,TZERO,CRIT,NC,MM,NNS                           CHEM  49
      IF(XT.LT.1.)GOTO333                                               CHEM  50
      NS=NC+NNS                                                         CHEM  51
    1 FORMAT(5F10.4,3I6)                                                CHEM  52
      MM1=MM                                                            CHEM  53
      READ 2,IHCODE,H,IPUNCH                                            CHEM  54
    2 FORMAT(I6,1F10.5,I3)                                              CHEM  55
C                                                                       CHEM  56
C                                                                       CHEM  57
C-----COMPUTE THE SIZE OF THE MATRIX                                    CHEM  58
C                                                                       CHEM  59
C                                                                       CHEM  60
      NA=MM+1+NS-NC+IHCODE                                              CHEM  61
C                                                                       CHEM  62
C     NA=SIZE OF MATRIX.  IT VARIES WITH THE NUMBER OF ELEMENTS         CHEM  63
C     AND THE NUMBER OF SOLIDS PRESENT IN THE SYSTEM.                   CHEM  64
C                                                                       CHEM  65
      DO 209 J=1,MM                                                     CHEM  66
C                                                                       CHEM  67
C                                                                       CHEM  68
```

```
C                                                                       CHEM  69
C----READ IN EMPIRICAL CONSTANTS FOR THE ENTHALPY FIT OF THE            CHEM  70
C     ELEMENTS.                                                         CHEM  71
C                                                                       CHEM  72
C                                                                       CHEM  73
C     S1 THRU S5=EMPIRICAL CONSTANTS FOR HEAT CAPACITY OF ELEMENTS      CHEM  74
C                                  (ABOVE 1000 OK)                      CHEM  75
C     A11 THRU A55=EMPIRICAL CONSTANTS FOR HEAT CAPACITY OF ELEMENTS    CHEM  76
C                                 (UP TO 1000 OK)                       CHEM  77
C                                                                       CHEM  78
      READ2111,S1(J),S2(J),S3(J),S4(J),S5(J),S6(J),JCODE(J)             CHEM  79
 2111 FORMAT(6E10.4,I3)                                                 CHEM  80
  210 FORMAT(7E10.8)                                                    CHEM  81
C                                                                       CHEM  82
      READ 210,A11(J),A22(J),A33(J),A44(J),A55(J),A66(J)                CHEM  83
  209 CONTINUE                                                          CHEM  84
C                                                                       CHEM  85
C                                                                       CHEM  86
C     NC IS THE TOTAL NUMBER OF MOLES OF GASES USED IN THE ORIGINAL INPUCHEM  87
C     NN WILL DIFFER FROM NC ONLY WHEN TRACE SPECIES ARE ELIMINATED FROMCHEM  88
C     THE COMPUTATIONS WHILE BEING HELD IN A TEMPORARY LOCATION UNTIL WECHEM  89
C     ARE REASONABLY SURE THAT WE ARE VERY CLOSE TO THE MINIMUM.        CHEM  90
C     NS IS THE TOTAL NUMBER OF MOLES OF GASES + SOLIDS BEING READ IN.  CHEM  91
C     IT WILL DIFFER FROM NQ ONLY WHEN TRACE SPECIES APPEAR.            CHEM  92
C                                                                       CHEM  93
C                                                                       CHEM  94
      KREAD=0                                                           CHEM  95
      NQ=NS                                                             CHEM  96
      NN=NC                                                             CHEM  97
C                                                                       CHEM  98
C                                                                       CHEM  99
C-----READ MOLECULAR WEIGHT,INITIAL GUESS,NAME OF SPECIE,AND CODE       CHEM 100
C     TO DETERMINE WETHER THE SPECIE IS ASOLID OR A GAS                 CHEM 101
C                                                                       CHEM 102
```

```
C                                                                       CHEM 103
C     NC=NO. OF GAS COMPONENTS                                          CHEM 104
C     NS=NO. OF CONDENSED PLUS GAS COMPONENTS                           CHEM 105
C     MM=NO. OF ELEMENTS                                                CHEM 106
C     TZERO=REFERENCE TEMPERATURE (298.15 OK)                           CHEM 107
C     RR=1.98726(CAL/GM-MOLE-OK)                                        CHEM 108
C     ICODE=0 (GAS),   =1 (SOLID)                                       CHEM 109
C     SPCIE1 AND SPCIE2 ARE THE SPECIES IDENTIFICATION NAME             CHEM 110
C                                                                       CHEM 111
      DO 212 I=1,NS                                                     CHEM 112
      READ 208,TLOW(I),XMW(I),Y(I),SPCIE1(I),SPCIE2(I),                 CHEM 113
     1         ICODE(I)                                                 CHEM 114
  208 FORMAT(10X,3E10.4,2X,2A3,I4)                                      CHEM 115
C                                                                       CHEM 116
C                                                                       CHEM 117
C-----READ IN EMPIRICAL CONSTANTS FOR THE ENTHALPY,FREE ENERGY          CHEM 118
C     AND ENTROPY FIT OF THE CHEMICAL SPECIES.                          CHEM 119
C                                                                       CHEM 120
C                                                                       CHEM 121
C                                                                       CHEM 122
C     AI THRU GI=EMPIRICAL CONSTANTS FOR HEAT CAPACITY (ABOVE 1000 OK)  CHEM 123
C                                                                       CHEM 124
      READ 210, AI(I),BI(I),CI(I),DI(I),EI(I),FI(I),GI(I)               CHEM 125
C                                                                       CHEM 126
C     AII THRU GII=EMPIRICAL CONSTANTS FOR HEAT CAPACITY (UP TO 1000 OK)CHEM 127
C                                                                       CHEM 128
      READ 210,AII(I),BII(I),CII(I),DII(I),EII(I),FII(I),GII(I)          CHEM 129
C                                                                       CHEM 130
C                                                                       CHEM 131
C----READ IN THE FORMULA NUMBER                                         CHEM 132
C                                                                       CHEM 133
C                                                                       CHEM 134
C                                                                       CHEM 135
C     AA(I,J)=FORMULA NUMBER. IT GIVES THE GRAM ATOMS OF ELEMENT        CHEM 136
```

```
C      J IN SPECIE I.                                                    CHEM 137
C                                                                        CHEM 138
       READ 210,(AA(I,J),J=1,MM)                                         CHEM 139
  212 CONTINUE                                                           CHEM 140
C                                                                        CHEM 141
C-----READ THE PRESSURE OF THE SYSTEM.                                   CHEM 142
C                                                                        CHEM 143
       READ3,RR,P                                                        CHEM 144
    3 FORMAT(2F14.8)                                                     CHEM 145
C                                                                        CHEM 146
C                                                                        CHEM 147
C-----READ IN THE NUMBER OF ITERATIONS AFTER WHICH TRACE SPECIES         CHEM 148
C      SHOULD BE CHECKED.                                                CHEM 149
C                                                                        CHEM 150
C                                                                        CHEM 151
       READ6,NFREQ                                                       CHEM 152
    6 FORMAT(3I6)                                                        CHEM 153
C                                                                        CHEM 154
C      CRIT=CRITERIA FOR CONVERGENCE.                                    CHEM 155
C                                                                        CHEM 156
       XBETA=CRIT                                                        CHEM 157
       KSEND=0                                                           CHEM 158
       KSEND1=0                                                          CHEM 159
       KORE=0                                                            CHEM 160
       KOUT=0                                                            CHEM 161
       BETA=0.                                                           CHEM 162
       T=XT                                                              CHEM 163
       KCODE=0                                                           CHEM 164
       LL=NN+I                                                           CHEM 165
C                                                                        CHEM 166
C                                                                        CHEM 167
C      MLFRC=MOLE FRACTION(INCLUDING SOLIDS)                             CHEM 168
C                                                                        CHEM 169
       SUM=0.                                                            CHEM 170
```

```
      DO 434 I=1,NQ                                                     CHEM 171
 434  SUM=SUM+Y(I)                                                      CHEM 172
C                                                                       CHEM 173
C-----CALCULATE THE GRAM-ATOMS OF EACH ELEMENT.  THIS IS THE            CHEM 174
C     MATERIAL BALANCE CONSTRAINT ON THE FREE ENERGY EQUATION           CHEM 175
C     BB(J) WILL STAY CONSTANT THROUGHOUT THE CALCULATIONS.  VALUES     CHEM 176
C     OF Y(I) SHOULD BE IN STOCHIOMETRIC PROPORTION.                    CHEM 177
C                                                                       CHEM 178
C                                                                       CHEM 179
C     BB(J)=GRAM ATOMS OF EACH ELEMENT                                  CHEM 180
C                                                                       CHEM 181
C                                                                       CHEM 182
      DO320J=1,MM                                                       CHEM 183
      BB(J)=0.0                                                         CHEM 184
      DO 320 I=1,NQ                                                     CHEM 185
      BB(J)=BB(J)+AA(I,J)*Y(I)                                          CHEM 186
  320 CONTINUE                                                          CHEM 187
C                                                                       CHEM 188
C                                                                       CHEM 189
C-----CHECK TO DETERMINE IF THERE ARE ANY SOLIDS IN THE SYSTEM.         CHEM 190
C                                                                       CHEM 191
C                                                                       CHEM 192
      DO 433 I=1,NQ                                                     CHEM 193
      IF(ICODE(I).EQ.0)GOTO433                                          CHEM 194
      KCODE=1                                                           CHEM 195
  433 CONTINUE                                                          CHEM 196
C                                                                       CHEM 197
C                                                                       CHEM 198
C----IF THERE IS NOT AN ENERGY CONSTRAINT GO TO 500.                    CHEM 199
C                                                                       CHEM 200
C                                                                       CHEM 201
      IF(IHCODE.EQ.0)GOTO500                                            CHEM 202
      MM=MM+1                                                           CHEM 203
      BB(MM)=H/SUM                                                      CHEM 204
```

```
  500 PRINT4                                                            CHEM 205
    4 FORMAT(1H1,18X,5HFO/RT,11X,12HINITIAL Y(I))                       CHEM 206
      KX=0                                                              CHEM 207
      CALL THERMO                                                       CHEM 208
C                                                                       CHEM 209
C                                                                       CHEM 210
C-----THERMO SUBROUTINE CALCULATES THE FREE ENRGY FUNCION,THE HEAT OF   CHEM 211
C     FORMATION OF EVERY CHEMICAL SPECIE AT ANY TEMPERATURE T,AND THE   CHEM 212
C     SENSIBLE ENTHALPY CHANGE PER MOLE OF EACH SPECIE.                 CHEM 213
C                                                                       CHEM 214
C                                                                       CHEM 215
      DO 206 I=1,NQ                                                     CHEM 216
      PRINT 14,I,SPCIE1(I),SPCIE2(I),FORT(I),Y(I)                       CHEM 217
   14 FORMAT(1X,I3,1X,2A3,2E18.7)                                       CHEM 218
  206 CONTINUE                                                          CHEM 219
   45 NTEST=NFREQ                                                       CHEM 220
      NT=1                                                              CHEM 221
C                                                                       CHEM 222
C                                                                       CHEM 223
C-----BETWEEN STATEMENT 300 TO 1050 THE R MATRIX AND THE VECTOR         CHEM 224
C     B ARE CALCUALTED.                                                 CHEM 225
C                                                                       CHEM 226
C                                                                       CHEM 227
  300 YBAR=0.                                                           CHEM 228
      IF(IHCODE.EQ.0)GOTO150                                            CHEM 229
      DO 207 I=1,NQ                                                     CHEM 230
      AA(I,MM)=ENT1(I)                                                  CHEM 231
  207 CONTINUE                                                          CHEM 232
  150 DO50I=1,NN                                                        CHEM 233
C                                                                       CHEM 234
C                                                                       CHEM 235
C     YBAR IS THE TOTAL NUMBER OF MOLES OF GAS SPECIES                  CHEM 236
C                                                                       CHEM 237
C                                                                       CHEM 238
```

```
   50 YBAR=YBAR+Y(I)                                                    CHEM 239
      DO10I=1,NN                                                        CHEM 240
      FAC=Y(I)/YBAR                                                     CHEM 241
      IF(FAC.LT.1.E-73)FAC=1.E-73                                       CHEM 242
C                                                                       CHEM 243
C                                                                       CHEM 244
C-----CALCULATE THE FREE ENERGY PARAMETER OF THE GAS SPECIES            CHEM 245
C     TO BE MINIMIZE                                                    CHEM 246
C                                                                       CHEM 247
C                                                                       CHEM 248
      FY(I)=Y(I)*(C(I)+ALOG(FAC))                                       CHEM 249
   10 CONTINUE                                                          CHEM 250
      IF(KCODE.EQ.0)GOTO111                                             CHEM 251
C                                                                       CHEM 252
C                                                                       CHEM 253
C-----IF THERE ARE NO SOLIDS PROCEED TO STATEMENT 111                   CHEM 254
C                                                                       CHEM 255
C                                                                       CHEM 256
C                                                                       CHEM 257
C-----CALCULATION OF THE FREE ENERGY PARAMENTER FOR SOLIDS              CHEM 258
C                                                                       CHEM 259
C                                                                       CHEM 260
      DO 11 I=LL,NQ                                                     CHEM 261
      FY(I)=Y(I)*FORT(I)                                                CHEM 262
   11 CONTINUE                                                          CHEM 263
C                                                                       CHEM 264
C                                                                       CHEM 265
C-----PROCEED TO CONSTRUCT THE R MATRIX                                 CHEM 266
C                                                                       CHEM 267
C                                                                       CHEM 268
  111 DO30J=1,MM1                                                       CHEM 269
      DO30K=J,MM1                                                       CHEM 270
      SUM=0.                                                            CHEM 271
      DO20I=1,NN                                                        CHEM 272
```

```
   20 SUM=SUM+AA(I,J)*AA(I,K)*Y(I)                                  CHEM 273
      R(J,K)=SUM                                                    CHEM 274
      R(K,J)=SUM                                                    CHEM 275
   30 CONTINUE                                                      CHEM 276
C                                                                   CHEM 277
C                                                                   CHEM 278
C-----GO TO 3000 IF THERE IS NOT AN ENERGY BALANCE CONSTRAINT       CHEM 279
C                                                                   CHEM 280
C                                                                   CHEM 281
      IF(IHCODE.EQ.0)GOTO3000                                       CHEM 282
      DO 3001 K=1,MM                                                CHEM 283
      SUM=0.                                                        CHEM 284
      DO 3002 I=1,NN                                                CHEM 285
 3002 SUM=SUM+AA(I,K)*AA(I,MM)*Y(I)                                 CHEM 286
      R(K,MM)=SUM                                                   CHEM 287
      R(MM,K)=SUM                                                   CHEM 288
 3001 CONTINUE                                                      CHEM 289
 3000 JJ=MM+1                                                       CHEM 290
      DO 103 K=1,MM                                                 CHEM 291
      SUM=0.                                                        CHEM 292
      DO 101 I=1,NN                                                 CHEM 293
  101 SUM=SUM+AA(I,K)*Y(I)                                          CHEM 294
      R(K,JJ)=SUM                                                   CHEM 295
      R(JJ,K)=SUM                                                   CHEM 296
  103 CONTINUE                                                      CHEM 297
      KL=NS-NC+JJ                                                   CHEM 298
      DO 1044 J=JJ,KL                                               CHEM 299
      DO 1045 K=JJ,KL                                               CHEM 300
 1045 R(J,K)=0.0                                                    CHEM 301
 1044 CONTINUE                                                      CHEM 302
      DO70J=1,MM                                                    CHEM 303
C                                                                   CHEM 304
C                                                                   CHEM 305
C ----PROCEED TO CALCULATE THE VECTOR B.                            CHEM 306
```

```
C                                                                       CHEM 307
C                                                                       CHEM 308
      SUM=0.                                                            CHEM 309
      DO130I=1,NN                                                       CHEM 310
  130 SUM=SUM+AA(I,J)*FY(I)                                             CHEM 311
   70 B(J,1)=SUM+BB(J)                                                  CHEM 312
      SUM=0.                                                            CHEM 313
      DO80I=1,NN                                                        CHEM 314
   80 SUM=SUM+FY(I)                                                     CHEM 315
      B(JJ,1)=SUM                                                       CHEM 316
      IF(KCODE.EQ.0)GOTO1050                                            CHEM 317
      KK=MM+1                                                           CHEM 318
      DO 29 I=LL,NQ                                                     CHEM 319
      KK=KK+1                                                           CHEM 320
      DO 29 J=1,MM                                                      CHEM 321
      R(J,KK)=AA(I,J)                                                   CHEM 322
      R(KK,J)=R(J,KK)                                                   CHEM 323
   29 CONTINUE                                                          CHEM 324
      KM=MM+1                                                           CHEM 325
      DO 1053 I=LL,NQ                                                   CHEM 326
      KM=KM+1                                                           CHEM 327
 1053 B(KM,1)=FORT(I)                                                   CHEM 328
 1050 CONTINUE                                                          CHEM 329
      IF(KCODE.EQ.0)R(JJ,JJ)=0.                                         CHEM 330
C                                                                       CHEM 331
C                                                                       CHEM 332
C-----MATRIX INVERSION IS CALLED TO PROVIDE THE SOLUTION FOR            CHEM 333
C     THE LINEARIZED EQUATIONS. THE SOLUTION OF THE EQUATIONS           CHEM 334
C     GIVES THE LAGRANGIAN MULTIPLIERS NEEDED TO COMPUTE THE MOLES      CHEM 335
C     OF EACH GAS SPECIES.  THE SOLUTION OF THE EQUATIONS GIVES,        CHEM 336
C     IN ADDITION, THE MOLES OF EACH SOLID SPECIE.                      CHEM 337
C                                                                       CHEM 338
C                                                                       CHEM 339
      N=NA                                                              CHEM 340
```

```
      M=MA                                                              CHEM 341
      CALL MATINV(R,NA,B,MA,NMAX)                                       CHEM 342
      DO100I=1,JJ                                                       CHEM 343
C                                                                       CHEM 344
C     PI(I)=LAGRANGINA MULTIPLIERS                                      CHEM 345
C                                                                       CHEM 346
  100 PI(I)=B(I,M)                                                      CHEM 347
      U=PI(JJ)                                                          CHEM 348
      XBAR=U*YBAR                                                       CHEM 349
      IF(KCODE.EQ.0)GOTO59                                              CHEM 350
      KK=MM+2                                                           CHEM 351
      LW=LL                                                             CHEM 352
      DO 1002 J=KK,KL                                                   CHEM 353
      X(LW)=B(J,M)                                                      CHEM 354
 1002 LW=LW+1                                                           CHEM 355
C                                                                       CHEM 356
C                                                                       CHEM 357
C-----BETWEEN STATEMENT 59 TO 110 A PROCEDURE IS FOLLOW TO              CHEM 358
C     COMPUTE THE NECESSARY DATA TO CALCULATE THE MOLES OF EACH         CHEM 359
C     GAS SPECIE.                                                       CHEM 360
C                                                                       CHEM 361
C                                                                       CHEM 362
   59 DO60I=1,NN                                                        CHEM 363
   60 FSUM(I)=-FY(I)+(Y(I)/YBAR)*XBAR                                   CHEM 364
      DO110I=1,NN                                                       CHEM 365
      PSUM=0.                                                           CHEM 366
      DO120J=1,MM                                                       CHEM 367
  120 PSUM=PSUM+PI(J)*AA(I,J)                                           CHEM 368
      YSUM(I)=PSUM*Y(I)                                                 CHEM 369
C                                                                       CHEM 370
C                                                                       CHEM 371
C-----CALCULATE THE MOLES OF GASEOUS SPECIES                            CHEM 372
C                                                                       CHEM 373
C                                                                       CHEM 374
```

```
  110 X(I)=FSUM(I)+YSUM(I)                                          CHEM 375
C                                                                   CHEM 376
C                                                                   CHEM 377
C-----COMPUTE THE CONVERGENCE PARAMENTER XLAMBD                     CHEM 378
C                                                                   CHEM 379
C                                                                   CHEM 380
      XLAMBD=1.                                                     CHEM 381
      DO 86 I=1,NQ                                                  CHEM 382
      DELT(I)=X(I)-Y(I)                                             CHEM 383
      IF(DELT(I).GE.0.)GOTO86                                       CHEM 384
      IF(X(I).GT.0.)GOTO86                                          CHEM 385
      XLAM(I)=-Y(I)/DELT(I)                                         CHEM 386
      XLAMBD=AMIN1(XLAMBD,XLAM(I))                                  CHEM 387
      XLAMBD=.99*XLAMBD                                             CHEM 388
   86 CONTINUE                                                      CHEM 389
      XLAM1=XLAMBD                                                  CHEM 390
      IF(XLAM1.EQ.0.)XLAM1=1.E-5                                    CHEM 391
      DEBAR=0.                                                      CHEM 392
      DO87I=1,NN                                                    CHEM 393
   87 DEBAR=DEBAR+DELT(I)                                           CHEM 394
C                                                                   CHEM 395
C                                                                   CHEM 396
C                                                                   CHEM 397
C                                                                   CHEM 398
C-----DETERMINE THE SIZE OF THE UNIT VECTOR XLAMBD.                 CHEM 399
C     APPLY THE CORRECTIONS TO OBTAIN A NEW SET OF ESTIMATES FOR THE CHEM 400
C     NEXT ITERATION. WHEN THE VALUE OF XLAMBD IS VERY SMALL SET THE CHEM 401
C     VALUES OF Y(I) EQUAL TO X(I) TO AVOID USING THE SAME VALUES OF CHEM 402
C     Y(I) AS WAS USED IN THE PREVIOUS ITERATION                    CHEM 403
C                                                                   CHEM 404
C                                                                   CHEM 405
C                                                                   CHEM 406
C                                                                   CHEM 407
C-----DETERMINE THE FREE ENERGY GRADIENT.  IF POSITIVE REDUCE XLAMBDA CHEM 408
```

```
C
C
   93 DFDL=0.
C
C     DFDL=FREE ENERGY GRADIENT
C
      DO88I=1,NQ
      IF(ICODE(I).EQ.1)GOTO83
   96 FAC=(Y(I)+XLAMBD*DELT(I))/(YBAR+XLAMBD*DEBAR)
   98 IF(FAC.GT.0.)GOTO82
  991 XLAMBD=.9*XLAMBD
      IF(XLAMBD.GT.1.0E-09)GOTO96
      IF(FAC.LT.1.E-73)FAC=1.E-73
   82 DFDL=DFDL+DELT(I)*(C(I)+ALOG(FAC))
      IF(ICODE(I).EQ.1)GOTO88
      AAA(I)=DELT(I)*(C(I)+ALOG(FAC))
      GOTO88
   83 DFDL=DFDL+DELT(I)*FORT(I)
   88 CONTINUE
      IF(DFDL.LT.0.000)GOTO89
      XLAMBD=.8*XLAMBD
      IF(XLAMBD.GT.1.0E-08)GOTO93
      DO 881 I=1,NN
  881 CONTINUE
C
C
C-----THE VALUE OF XLAMBD THAT ASSURES CONVERGENCE HAS BEEN FOUND
C
C
   89 DO76I=1,NQ
      IF(XLAMBD.GT.1.E-6)GOTO90
      IF(DFDL.LT.0.)GOTO90
      IF(XLAM1.LT.1.E-6)XLAM1=1.E-6
C
```

```
C                                                                       CHEM 443
C-----CALCUALTE THE NEW COMPOSITION FOR THE NEXT ITERATION              CHEM 444
C                                                                       CHEM 445
C                                                                       CHEM 446
      Y(I)=Y(I)+XLAM1*DELT(I)*.1                                        CHEM 447
      GOTO900                                                           CHEM 448
   90 CONTINUE                                                          CHEM 449
      Y(I)=Y(I)+XLAMBD*DELT(I)                                          CHEM 450
  900 CONTINUE                                                          CHEM 451
      IF(Y(I).LT.0.)Y(I)=1.E-73                                         CHEM 452
   76 CONTINUE                                                          CHEM 453
      SUMY=0.                                                           CHEM 454
      SUMY1=0.                                                          CHEM 455
      DO370I=1,NN                                                       CHEM 456
  370 SUMY=SUMY+Y(I)                                                    CHEM 457
      IF(KCODE.EQ.0)GOTO372                                             CHEM 458
      DO 371 I=LL,NQ                                                    CHEM 459
  371 SUMY1=SUMY1+Y(I)                                                  CHEM 460
  372 SUMY1=SUMY1+SUMY                                                  CHEM 461
      DO340I=1,NQ                                                       CHEM 462
      PERC(I)=(Y(I)/SUMY)*100.                                          CHEM 463
      MLFRC(I)=Y(I)/SUMY1                                               CHEM 464
 340  PERC1(I)=MLFRC(I)*100.00                                          CHEM 465
C                                                                       CHEM 466
C                                                                       CHEM 467
C-----CHECK IF CONVERGENCE CRITERIA HAS BEEN MET. IF NOT GO BACK TO     CHEM 468
C     STATEMENT 300.                                                    CHEM 469
C                                                                       CHEM 470
C                                                                       CHEM 471
  350 BETA=0.                                                           CHEM 472
      GSUM2=0.                                                          CHEM 473
      DO 341 I=1,NQ                                                     CHEM 474
C     IF(KX.EQ.0.AND.NT.LT.NFREQ)GOTO3410                               CHEM 475
      IF(Y(I).LT.1.E-30)GOTO534                                         CHEM 476
```

```
 3410 IF(ICODE(I).EQ.1)GOTO342                                          CHEM 477
      FAC=Y(I)/SUMY                                                     CHEM 478
      IF(FAC.LT.1.E-73)FAC=1.E-73                                       CHEM 479
      FY(I)=Y(I)*(C(I)+ALOG(FAC))                                       CHEM 480
      GSUM2=GSUM2+FY(I)                                                 CHEM 481
      GOTO341                                                           CHEM 482
  342 FY(I)=Y(I)*FORT(I)                                                CHEM 483
      GSUM2=GSUM2+FY(I)                                                 CHEM 484
  341 CONTINUE                                                          CHEM 485
      IF(XLAMBD.EQ.0.)GOTO534                                           CHEM 486
 3411 DO85I=1,NQ                                                        CHEM 487
   85 BETA=BETA+ABS(DELT(I))                                            CHEM 488
      IF(DFDL.GT.0..AND.XLAM1.GE.0.9990)GOTO534                         CHEM 489
      IF(BETA.LT.XBETA)GOTO800                                          CHEM 490
  532 IF(NTEST.NE.NT)GOTO560                                            CHEM 491
  533 NTEST=NT+NFREQ                                                    CHEM 492
  534 KCALL=1                                                           CHEM 493
      INIT=LL                                                           CHEM 494
      NCOUNT=NQ                                                         CHEM 495
C                                                                       CHEM 496
C                                                                       CHEM 497
C-----PROCEED TO CHECK WHETHER THERE ARE TRACE SPECIES                  CHEM 498
C                                                                       CHEM 499
C                                                                       CHEM 500
      CALL HOLD1(KCALL,INIT,NCOUNT,LL)                                  CHEM 501
  560 IF(NT.GE.MAXNT)GOTO600                                            CHEM 502
      NT=NT+1                                                           CHEM 503
C                                                                       CHEM 504
C                                                                       CHEM 505
C-----IF THE NUMBER OF ITERATIONS EXCEED 900 STOP COMPUTATIONS          CHEM 506
C                                                                       CHEM 507
C                                                                       CHEM 508
      IF(NT.GT.900)GOTO333                                              CHEM 509
      GOTO300                                                           CHEM 510
```

```
C                                                                       CHEM 511
C                                                                       CHEM 512
C-----ADJUST CONVERGENCE CRITERIA. THEY ARE TOO STRINGENT.              CHEM 513
C                                                                       CHEM 514
C                                                                       CHEM 515
  600 XBETA=XBETA+.001                                                  CHEM 516
      MAXNT=MAXNT+10                                                    CHEM 517
      NT=NT+1                                                           CHEM 518
      GOTO300                                                           CHEM 519
  800 IF(KOUT.NE.1)GOTO801                                              CHEM 520
      IF(IN.EQ.NC)GOTO801                                               CHEM 521
C                                                                       CHEM 522
C                                                                       CHEM 523
C-----COMPUTE THE VALUES OF THE TRACE SPECIES THAT WERE LEFT OUT OF     CHEM 524
C     COMPUTATIONS.                                                     CHEM 525
C                                                                       CHEM 526
C                                                                       CHEM 527
      CALL TRACE(PI)                                                    CHEM 528
  802 NN=NC                                                             CHEM 529
      NQ=NS                                                             CHEM 530
      KOUT=0                                                            CHEM 531
      KRTRN=0                                                           CHEM 532
C***********************************************************************CHEM 533
C***********************************************************************CHEM 534
C                                                                      * CHEM 535
C                                                                      * CHEM 536
C-----CONVERGENCE HAS BEEN ACHIEVED.  PRINT OUTPUT                     * CHEM 537
C                                                                      * CHEM 538
C                                                                      * CHEM 539
C***********************************************************************CHEM 540
C***********************************************************************CHEM 541
  801 PRINT 16,NT,U                                                     CHEM 542
   16 FORMAT(//1X,30HNT = NO. ITERATIONS REQUIRED = I5,5X,              CHEM 543
     1'U=X/Y='1F15.7//)                                                 CHEM 544
```

```
      DO 2190 J=1,MM                                                    CHEM 545
      PRINT 2189,BB(J)                                                  CHEM 546
 2189 FORMAT(1X,6HBB(J)=,F15.8)                                         CHEM 547
 2190 CONTINUE                                                          CHEM 548
      PRINT201,BETA,SUMY1,H                                             CHEM 549
  201 FORMAT(//1X,7HBETA = E12.4,5X,' TOTAL NO. OF MOLES='F8.4,         CHEM 550
     15X,'H='E13.6//)                                                   CHEM 551
      PRINT 161,GSUM2                                                   CHEM 552
  161 FORMAT(1X,47HFREE ENERGY F(Y) OF THE SYSTEM AT EQUILIBRIUM =E16.8)CHEM 553
      PRINT204,P,T                                                      CHEM 554
  204 FORMAT(   ///1X, 9HPRESSURE=E13.5,5X,6HTEMP =E13.5//)             CHEM 555
      PRINT32                                                           CHEM 556
   32 FORMAT(//6X,'I',21X,'Y(I)',9X,'MOLE FRACTION',5X,                 CHEM 557
     1'MASS FRACTION')                                                  CHEM 558
      DO580I=1,NQ                                                       CHEM 559
      XMOL(I)=PERC(I)/100.                                              CHEM 560
  580 CONTINUE                                                          CHEM 561
      ENTRPY=0.                                                         CHEM 562
      XMWGAS=0.                                                         CHEM 563
      TMASMX=0.                                                         CHEM 564
      TMASS=0.                                                          CHEM 565
      DO81I=1,NQ                                                        CHEM 566
      IF(ICODE(I).EQ.1)GOTO790                                          CHEM 567
      TMASS=TMASS+XMW(I)*Y(I)                                           CHEM 568
      XXXX=XMOL(I)*XMW(I)                                               CHEM 569
      XXX=P*XMOL(I)                                                     CHEM 570
      S(I)=S(I)-RR*ALOG(XXX)                                            CHEM 571
      ENTRPY=ENTRPY+S(I)*XMOL(I)                                        CHEM 572
      XMWGAS=XMWGAS+XMOL(I)*XMW(I)                                      CHEM 573
      GOTO81                                                            CHEM 574
 790  TMASMX=TMASMX+XMW(I)*Y(I)                                         CHEM 575
   81 CONTINUE                                                          CHEM 576
      TMASMX=TMASMX+TMASS                                               CHEM 577
      DO 191I=1,NQ                                                      CHEM 578
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```
      XMAS1(I)=Y(I)*XMW(I)/TMASMX                                       CHEM 579
      XMASS(I)=XMW(I)*XMOL(I)/XMWGAS                                    CHEM 580
  191 CONTINUE                                                          CHEM 581
      DO44I=1,NQ                                                        CHEM 582
      IF(IPUNCH.EQ.0)GOTO43                                             CHEM 583
      IF(XMOL(I).LT.1.0000E-4)GOTO43                                    CHEM 584
      PUNCH 46,XMOL(I),SPCIE1(I),SPCIE2(I)                              CHEM 585
   46 FORMAT(2E14.7,10X,2A3)                                            CHEM 586
   43 PRINT 19,I,SPCIE1(I),SPCIE2(I),Y(I),XMOL(I),XMASS(I)              CHEM 587
   44 CONTINUE                                                          CHEM 588
19    FORMAT(1X,I6,3X,2A3,2X,3E18.7)                                   CHEM 589
      ENTGAS=0.                                                         CHEM 590
      PRINT12                                                           CHEM 591
12    FORMAT( ///36X,'MASS FRACTION',/15X,'HEAT OF FORMATION  ',2X,     CHEM 592
     1'OF THE MIXTURE',5X,'ENTROPY')                                    CHEM 593
      DO 781 I=1,NQ                                                     CHEM 594
  781 ENTGAS=ENTGAS+ENT1(I)*PERC(I)/100.                                CHEM 595
      DO 79 I=1,NQ                                                      CHEM 596
79    PRINT 24, I,SPCIE1(I),SPCIE2(I),ENT(I),XMAS1(I),S(I)              CHEM 597
   24 FORMAT(1X,I5,3X,2A3,3E17.7)                                       CHEM 598
      ENTRPY=ENTRPY/XMWGAS                                              CHEM 599
      ENTGAS=ENTGAS/XMWGAS                                              CHEM 600
      PRINT18,ENTGAS                                                    CHEM 601
   18 FORMAT(//1X,'ENTHALPY OF GAS MIXTURE(CAL/GM-MOLE='E17.7)          CHEM 602
      PRINT17,XMWGAS,ENTRPY                                             CHEM 603
   17 FORMAT(//1X,28HMOLECULAR WEIGHT OF GAS MIX=E16.8,4X,              CHEM 604
     1'ENTROPY( CAL/(GM-MOLE-OK) )='E17.6//)                            CHEM 605
      XBETA=CRIT                                                        CHEM 606
      LL=NN+1                                                           CHEM 607
      NTEST=NFREQ                                                       CHEM 608
      KSOLID=0                                                          CHEM 609
      KX=0                                                              CHEM 610
      IF(IHCODE.EQ.0)GOTO332                                            CHEM 611
      H=H-1000.                                                         CHEM 612
```

```
      BB(MM)=H/SUMY1                                                    CHEM 613
      IF(H.LT.(-30000.))GOTO332                                         CHEM 614
      IF(IHCODE.EQ.1)GOTO500                                            CHEM 615
332   T=T+TINC                                                          CHEM 616
      IF(T.GE.3373.)TINC=10.                                            CHEM 617
      IF(T.GE.TMAX)GOTO5                                                CHEM 618
      GOTO500                                                           CHEM 619
 333  PRINT 5119                                                        CHEM 620
5119  FORMAT(1H1)                                                       CHEM 621
      STOP                                                              CHEM 622
      END                                                               CHEM 623
```

```
      SUBROUTINE THERMO                                                 THER   1
C                                                                       THER   2
C                                                                       THER   3
C     FORMATION OF EVERY CHEMICAL SPECIE AT ANY TEMPERATURE T,AND THE   THER   4
C     SENSIBLE ENTHALPY CHANGE PER MOLE OF EACH SPECIE.                 THER   5
C                                                                       THER   6
C                                                                       THER   7
      COMMON/KA/ICODE(40),SPCIE1(40),SPCIE2(40),AA(40,5),               THER   8
     1          ENT1(40),ENT(40)                                        THER   9
      COMMON/KB/AI(40),BI(40),CI(40),DI(40),EI(40),FI(40),              THER  10
     1       GI(40),AII(40),BII(40),CII(40),DII(40),EII(40),            THER  11
     2       FII(40),GII(40),DELH(40),FORT(40),C(40),TLOW(40),          THER  12
     3       Y(40),XMW(40),MLFRC(40)                                    THER  13
      COMMON/KBB/CPDT1(5),PERC(40),PERC1(40)                            THER  14
      COMMON/KE/S1(5),S2(5),S3(5),S4(5),S5(5),A11(5),A22(5),            THER  15
     1       A33(5),A44(5),A55(5),S6(5),A66(5),JCODE(5),S(40)           THER  16
      COMMON/KF/NC,NS,MM,RR,MM1,NQ,NN,KW,IN,KOUNT,KCODE,KSOLID          THER  17
      COMMON/KG/T,TZERO,TZERO1,TZERO2,TZERO3,TZERO4,TZERO5,P            THER  18
      REAL MLFRC                                                        THER  19
C                                                                       THER  20
C     T=TEMPERATURE IN OK                                               THER  21
C                                                                       THER  22
      T1=T                                                              THER  23
      T2=T1*T                                                           THER  24
      T3=T2*T                                                           THER  25
      T4=T3*T                                                           THER  26
      T5=T4*T                                                           THER  27
      A1=T                                                              THER  28
      A2=T2/2.                                                          THER  29
      A3=T3/3.                                                          THER  30
      A4=T4/4.                                                          THER  31
      A5=T5/5.                                                          THER  32
C                                                                       THER  33
C                                                                       THER  34
```

```
C-----CALCUALTE THE FREE ENERGY FUNCTION FORT(I), THE ENTROPY S(I),      THER  35
C     AND THE CHEMICAL ENERGY ENT1(I)                                    THER  36
C                                                                        THER  37
C                                                                        THER  38
C                                                                        THER  39
C     FORT(I)=FREE ENERGY FUNCTION                                       THER  40
C     S(I)=ENTROPY                                                       THER  41
C     ENT1(I)=HEAT OF FORMATION AT 298 OK + THE SENSIBLE                 THER  42
C     ENTHALPY GAIN FROM 298 TO T.                                       THER  43
C                                                                        THER  44
      NQ=NS                                                              THER  45
      DO 41 I=1,NQ                                                       THER  46
      IF(T.GT.TLOW(I))GOTO6205                                           THER  47
      FORT(I)=AII(I)*(1.-ALOG(T))-BII(I)*T/2.-CII(I)*T2/6.-DII(I)*T3/12.THER  48
     1        -EII(I)*T4/20.+FII(I)/T-GII(I)                             THER  49
      S(I)=(AII(I)*ALOG(T)+BII(I)*T+CII(I)*T2/2.+DII(I)*T3/3.+EII(I)*T4/THER  50
     14.+GII(I))*RR                                                      THER  51
      ENT1(I)=(AII(I)*A1+BII(I)*A2+CII(I)*A3+DII(I)*A4+EII(I)*A5         THER  52
     1+FII(I))*RR                                                        THER  53
      IF(ICODE(I).EQ.1)GOTO41                                            THER  54
      C(I)=FORT(I)+ALOG(P)                                               THER  55
      GOTO41                                                             THER  56
 6205 FORT(I)=AI(I)*(1.-ALOG(T))-BI(I)*T/2.-CI(I)*T2/6.-DI(I)*T3/12.     THER  57
     1        -EI(I)*T4/20.+FI(I)/T-GI(I)                                THER  58
      S(I)=AI(I)*ALOG(T)+BI(I)*T+CI(I)*T2/2.+DI(I)*T3/3.+EI(I)*T4/4.+    THER  59
     1GI(I)                                                              THER  60
      S(I)=S(I)*RR                                                       THER  61
      ENT1(I)=(AI(I)*A1+BI(I)*A2+CI(I)*A3+DI(I)*A4+EI(I)*A5              THER  62
     1+FI(I))*RR                                                         THER  63
      IF(ICODE(I).EQ.1)GOTO41                                            THER  64
      C(I)=FORT(I)+ALOG(P)                                               THER  65
   41 CONTINUE                                                           THER  66
      DO 78I=1,NQ                                                        THER  67
C     ELEMENTS FOR TEMPERATURES GREATER THAN 1000(OK)                    THER  68
```

```
      IF(I.GT.1)GOTO6291                                                THER  69
      IF(T.LT.TLOW(I))GOTO6207                                          THER  70
C                                                                       THER  71
C                                                                       THER  72
C-----CALCULATE THE SENSIBLE ENTHALPY OF THE CONSTITUENT                THER  73
C                                                                       THER  74
C                                                                       THER  75
      DO 296J=1,MM1                                                     THER  76
      CPDT1(J)=(S1(J)*A1+S2(J)*A2+S3(J)*A3+S4(J)*A4+S5(J)*A5            THER  77
     1        +S6(J))*RR                                                THER  78
  296 CONTINUE                                                          THER  79
      GOTO6291                                                          THER  80
C                                                                       THER  81
C                                                                       THER  82
C-----CALCULATE THE SENSIBLE ENTHALPY OF THE CONSTITUENT                THER  83
C     ELEMENTS FOR TEMPERATURES LESS THAN 1000(OK).                     THER  84
C                                                                       THER  85
C                                                                       THER  86
 6207 DO297J=1,MM1                                                      THER  87
      CPDT1(J)=(A11(J)*A1+A22(J)*A2+A33(J)*A3+A44(J)*A4                 THER  88
     1        +A55(J)*A5+A66(J))*RR                                     THER  89
  297 CONTINUE                                                          THER  90
C                                                                       THER  91
C     RSUM IS THE SENSIBLE ENTHALPY OF THE ELEMENTS OF THE ITH SPECIE   THER  92
C     AT TEMPERATURE T(OK),WITH RESPECT TO THE STANDARD STATE(P=1ATM,   THER  93
C     TZERO=298.15OK)                                                   THER  94
C                                                                       THER  95
C                                                                       THER  96
C-----COMPUTE THE HEAT OF FORMATION OF EACH CHEMICAL SPECIE             THER  97
C                                                                       THER  98
C                                                                       THER  99
C                                                                       THER 100
C     ENT(I)=HEAT OF FORMATION OF EACH CHEMICAL SPECIE AT TEMPERATURE   THER 101
C     T.                                                                THER 102
```

```
C                                                                       THER 103
 6291 RSUM=0.                                                           THER 104
      DO 398 J=1,MM1                                                    THER 105
      IF(JCODE(J).EQ.1)GOTO393                                          THER 106
      RSUM=RSUM+0.5*AA(I,J)*CPDT1(J)                                    THER 107
      GO TO 398                                                         THER 108
  393 RSUM=RSUM+AA(I,J)*CPDT1(J)                                        THER 109
  398 CONTINUE                                                          THER 110
      ENT(I)=ENT1(I)-RSUM                                               THER 111
      IF(ABS(ENT(I)).LT.3.)ENT(I)=0.                                    THER 112
   78 CONTINUE                                                          THER 113
      RETURN                                                            THER 114
      END                                                               THER 115
```

```
      SUBROUTINE HOLD1(KCALL,INIT,NCOUNT,LL)                            HOLD   1
C                                                                       HOLD   2
C     THIS SUBROUTINE ELIMINATES THE TRACE SPECIES FROM THE COMPUTATIONSHOLD   3
C     AND HOLD THEM IN STORAGE UNTIL THE END.                           HOLD   4
C                                                                       HOLD   5
      COMMON/KA/ICODE(40),SPCIE1(40),SPCIE2(40),AA(40,5),               HOLD   6
     1          ENT1(40),ENT(40)                                        HOLD   7
      COMMON/KB/AI(40),BI(40),CI(40),DI(40),EI(40),FI(40),              HOLD   8
     1       GI(40),AII(40),BII(40),CII(40),DII(40),EII(40),            HOLD   9
     2       FII(40),GII(40),DELH(40),FORT(40),C(40),TLOW(40),          HOLD  10
     3       Y(40),XMW(40),MLFRC(40)                                    HOLD  11
      COMMON/KBB/CPDT1(5),PERC(40),PERC1(40)                            HOLD  12
      COMMON/KC/IICODE(40),XPCIE1(40),XPCIE2(40),XAA(40,5),             HOLD  13
     1           XENT(40),XENT1(40)                                     HOLD  14
      COMMON/KD/XAI(40),XBI(40),XCI(40),XDI(40),XEI(40),                HOLD  15
     1       XFI(40),XGI(40),XAII(40),XBII(40),XCII(40),                HOLD  16
     2       XDII(40),XEII(40),XFII(40),XGII(40),XMLFR(40)              HOLD  17
      COMMON/KDD/XDELH(40),XCPDT(40),XCPDT1(05),XFORT(40),              HOLD  18
     1XY(40),XC(40),XTLOW(40),XXMW(40),XPERC(40),XPERC1(40)             HOLD  19
      COMMON/KF/NC,NS,MM,RR,MM1,NQ,NN,KW,IN,KOUT,KCODE,KSOLID           HOLD  20
      DIMENSION YX(40)                                                  HOLD  21
      REAL MLFRC                                                        HOLD  22
      IF(KCALL.EQ.2)GOTO5050                                            HOLD  23
      DO530J=1,NN                                                       HOLD  24
      YMAX=0.                                                           HOLD  25
      DO520L=1,NN                                                       HOLD  26
  520 YMAX=AMAX1(YMAX,Y(L))                                             HOLD  27
      DO530K=1,NN                                                       HOLD  28
      YX(K)=Y(K)/YMAX                                                   HOLD  29
      IF(ABS(YX(K)-1.).GT.1.E-6)GOTO530                                 HOLD  30
      Y(K)=0.                                                           HOLD  31
      XY(J)=YMAX                                                        HOLD  32
      XAI(J)=AI(K)                                                      HOLD  33
      XAII(J)=AII(K)                                                    HOLD  34
```

```
      XBI(J)=BI(K)                                                      HOLD  35
      XBII(J)=BII(K)                                                    HOLD  36
      XCI(J)=CI(K)                                                      HOLD  37
      XCII(J)=CII(K)                                                    HOLD  38
      XDI(J)=DI(K)                                                      HOLD  39
      XDII(J)=DII(K)                                                    HOLD  40
      XEI(J)=EI(K)                                                      HOLD  41
      XEII(J)=EII(K)                                                    HOLD  42
      XFI(J)=FI(K)                                                      HOLD  43
      XFII(J)=FII(K)                                                    HOLD  44
      XGI(J)=GI(K)                                                      HOLD  45
      XGII(J)=GII(K)                                                    HOLD  46
      XC(J)=C(K)                                                        HOLD  47
      XPERC(J)=PERC(K)                                                  HOLD  48
      XPERC1(J)=PERC1(K)                                                HOLD  49
      XMLFR(J)=MLFRC(K)                                                 HOLD  50
      XFORT(J)=FORT(K)                                                  HOLD  51
      XENT(J)=ENT(K)                                                    HOLD  52
      XENT1(J)=ENT1(K)                                                  HOLD  53
      XTLOW(J)=TLOW(K)                                                  HOLD  54
      XDELH(J)=DELH(K)                                                  HOLD  55
      XXMW(J)=XMW(K)                                                    HOLD  56
      XPCIE1(J)=SPCIE1(K)                                               HOLD  57
      XPCIE2(J)=SPCIE2(K)                                               HOLD  58
      IICODE(J)=ICODE(K)                                                HOLD  59
      DO540I=1,MM                                                       HOLD  60
  540 XAA(J,I)=AA(K,I)                                                  HOLD  61
  530 CONTINUE                                                          HOLD  62
      L1=NN                                                             HOLD  63
  521 DO 510 I=1,L1                                                     HOLD  64
       AI(I)=XAI(I)                                                     HOLD  65
      AII(I)=XAII(I)                                                    HOLD  66
      BI(I)=XBI(I)                                                      HOLD  67
      BII(I)=XBII(I)                                                    HOLD  68
```

```
      CI(I)=XCI(I)                                                      HOLD  69
      CII(I)=XCII(I)                                                    HOLD  70
      DI(I)=XDI(I)                                                      HOLD  71
      DII(I)=XDII(I)                                                    HOLD  72
      EI(I)=XEI(I)                                                      HOLD  73
      EII(I)=XEII(I)                                                    HOLD  74
      FI(I)=XFI(I)                                                      HOLD  75
      FII(I)=XFII(I)                                                    HOLD  76
      GI(I)=XGI(I)                                                      HOLD  77
      GII(I)=XGII(I)                                                    HOLD  78
      SPCIE1(I)=XPCIE1(I)                                               HOLD  79
      SPCIE2(I)=XPCIE2(I)                                               HOLD  80
      FORT(I)=XFORT(I)                                                  HOLD  81
      ENT(I)=XENT(I)                                                    HOLD  82
      ENT1(I)=XENT1(I)                                                  HOLD  83
      TLOW(I)=XTLOW(I)                                                  HOLD  84
      DELH(I)=XDELH(I)                                                  HOLD  85
      XMW(I)=XXMW(I)                                                    HOLD  86
      ICODE(I)=IICODE(I)                                                HOLD  87
      PERC(I)=XPERC(I)                                                  HOLD  88
      PERC1(I)=XPERC1(I)                                                HOLD  89
      MLFRC(I)=XMLFR(I)                                                 HOLD  90
      IF(ICODE(I).EQ.1)GOTO5211                                         HOLD  91
      C(I)=XC(I)                                                        HOLD  92
 5211 DO 590 J=1,MM                                                     HOLD  93
  590 AA(I,J)=XAA(I,J)                                                  HOLD  94
      KOUT=1                                                            HOLD  95
  510 Y(I)=XY(I)                                                        HOLD  96
      KW=0                                                              HOLD  97
      IN=NN                                                             HOLD  98
      DO550I=1,NN                                                       HOLD  99
      IF(PERC(I).GT.1.E-9)GOTO550                                       HOLD 100
 5500 IN=IN-1                                                           HOLD 101
      KW=KW+1                                                           HOLD 102
```

```
  550 CONTINUE                                                          HOLD 103
      NN=IN                                                             HOLD 104
      NL=NN+1                                                           HOLD 105
      IF(KCODE.EQ.0)GOTO5600                                            HOLD 106
 5050 DO 507 I=INIT,NCOUNT                                              HOLD 107
      IF(KCALL.EQ.2)GOTO5051                                            HOLD 108
      AI(NL)=AI(I)                                                      HOLD 109
      AII(NL)=AII(I)                                                    HOLD 110
      BI(NL)=BI(I)                                                      HOLD 111
      BII(NL)=BII(I)                                                    HOLD 112
      CI(NL)=CI(I)                                                      HOLD 113
      CII(NL)=CII(I)                                                    HOLD 114
      DI(NL)=DI(I)                                                      HOLD 115
      DII(NL)=DII(I)                                                    HOLD 116
      EI(NL)=EI(I)                                                      HOLD 117
      EII(NL)=EII(I)                                                    HOLD 118
      FI(NL)=FI(I)                                                      HOLD 119
      FII(NL)=FII(I)                                                    HOLD 120
      GI(NL)=GI(I)                                                      HOLD 121
      GII(NL)=GII(I)                                                    HOLD 122
      SPCIE1(NL)=SPCIE1(I)                                              HOLD 123
      SPCIE2(NL)=SPCIE2(I)                                              HOLD 124
      FORT(NL)=FORT(I)                                                  HOLD 125
      ICODE(NL)=ICODE(I)                                                HOLD 126
      XMW(NL)=XMW(I)                                                    HOLD 127
      ENT(NL)=ENT(I)                                                    HOLD 128
      ENT1(NL)=ENT1(I)                                                  HOLD 129
      TLOW(NL)=TLOW(I)                                                  HOLD 130
      DELH(NL)=DELH(I)                                                  HOLD 131
      PERC(NL)=PERC(I)                                                  HOLD 132
      PERC1(NL)=PERC1(I)                                                HOLD 133
      MLFRC(NL)=MLFRC(I)                                                HOLD 134
      IF(KSOLID.EQ.1)GOTO551                                            HOLD 135
 5051 XAI(I)=AI(I)                                                      HOLD 136
```

```
      XAII(I)=AII(I)                                                    HOLD 137
      XBI(I)=BI(I)                                                      HOLD 138
      XBII(I)=BII(I)                                                    HOLD 139
      XCI(I)=CI(I)                                                      HOLD 140
      XCII(I)=CII(I)                                                    HOLD 141
      XDI(I)=DI(I)                                                      HOLD 142
      XDII(I)=DII(I)                                                    HOLD 143
      XEI(I)=EI(I)                                                      HOLD 144
      XEII(I)=EII(I)                                                    HOLD 145
      XFI(I)=FI(I)                                                      HOLD 146
      XFII(I)=FII(I)                                                    HOLD 147
      XGI(I)=GI(I)                                                      HOLD 148
      XGII(I)=GII(I)                                                    HOLD 149
      XPCIE1(I)=SPCIE1(I)                                               HOLD 150
      XPCIE2(I)=SPCIE2(I)                                               HOLD 151
      XPERC(I)=PERC(I)                                                  HOLD 152
      XPERC1(I)=PERC1(I)                                                HOLD 153
      XMLFR(I)=MLFRC(I)                                                 HOLD 154
      XFORT(I)=FORT(I)                                                  HOLD 155
      IICODE(I)=ICODE(I)                                                HOLD 156
      XXMW(I)=XMW(I)                                                    HOLD 157
      XTLOW(I)=TLOW(I)                                                  HOLD 158
      XDELH(I)=DELH(I)                                                  HOLD 159
      IF(KCALL.EQ.2)GOTO551                                             HOLD 160
      XENT(I)=ENT(I)                                                    HOLD 161
      XENT1(I)=ENT1(I)                                                  HOLD 162
  551 DO 591 J=1,MM                                                     HOLD 163
      IF(KCALL.EQ.2)GOTO5510                                            HOLD 164
      AA(NL,J)=AA(I,J)                                                  HOLD 165
      IF(KSOLID.EQ.1)GOTO591                                            HOLD 166
 5510 XAA(I,J)=AA(I,J)                                                  HOLD 167
  591 CONTINUE                                                          HOLD 168
      IF(KCALL.EQ.2)GOTO560                                             HOLD 169
      Y(NL)=Y(I)                                                        HOLD 170
```

```
      NL=NL+1                                                           HOLD 171
  507 CONTINUE                                                          HOLD 172
      KSOLID=1                                                          HOLD 173
 5600 LL=NN+1                                                           HOLD 174
      NQ=NQ-KW                                                          HOLD 175
      IF(KCODE.EQ.0)NQ=NN                                               HOLD 176
  560 RETURN                                                            HOLD 177
      END                                                               HOLD 178
```

```
      SUBROUTINE TRACE (PI)                                             TRAC   1
      COMMON/KA/ICODE(40),SPCIE1(40),SPCIE2(40),AA(40,5),               TRAC   2
     1          ENT1(40),ENT(40)                                        TRAC   3
      COMMON/KB/AI(40),BI(40),CI(40),DI(40),EI(40),FI(40),              TRAC   4
     1       GI(40),AII(40),BII(40),CII(40),DII(40),EII(40),            TRAC   5
     2       FII(40),GII(40),DELH(40),FORT(40),C(40),TLOW(40),          TRAC   6
     3       Y(40),XMW(40),MLFRC(40)                                    TRAC   7
      COMMON/KBB/CPDT1(5),PERC(40),PERC1(40)                            TRAC   8
      COMMON/KC/IICODE(40),XPCIE1(40),XPCIE2(40),XAA(40,5),             TRAC   9
     1           XENT(40),XENT1(40)                                     TRAC  10
      COMMON/KD/XAI(40),XBI(40),XCI(40),XDI(40),XEI(40),                TRAC  11
     1       XFI(40),XGI(40),XAII(40),XBII(40),XCII(40),                TRAC  12
     2       XDII(40),XEII(40),XFII(40),XGII(40),XMLFR(40)              TRAC  13
      COMMON/KDD/XDELH(40),XCPDT(40),XCPDT1(05),XFORT(40),              TRAC  14
     1XY(40),XC(40),XTLOW(40),XXMW(40),XPERC(40),XPERC1(40)             TRAC  15
      COMMON/KF/NC,NS,MM,RR,MM1,NQ,NN,KW,IN,KOUT,KCODE,KSOLID           TRAC  16
      DIMENSION YTRACE(40),PI(7)                                        TRAC  17
      REAL MLFRC                                                        TRAC  18
      L1=IN+1                                                           TRAC  19
C                                                                       TRAC  20
C     STORE THE VALUES OF Y(I) OF THE SOLID SPECIES BEFORE BEING ERASED TRAC  21
C     BY THE CALCULATIONS OF THE TRACE SPECIES WHICH FOLLOWS.           TRAC  22
C                                                                       TRAC  23
      IF(KCODE.EQ.0)GOTO7428                                            TRAC  24
      NP=NC+1                                                           TRAC  25
      L4=NN+1                                                           TRAC  26
      DO 7427 I=L4,NQ                                                   TRAC  27
      XY(NP)=Y(I)                                                       TRAC  28
      XPERC(NP)=PERC(I)                                                 TRAC  29
      XMLFR(NP)=MLFRC(I)                                                TRAC  30
      XPERC1(NP)=PERC1(I)                                               TRAC  31
 7427 NP=NP+1                                                           TRAC  32
 7428 YBAR=0.                                                           TRAC  33
C                                                                       TRAC  34
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C     PROCEED TO CALCULATE THE TRACE SPECIES.                          TRAC  35
C                                                                      TRAC  36
C                                                                      TRAC  37
      DO 7429 I=1,NN                                                   TRAC  38
 7429 YBAR=YBAR+Y(I)                                                   TRAC  39
       DO 7433 I=L1,NC                                                 TRAC  40
      SUM=0.                                                           TRAC  41
      DO 7430 J=1,MM1                                                  TRAC  42
 7430 SUM=SUM+XAA(I,J)*PI(J)                                           TRAC  43
      SUM1=-C(I)+SUM                                                   TRAC  44
      IF(SUM1.LT.0.)GOTO7431                                           TRAC  45
      YTRACE(I)=YBAR*(EXP(SUM1))                                       TRAC  46
      GOTO7432                                                         TRAC  47
 7431 SUM2=-SUM1                                                       TRAC  48
      YTRACE(I)=YBAR*(1./(EXP(SUM2)))                                  TRAC  49
      XPERC(I)=(YTRACE(I)/YBAR)*100.                                   TRAC  50
 7432 XY(I)=YTRACE(I)                                                  TRAC  51
 7433 CONTINUE                                                         TRAC  52
      DO 7434 I=1,NN                                                   TRAC  53
      XPERC(I)=PERC(I)                                                 TRAC  54
 7434 XY(I)=Y(I)                                                       TRAC  55
      L1=NS                                                            TRAC  56
  521 DO 510 I=1,L1                                                    TRAC  57
       AI(I)=XAI(I)                                                    TRAC  58
      AII(I)=XAII(I)                                                   TRAC  59
      BI(I)=XBI(I)                                                     TRAC  60
      BII(I)=XBII(I)                                                   TRAC  61
      CI(I)=XCI(I)                                                     TRAC  62
      CII(I)=XCII(I)                                                   TRAC  63
      DI(I)=XDI(I)                                                     TRAC  64
      DII(I)=XDII(I)                                                   TRAC  65
      EI(I)=XEI(I)                                                     TRAC  66
      EII(I)=XEII(I)                                                   TRAC  67
      FI(I)=XFI(I)                                                     TRAC  68
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      FII(I)=XFII(I)                                                    TRAC  69
      GI(I)=XGI(I)                                                      TRAC  70
      GII(I)=XGII(I)                                                    TRAC  71
      SPCIE1(I)=XPCIE1(I)                                               TRAC  72
      SPCIE2(I)=XPCIE2(I)                                               TRAC  73
      FORT(I)=XFORT(I)                                                  TRAC  74
      ENT(I)=XENT(I)                                                    TRAC  75
      ENT1(I)=XENT1(I)                                                  TRAC  76
      TLOW(I)=XTLOW(I)                                                  TRAC  77
      DELH(I)=XDELH(I)                                                  TRAC  78
      XMW(I)=XXMW(I)                                                    TRAC  79
      ICODE(I)=IICODE(I)                                                TRAC  80
      PERC(I)=XPERC(I)                                                  TRAC  81
      PERC1(I)=XPERC1(I)                                                TRAC  82
      MLFRC(I)=XMLFR(I)                                                 TRAC  83
      IF(ICODE(I).EQ.1)GOTO5211                                         TRAC  84
      C(I)=XC(I)                                                        TRAC  85
 5211 DO 590 J=1,MM                                                     TRAC  86
  590 AA(I,J)=XAA(I,J)                                                  TRAC  87
  510 Y(I)=XY(I)                                                        TRAC  88
      RETURN                                                            TRAC  89
      END                                                               TRAC  90
```

```
      SUBROUTINE MATINV(A,N,B,M,NMAX)                                   MATI   1
C                                                                       MATI   2
C                                                                       MATI   3
C     MATRIX INVERSION WITH ACCOMPANYING SOLUTION OF LINEAR EQUATIONS   MATI   4
      DIMENSION A(7,7),B(7,1),IPIVOT(7),INDEX(7,2)                      MATI   5
      EQUIVALENCE (IROW,JROW), (ICOLUM,JCOLUM), (AMAX,T,SWAP)           MATI   6
C                                                                       MATI   7
C     INITIALIZATION                                                    MATI   8
C                                                                       MATI   9
    5 ISCALE=0                                                          MATI  10
    6 R1=10.0**18                                                       MATI  11
    7 R2=1.0/R1                                                         MATI  12
   10 DETERM=1.0                                                        MATI  13
   15  DO 20 J=1,N                                                      MATI  14
   20 IPIVOT(J)=0                                                       MATI  15
   30 DO 550 I=1,N                                                      MATI  16
C                                                                       MATI  17
C     SEARCH FOR PIVOT ELEMENT                                          MATI  18
C                                                                       MATI  19
   40 AMAX=0.0                                                          MATI  20
   45 DO 105 J=1,N                                                      MATI  21
   50 IF (IPIVOT(J)-1)60,105,60                                         MATI  22
   60 DO 100 K=1,N                                                      MATI  23
   70 IF (IPIVOT(K)-1)80,100,740                                        MATI  24
   80 IF (ABS(AMAX)-ABS(A(J,K)))85,100,100                              MATI  25
   85 IROW=J                                                            MATI  26
   90 ICOLUM=K                                                          MATI  27
   95 AMAX=A(J,K)                                                       MATI  28
  100 CONTINUE                                                          MATI  29
  105 CONTINUE                                                          MATI  30
      IF (AMAX)110,106,110                                              MATI  31
  106 DETERM=0.0                                                        MATI  32
      ISCALE=0                                                          MATI  33
      GO TO 740                                                         MATI  34
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```
  110 IPIVOT(ICOLUM)=IPIVOT(ICOLUM)+1                                   MATI  35
C                                                                       MATI  36
C     INTERCHANGE ROWS TO PUT PIVOT ELEMENT ON DIAGONAL                 MATI  37
C                                                                       MATI  38
  130 IF (IROW-ICOLUM)140,260,140                                       MATI  39
  140 DETERM=-DETERM                                                    MATI  40
  150 DO 200 L=1,N                                                      MATI  41
  160 SWAP=A(IROW,L)                                                    MATI  42
  170 A(IROW,L)=A(ICOLUM,L)                                             MATI  43
  200 A(ICOLUM,L)=SWAP                                                  MATI  44
  205 IF(M)260,260,210                                                  MATI  45
  210 DO 250 L=1,M                                                      MATI  46
  220 SWAP=B(IROW,L)                                                    MATI  47
  230 B(IROW,L)=B(ICOLUM,L)                                             MATI  48
  250 B(ICOLUM,L)=SWAP                                                  MATI  49
  260 INDEX(I,1)=IROW                                                   MATI  50
  270 INDEX(I,2)=ICOLUM                                                 MATI  51
  310 PIVOT=A(ICOLUM,ICOLUM)                                            MATI  52
C                                                                       MATI  53
C     SCALE THE DETERMINANT                                             MATI  54
C                                                                       MATI  55
 1000 PIVOTI=PIVOT                                                      MATI  56
 1005 IF(ABS(DETERM)-R1)1030,1010,1010                                  MATI  57
 1010 DETERM=DETERM/R1                                                  MATI  58
      ISCALE=ISCALE+1                                                   MATI  59
      IF(ABS(DETERM)-R1)1060,1020,1020                                  MATI  60
 1020 DETERM=DETERM/R1                                                  MATI  61
      ISCALE=ISCALE+1                                                   MATI  62
      GO TO 1060                                                        MATI  63
 1030 IF(ABS(DETERM)-R2)1040,1040,1060                                  MATI  64
 1040 DETERM=DETERM*R1                                                  MATI  65
      ISCALE=ISCALE-1                                                   MATI  66
      IF(ABS(DETERM)-R2)1050,1050,1060                                  MATI  67
 1050 DETERM=DETERM*R1                                                  MATI  68
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```
      ISCALE=ISCALE-1                                                   MATI  69
 1060 IF(ABS(PIVOTI)-R1)1090,1070,1070                                  MATI  70
 1070 PIVOTI=PIVOTI/R1                                                  MATI  71
      ISCALE=ISCALE+1                                                   MATI  72
      IF(ABS(PIVOTI)-R1)320,1080,1080                                   MATI  73
 1080 PIVOTI=PIVOTI/R1                                                  MATI  74
      ISCALE=ISCALE+1                                                   MATI  75
      GO TO 320                                                         MATI  76
 1090 IF(ABS(PIVOTI)-R2)2000,2000,320                                   MATI  77
 2000 PIVOTI=PIVOTI*R1                                                  MATI  78
      ISCALE=ISCALE-1                                                   MATI  79
      IF(ABS(PIVOTI)-R2)2010,2010,320                                   MATI  80
 2010 PIVOTI=PIVOTI*R1                                                  MATI  81
      ISCALE=ISCALE-1                                                   MATI  82
  320 DETERM=DETERM*PIVOTI                                              MATI  83
C                                                                       MATI  84
C     DIVIDE PIVOT ROW BY PIVOT ELEMENT                                 MATI  85
C                                                                       MATI  86
  330 A(ICOLUM,ICOLUM)=1.0                                              MATI  87
  340 DO 350 L=1,N                                                      MATI  88
  350 A(ICOLUM,L)=A(ICOLUM,L)/PIVOT                                     MATI  89
  355 IF(M) 380,380,360                                                 MATI  90
  360 DO 370 L=1,M                                                      MATI  91
  370 B(ICOLUM,L)=B(ICOLUM,L)/PIVOT                                     MATI  92
C                                                                       MATI  93
C     REDUCE NON-PIVOT ROWS                                             MATI  94
C                                                                       MATI  95
  380 DO 550 L1=1,N                                                     MATI  96
  390 IF(L1-ICOLUM)400,550,400                                          MATI  97
  400 T=A(L1,ICOLUM)                                                    MATI  98
  420 A(L1,ICOLUM)=0.0                                                  MATI  99
  430 DO 450 L=1,N                                                      MATI 100
  450 A(L1,L)=A(L1,L)-A(ICOLUM,L)*T                                     MATI 101
  455 IF(M) 550,550,460                                                 MATI 102
```

```
  460 DO 500 L=1,M                                                  MATI 103
  500 B(L1,L)=B(L1,L)-B(ICOLUM,L)*T                                 MATI 104
  550 CONTINUE                                                      MATI 105
C                                                                   MATI 106
C     INTERCHANGE COLUMNS                                           MATI 107
  600 DO 710 I=1,N                                                  MATI 108
C                                                                   MATI 109
  610 L=N+1-I                                                       MATI 110
  620 IF(INDEX(L,1)-INDEX(L,2))630,710,630                          MATI 111
  630 JROW=INDEX(L,1)                                               MATI 112
  640 JCOLUM=INDEX(L,2)                                             MATI 113
  650 DO 705 K=1,N                                                  MATI 114
  660 SWAP=A(K,JROW)                                                MATI 115
  670 A(K,JROW)=A(K,JCOLUM)                                         MATI 116
  700 A(K,JCOLUM)=SWAP                                              MATI 117
  705 CONTINUE                                                      MATI 118
  710 CONTINUE                                                      MATI 119
  740 RETURN                                                        MATI 120
      END                                                           MATI 121
```

CHEMICAL EQUILIBRIUM ANALYSIS NOMENCLATURE

MAIN:

AA(I,J): Formula number. Gives the gram atoms of element J in Species I.

AI...GI: These are the seven empirical constants for the high temperature fit ($1000^{o}K$-$6000^{o}K$) for the free energy functions. The first five constants (AI through EI) are used for the heat capacity fit.

AII...GII: These are the seven empirical constants for the low temperature fit ($300^{o}K$-$1000^{o}K$) for the free energy function.

A11...A66: These are the six empirical constants for the Enthalpy fit of the constituent elements ($300^{o}K$-$1000^{o}K$).

B(J,1): Is the vector formed from the right hand side of Equations in Table 4-1.

BB(J): Gram atoms of the constituent element J.

BETA: Criteria for convergence. It varies if convergence has not been achieved after 100 iterations.

C(I): Defined by Equation (4-12).

CRIT: Initial criteria for convergence.

DELT(I): Difference between the values of Y(I) and the calculated value of X(I) (gram/moles).

DFDL: Is the gradient $dF/d\lambda$ defined by Equation (4-41).

DEBAR: Is the sum of DELT(I) (gram/moles).

ENT(I): Is the heat of formation of species I, (calories/gram-mole).

ENT1(I): The enthalpy of each species I, (calories/gram-mole).

ENTGAS: The total enthalpy of the gas mixture, (calories/gram-mole).

ENTRPY: The total entropy of the gas mixture, (calories/gram-mole ^{o}K).

FY(I): Defined by Equation (4-11).

FORT(I): Is $\overline{F}^{o}_{T}/RT$.

FSUM(I): Is the sum of the first two terms of the right hand side of Equation (4-32).

GSUM2: Is the total free energy of the system at equilibrium, (calories/gram-mole).

H: This variable is used for restricted equilibrium, and is the heat balance constraint (cal/gram-mole of polymer).

ICODE(I): Is a code used to identify whether a specie is a gas or a solid. If ICODE is zero, the species is a gas. If ICODE is one, the species is a solid.

IPUNCH: If IPUNCH is one, punch output. Otherwise, IPUNCH is zero.

JCODE: Is a code used to identify whether the reference state of the constituent elements are in the gas or in the solid state.

KOUT: When KOUT is zero, trace species computations are bypassed. When KOUT is one, trace species are computed after convergence to equilibrium has been achieved.

KCODE: When the system is an all gas system KCODE is

is zero. When there is a solid, KCODE is one. This is used to adjust the size of the matrix that needs to be inverted.

MM: Is the number of elements.

MAXNT: Number of iterations after which the criteria for convergence CRIT is adjusted.

MLFRC(I): Mole fraction of species I in the mixture.

NA: Is the size of the R matrix.

NC: Number of gas species read in.

NN: Number of gas species remaining after trace species are eliminated.

NQ: Is the total number of gas and solid species after trace species are eliminated.

NS: Is the total number of gas and solid species read in.

NT: Total number of iterations.

NFREQ: Number of iterations after which the system is checked for trace species.

P: Pressure of the system in atmosphere.

PI: The Lagrange Multipliers.

R: Is the matrix formed from the coefficients of the Equations in Table 4-1.

S(I): Entropy of species I.

S1...S6: These are the six empirical constants for the enthalpy fit of the constituent elements (1000°K-6000°K).

SPECIE(I): Specie identification number.

T: Temperature in ^{o}K.

TLOW(I): Maximum temperature of low temperature fit for species I.

X(I): Calculated value of the moles of species I.

XMW(I): Molecular weight of species I.

Y(I): Moles of Y(I) guessed; or improved values of Y(I), based on the calculated values of X(I).

THERMO: Only those variables not previously defined will be mentioned in this section. This subroutine calculates the thermodynamic properties of the gas-solid system.

ENT1(I): Enthalpy of species I. (Calories/gram-mole).

CPDT1(J): Sensible enthalpy gain by the constituent elements. (Calories/gram-mole).

HOLD1: This subroutine stores the variables of the trace species in temporary location.

IICODE(I): Temporary location of ICODE(I).

XAA(I,J): Temporary storage for AA(I,J).

XAI...XGI: Temporary storage location for AI...GI.

XC(I): Temporary storage location for C(I).

XXMW(I): Temporary storage location for XMW(I).

XFORT(I): Temporary location for FORT(I).

XPCIE1(I): Temporary storage location for SPCIE1(I).

TRACE: This subroutine computes the value of the trace species once convergence to the minimum free energy has been achieved.

YTRACE(I): Value of the moles of Y(I) calculated for

the trace species.

INPUT FORMAT FOR THE CHEMICAL EQUILIBRIUM PROGRAM

This program calculates the equilibrium composition of any system at specified temperatures and pressures. Multiple cases can be run with the same data base by specifying the initial temperature at which equilibrium composition is desired, the temperature increment and the final temperature.

CARD 1: FORMAT (5F10.4,3I6)	COLUMNS:
XT = Initial Temperature (^{o}K).	1-10
TMAX = Final Temperature (^{o}K).	11-20
TINC = Temperature Increment (^{o}K)	21-30
CRIT = Convergence Tolerance (0.001 moles is recommended).	31-40
TZERO = Reference Temperature (298.16^{o}K)	41-50
NC = Number of Gas Components	51-56
MM = Number of Elements	57-62
NNS = Number of Solid Species	63-68

CARD 2: FORMAT (I6, F10.5, I3)

IHCODE = 1 (Restrictive Equilibrium Option) otherwise, leave blank.	6
H = Enthalpy for Restrictive Equilibrium Option.	7-16
IPUNCH = 1, Punch Mole Fraction and species name, otherwise, leave blank.	19

CARD 3: Reads the empirical constants for the heat capacity of the reference elements for the temperature range

1000°K to 6000°K. These are stored in the constants S1 through S6. If the reference element is a solid, JCODE should be set to one. CARD 3 is read MM number of times.

CARD 3:	FORMAT (6E10.4, I3)	COLUMNS:
S1(J) =	Empirical constants for the heat capacity of the reference elements for the temperature range 1000°K to 6000°K.	1-10
S2(J) =		11-20
S3(J) =		11-20
S4(J) =		21-30
S5(J) =		31-40
S6(J) =		51-60
JCODE(J) =	Zero if reference element is a gas, one if it is a solid or a liquid.	66

CARD 4:	FORMAT (6E10.4)	
A11(J) =	Empirical constants for the heat capacity of the reference elements for the temperature range 298°K to 1000°K.	1-10
A22(J) =		11-20
A33(J) =		21-30
A44(J) =		31-40
A55(J) =		41-50
A66(J) =		51-60

CARD 4, as with CARD 3, is read in MM number of times.

CARD 5:	FORMAT (10x,3E10.4,2x,2A3,I4)	
TLOW(I) =	Maximum temperature of low temperature fit (usually 1000°K)	11-20
YMW(I) =	Molecular weight of species	21-30

		COLUMNS:
Y(I) =	Mole fraction of species	31-40
SPCIE1(I) =	Alphameric representation	
SPCIE2(I) =	of chemical species	41-43
ICODE(I) =	Zero for a gas, one for a solid or liquid species.	51

CARD 6: FORMAT (7E10.4)

AI(I) =	Empirical constants for the free energy fit of the chemical species for the temperature range of 1000°K to 6000°K.	1-10
BI(I) =		11-20
CI(I) =		21-30
DI(I) =		31-40
EI(I) =		41-50
FI(I) =		51-60
GI(I) =		61-70

CARD 7: FORMAT (7E10.4)

AII(I) =	Empirical constants for the free energy fit of the chemical species for the temperature range of 298°K to 1000 °K.	1-10
BII(I) =		11-20
CII(I) =		21-30
DII(I) =		31-40
EII(I) =		41-50
FII(I) =		51-60
GII(I) =		61-70

CARD 8: FORMAT (8E10.4)

AA(I,1) =	Formula number of the Ith species (continued).	1-10
AA(I,2) =		11-20

		COLUMNS:
AA(I,3) =	Formula number for the Ith species.	21-30
AA(I,4) =		31-40
AA(I,M) =		71-80

CARDS 5, 6, 7 and 8 are read.

CARD 9: FORMAT (2F14.8)

RR = 1.98726	1-14
P = Pressure in atmospheres.	15-28

CARD 10: FORMAT (I6)

NFREQ = Maximum number of iterations.	1-6

TABLE E-2. Typical Chemical Equilibrium Input Data

```
                                                                                DATA   1
    10     2     4     1     2        5500.                                     DATA   2
     2160.                500.        .8 0.3500000 .00000100                   DATA   3
       .50000E9       .50000E5   .4805555E-12   0.90                            DATA   4
  3000.0E0   1073.00     2.E-4                                                  DATA   5
1.363252E01.85605E-3-7.6675E-7.151043E-9-1.139E-14-6.49672E2  1                 DATA   6
-.712442E07.34065E-3-5.5262E-61.51400E-9-2.382E-14-6.80533E1                    DATA   7
3.043690E06.11871E-4-7.3994E-9-2.033E-112.4594E-15-8.54910E2  0                 DATA   8
2.846085E04.19321E-3-9.6119E-69.51227E-9-3.309E-12-9.67253E2                    DATA   9
3.597613E07.81456E-4-2.2387E-74.2490E-11-3.346E-15-1.19279E3  0                 DATA  10
3.718995E0-2.5167E-38.58374E-6-8.2999E-92.7082E-12-1.10577E3                    DATA  11
2.220792E01.74309E-3-1.2008E-65.0841E-10-8.169E-14-7.49661E2  1                 DATA  12
4.245929E01.11866E-2-1.9539E-51.6109E-08-4.991E-12-4.80666E2                    DATA  13
          1000.00E0  15.0350E0 .30420E-4   CH3     0                            DATA  14
2.802766E06.25045E-3-2.2892E-63.8993E-10-2.528E-141.578749E45.684117E0          DATA  15
3.399505E04.26783E-32.03327E-7-1.155E-094.1288E-131.564979E42.703747E0          DATA  16
1.00000E0  3.00000E0                                                            DATA  17
          1000.00E0  1.6043E01 .38328E-3   CH4     0                            DATA  18
 1.18000E0 1.0950E-2-4.0620E-6 7.137E-10-4.749E-14-9.8556E03 1.2506E01          DATA  19
4.249768E0-6.9127E-3 3.1602E-5-2.9715E-89.5103E-12-1.01866E4-9.1755E-1          DATA  20
1.00000E0  4.00000E0                                                            DATA  21
          1000.00E0  2.6038E01 .17288E-2  C2H2     0                            DATA  22
 4.4966E00 5.2698E-3-1.840E-063.1054E-10-2.000E-142.5637E004-3.14481E0          DATA  23
7.90333E-1 2.3466E-2-3.5542E-5 2.7951E-8-8.448E-12 2.6255E04 1.4005E01          DATA  24
2.00000E0  2.00000E0                                                            DATA  25
          1000.00E0  2.01600E0 2.00385E0    H2     0                            DATA  26
3.04369E00 6.1187E-4 -7.399E-9 -2.03E-11 2.459E-15-8.5491E02 -1.648E00          DATA  27
2.846085E04.1932E-03-9.6119E-69.5123E-09-3.309E-12-9.67254E2 -1.4118E0          DATA  28
      0.E0      2.E0                                                            DATA  29
          1000.00E0  1.00800E0 .47481E-2     H     0                            DATA  30
2.500000E0 0.00000E0 0.00000E0 0.00000E0 0.00000E02.547050E4-4.6001E-1          DATA  31
2.500000E0 0.00000E0 0.00000E0 0.00000E0 0.00000E02.547050E4-4.6001E-1          DATA  32
      0.E0      1.E0                                                            DATA  33
          1000.00E0  18.0160E0 .10954E-3   H2O     0                            DATA  34
```

```
 2.67075E0 3.0317E-3 -8.535E-7 1.179E-10-6.197E-15-2.9889E04 6.88383E0  DATA   35
4.15650E00-1.7244E-35.6982E-06-4.5930E-91.4234E-12-3.02888E4-6.8616E-1  DATA   36
      0.E0      2.0E0       1.E0                                       DATA   37
          1000.00E0  2.8011E01 1.97510E0    CO      0                  DATA   38
 2.9512E00 1.5526E-3-6.1911E-7 1.135E-10-7.788E-15-1.4232E04 6.5314E00  DATA   39
3.787133E0-2.171E-035.07573E-6-3.4738E-97.7217E-13-1.43635E4 2.63355E0  DATA   40
      1.E0       0.E0      1.0E0                                       DATA   41
          1000.00E0  44.011E0  .23651E-4   CO2     0                  DATA   42
 4.4129E003.1923E-03 -1.298E-6 2.415E-10-1.674E-14-4.8944E04-7.2876E-1  DATA   43
2.170100E0 1.0378E-2-1.0734E-56.34592E-9-1.628E-12-4.83526E4 1.06644E1  DATA   44
      1.E0       0.E0      2.0E0                                       DATA   45
          1000.00E0  29.09800  .17321E-3   SIH     0                  DATA   46
3.067823E01.50816E-3-5.8923E-7.108543E-9-7.476E-154.402100E45.916108E0  DATA   47
4.236578E0-4.3652E-39.69889E-6-7.5517E-92.0693E-124.385927E46.06156E-1  DATA   48
     0.0E0       1.E0       0.E0       1.E0                            DATA   49
          1000.00E0  44.0900E0 .306063E0   SIO     0                  DATA   50
3.729516E08.63359E-4-3.5894E-76.8213E-11-4.784E-15-1.20083E43.747283E0  DATA   51
3.349588E0-2.6538E-45.48140E-6-6.879E-092.6111E-12-1.17971E46.242183E0  DATA   52
     0.E0       0.E0       1.E0       1.E0                            DATA   53
          1000.00E0  28.0900E0 1.03944E0    SI      1                  DATA   54
2.220792E01.74309E-3-1.2008E-65.0841E-10-8.169E-14-7.49661E2-1.09166E1  DATA   55
4.245929E01.11866E-2-1.9539E-51.6109E-08-4.991E-12-4.80666E2-2.75544E0  DATA   56
     0.E0       0.E0       0.E0       1.E0                            DATA   57
          1000.00E0  12.000E0  2.32170E0     C      1                  DATA   58
1.36325E001.85605E-3-7.6675E-71.5104E-10-1.139E-14-6.4967E02-7.9890E00  DATA   59
-7.1244E-17.34065E-3-5.5262E-6 1.514E-09-2.382E-14-6.80533E1 2.79326E0  DATA   60
      1.E0       0.E0       0.E0       0.E0
```

TABLE E-3. Typical Results From the Chemical Equilibrium Program

		FO/RT	INITIAL Y(I)
1	CH3	-0.2125516E 02	0.9999996E-01
2	CH4	-0.3390263E 02	0.9999996E-01
3	C2H	-0.1620010E 01	0.9999996E-01
4	C2H2	-0.1795241E 02	0.9999996E-01
5	H2	-0.1946587E 02	0.5000000E 00
6	H	-0.3306983E 01	0.1817857E 01
7	H2O	-0.4199399E 02	0.5000000E-01
8	OH	-0.2355809E 02	0.9999996E-01
9	CO	-0.3433722E 02	0.1781250E 01
10	CO2	-0.5534689E 02	0.9999996E-01
11	C2H4	-0.3240714E 02	0.9999997E-07
12	SIH	-0.5337708E 01	0.9999997E-07
13	SIH4	-0.3107219E 02	0.9999997E-07
14	SIO	-0.3503526E 02	0.5000000E-01
15	SIO2	-0.5489357E 02	0.5000000E-01
16	SI	-0.5333599E 01	0.1245673E 01
17	C	-0.2770977E 01	0.1819402E 01

NT = NO. ITERATIONS REQUIRED = 15 U=X/Y= 0.9999992

BB(J)= 4.30065060
BB(J)= 4.01785469
BB(J)= 2.28124809
BB(J)= 1.34567261

BETA = 0.1358E-03 TOTAL NO. OF MOLES= 7.6533 H= 0.0

FREE ENERGY F(Y) OF THE SYSTEM AT EQUILIBRIUM = -0.13351440E 03

PRESSURE= 0.10000E 01 TEMP = 0.20000E 04

I		Y(I)	MOLE FRACTION	MASS FRACTION
1	H2	0.2003845E 01	0.4668565E 00	0.5539759E-01
2	CO	0.1975098E 01	0.4601589E 00	0.7586706E 00
3	SIO	0.3060627E 00	0.7130653E-01	0.1850488E 00
4	H	0.4748080E-02	0.1106209E-02	0.6563182E-04
5	C2H2	0.1728777E-02	0.4027709E-03	0.6172804E-03
6	CH4	0.3832877E-03	0.8929848E-04	0.8432310E-04
7	SIH	0.1732134E-03	0.4035531E-04	0.6911633E-04
8	H2O	0.1095384E-03	0.2552029E-04	0.2706204E-04
9	CH3	0.3042049E-04	0.7087376E-05	0.6271996E-05
10	CO2	0.2365047E-04	0.5510093E-05	0.1427371E-04
11	C2H4	0.5377922E-05	0.1252949E-05	0.2068926E-05
12	C2H	0.3443769E-05	0.8023304E-06	0.1182037E-05
13	SIH4	0.1743203E-05	0.4061320E-06	0.7678682E-06
14	SIO2	0.1158856E-05	0.2699907E-06	0.9549212E-06
15	OH	0.2662728E-07	0.6203628E-08	0.6210342E-08
16	SI	0.1039440E 01	0.2421690E 00	0.4003937E 00
17	C	0.2321698E 01	0.5409100E 00	0.3820527E 00

		HEAT OF FORMATION	MASS FRACTION OF THE MIXTURE	ENTROPY
1	H2	0.0	0.3107945E-01	0.7275468E 02
2	CO	-0.2842813E 05	0.4256333E 00	0.7500009E 02

3	SIO	-0.2500515E 05	0.1038171E 00	0.7741382E 02
4	H	0.5422250E 05	0.3682109E-04	0.9031674E 02
5	C2H2	0.5257357E 05	0.3463100E-03	0.6054889E 02
6	CH4	-0.2164932E 05	0.4730739E-04	0.5537646E 02
7	SIH	0.8607963E 05	0.3877601E-04	0.8336095E 02
8	H2O	-0.6012953E 05	0.1518250E-04	0.7891264E 02
9	CH3	0.3051525E 05	0.3518747E-05	0.8537036E 02
10	CO2	-0.9484888E 05	0.8007915E-05	0.9794763E 02
11	C2H4	0.8626629E 04	0.1160720E-05	0.1168788E 03
12	C2H	0.1145694E 06	0.6631526E-06	0.9015688E 02
13	SIH4	0.5439773E 04	0.4307934E-06	0.1118265E 03
14	SIO2	-0.8350925E 05	0.5357354E-06	0.9616628E 02
15	OH	0.8756605E 04	0.3484164E-08	0.1174121E 03
16	SI	0.0	0.2246310E 00	0.1605104E 02
17	C	0.0	0.2143411E 00	0.9754942E 01

ENTHALPY OF GAS MIXTURE(CAL/GM-MOLE= 0.4021755E 03

MOLECULAR WEIGHT OF GAS MIX= 0.16989594E 02 ENTROPY(CAL/(GM-MOLE-OK))= 0.436349E 01

APPENDIX F

METHOD FOR ESTIMATING PYROLYSIS PRODUCT COMPOSITION

Estimating the Pyrolysis Composition for a 40 Percent by Weight Nylon, 60 Percent by Weight Phenolic Resin

The most direct method of determining the products of degradation is the analysis by pyrolysis gas chromatography. This has been done by Sykes (1, 2) in which the hot degradation products were injected directly into the gas chromatograph. However, even with this procedure certain amount of condensation of heavy molecular weight species occur which remain unidentified and a possible source of error. The method has, however, reduced the total amount of unidentified material. Sykes has reported typical pyrolysis gas compositions for eighty-three percent of the total decomposition products evolved during the thermal degradation of nylon-phenolic resin composites (1, 2). The remaining seventeen percent was reported as an unidentified dark, tarry substance. This data is presented in Table F-1. The data of Friedman (5) for phenolic resin is presented in Table F-2 and there are fifteen percent unidentified materials. In addition, the data of Friedman (5) for nylon phenolic resin is presented in Table F-3. April (3) estimated a pyrolysis gas composition for his experimental work,

TABLE F-1: Pyrolysis product composition resulting from the degradation of a 40 percent nylon, 60 percent by weight phenolic resin, as reported by Sykes (2).

SPECIES	MASS FRACTION
Phenol	0.118
Methylphenol	0.064
Dimethylphenol	0.051
Trimethylphenol	0.041
Benzene	0.003
Toluene	0.001
Cyclopentanone	0.029
Hydrogen	0.010
Methane	0.010
Carbon Monoxide	0.021
Carbon Dioxide	0.067
Water	0.062
Ammonia	0.002
Unidentified	0.173
Carbon Residue	0.340

TABLE F-3: Pyrolysis product composition resulting from the degradation of nylon phenolic resin, as reported by Friedman (5).

SPECIES:	MASS FRACTION
Hydrogen	0.011
Methane	0.015
Ammonia	0.016
Water	0.064
Acetylene	0.066
Hydrogen Cyanide	0.022
Carbon Monoxide	0.071
Nitrogen	0.001
Ethylene	0.091
Ethane	0.001
Carbon Dioxide	0.023
Diacetylene	0.011
Acetone	0.010
Benzene	0.016
Toluene	0.011
Xylene	0.007
Isopropanol	0.018
Propane	0.015
Carbon Residue	0.529

TABLE F-2 Pyrolysis product composition resulting from the degradation of phenolic resin, as reported by Friedman (5).

SPECIES	MASS FRACTION
Carbon Dioxide	0.019
Carbon Monoxide	0.042
Benzene	0.004
Toluene	0.009
Phenol	0.181
Methylphenol	0.060
Methane	0.043
Water	0.114
Hydrogen	0.027
Unidentified	0.150
Carbon Residue	0.350

based on a comparison of the experimental and calculated heat of pyrolysis. His approach was, knowing the heat of pyrolysis, or heat of degradation, the heat of formation of these species and the reported analytically determined composition, estimate a new composition in such a way that the experimental and calculated values of the heat of pyrolysis agree within a few percent. His results are shown in Table F-4.

Since the compositions reported by Sykes (1, 2) and Friedman (5) have unidentified products and since the composition of April (3) does not agree with the elemental balance, a new composition based on the elemental balance constraints was arrived at in this research. The elemental composition for a 40 percent nylon, 60 percent by weight phenolic resin is shown in Table F-5. It is shown that for every 100 grams of polymer there are 73.80 grams of carbon, 7.36 grams of hydrogen, 3.95 grams of nytrogen and 14.89 grams of oxygen. The procedure is then to distribute the gram of these elements to each of the identified species in such a way that the elemental balance requirements are satisfied. A more detailed presentation is given by Hacker, et. al. (6).

Distribution of Oxygen Element

To accomplish the distribution of the oxygen element, an initial estimate based on the data of Table F-2 through Table F-4 is used. Table F-6 shows the initial estimate

TABLE F-4: Estimated pyrolysis gas composition of April (3).

SPECIES	MASS FRACTION
Hydrogen	0.036
Water	0.478
Methane	0.058
Phenol	0.241
Carbon Monoxide	0.057
Dimethylphenol	0.087
Carbon Dioxide	0.025
Toluene	0.012
Benzene	0.006

TABLE F-5: Elemental composition of a 40 percent nylon, 60 percent by weight phenolic resin composite.

ELEMENT	MOLES ELEMENT / MOLE OF POLYMER	MASS ELEMENT / 100 GRAMS OF POLYMER
C	8.19	73.80
H	9.87	7.36
N	0.376	3.95
O	1.240	14.89

TABLE F-6: Initial and final estimates of the composition of the oxygen containing species.

	INITIAL ESTIMATE (%)	FINAL ESTIMATE (%)
Phenol	25	23.13
Water	7.5	7.20
Carbon Dioxide	5	4.61
Carbon Monoxide	5	4.66

and the adjusted final estimate which satisfies the elemental balance on oxygen. The dimethyl phenol, and trimethyl phenol were lumped into phenol for lack of thermodynamic data on these species. The total number of grams distributed among these species is 14.89.

Distribution of Hydrogen

The number of grams of hydrogen to be distributed among the hydrogen containing species is 7.36. However, only 4.80 grams are available since 2.86 grams were already distributed in phenol and water. The results of this distribution is shown in Table F-7.

Distribution of Nitrogen

The only nitrogen containing species is Nitrogen (N_2) and the grams are 3.95 as shown in Table F-5.

Distribution of Carbon

The total grams of carbon available is 73.80. Of these, 34.50 have been distributed among some of the oxygen and hydrogen containing species, which are also carbon containing species. Hence, this leaves 39.30 grams of carbon which are to be assigned to the carbon species. The composition of all the species is presented in Table F-8.

TABLE F-7: Initial and final estimate of the composition of the hydrogen containing species.

	INITIAL ESTIMATE (%)	FINAL ESTIMATE (%)
Methane	3	3.87
Acetylene	3	3.89
Ethylene	3	3.89
Ethane	0.5	0.65
Benzene	2	2.58
Hydrogen	2	2.58

TABLE F-8: Estimate of the representative composition of the pyrolysis products for a 40 percent nylon, 60 percent by weight phenolic resin ablative composite.

Species	Mass Percent	Mole Percent
H_2	2.57	20.92
CH_4	3.86	3.90
C_2H_2	3.88	2.41
C_2H_4	3.88	2.24
C_2H_6	0.64	.35
C_6H_6	2.57	.53
C_6H_6OH	23.10	3.97
CO	4.65	2.40
CO_2	4.60	1.69
H_2O	7.29	6.45
N_2	3.95	2.20
C(solid)	39.01	52.94

Element	Elemental Composition (mass percent)
C	73.80
H	7.36
O	3.95
N	14.89
Total	100.00

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APPENDIX G

RESTRICTIVE EQUILIBRIUM ANALYSIS

In Chapter IV the equations for the chemical equilibrium analysis were developed. The analysis developed in Chapter IV consists of finding the equilibrium composition of a multicomponent, polyphase system by minimizing the free energy.

In reference (1) a method developed by del Valle and Pike was proposed whereby a restricted equilibrium state is defined. This equilibrium state is defined by adding to the free energy minimization algorithm an additional constraint; this constraint is in the nature of an energy balance constraint.

This constraint adds one extra equation to the free energy minimization technique. This technique was implemented at the suggestion of Swann from NASA (2). The reason for his suggestion was that at low temperatures the equilibrium composition of the degradation products of nylon-phenolic resins are not in agreement with experimentally determined values. In trying to improve the agreement the approach briefly described in this appendix was proposed. Therefore, it was developed for heuristic reasons and not for its theoretical value.

Heat Balance Constraint

The heat of pyrolysis of a degrading plastic can be

computed using the following equation (3):

$$\Delta H_{pyr} = \sum_{i=1}^{q} \{x_{p,i} \Delta H_{f,i} + \int_{298\ K}^{T_p} x_{p,i} C_{p,i}\, dT\} -$$

$$\sum_{j=1}^{l} \{x_{r,j} \Delta H_{f,j} + \int_{298^oK}^{T_p} x_{r,j} C_{p,j}\, dT\} \qquad \text{(G-1)}$$

where the subscript p and r denote products and reactants respectively, q the total number of species present in the pyrolysis products and l the total number of components in the ablative composite. For nylon-phenolic resin composites, the temperature, T_r, where the degradation starts, is approximately 300°C, and the final temperature is approximately 1000°C. Pyrolysis products are generated over this temperature range and T_p is the appropriate average temperature which gives the correct energy associated with the pyrolysis products. It was determined to be 700°C as a weighted average based on the mass loss rate (3). Rearranging Equation G-1 gives,

$$\Delta H_{pyr} + \sum_{j=1}^{l} \{H_{r,j} \Delta H_{f,j} + \int_{298^oK}^{T_r} x_{r,j} C_{p,j}\, dT\} =$$

$$- \sum_{i=1}^{q} \{x_{p,i} \Delta H_{j,i} + \int_{298^oK}^{T_p} x_{p,i} C_{p,i}\, dT\} \qquad \text{(G-2)}$$

The left hand side of Equation (G-2) is known from experimentally determined values. Lets define b_{m+1} as the left hand side, and let's drop the subscript p on the X's since we are going to deal only with the products.

$$b_{m+1} = \sum_{i=1}^{q} \{ x_i \ \Delta H_{f,i} + \int_{298^oK}^{T_p} x_i \ C_{p,i} \ dT\} \qquad \text{(G-3)}$$

Notice that the X_i's are unknown. However, the right hand side of the equation which is unknown must satisfy the left hand side which is known. Equation (G-3) can be expanded to the form below:

$$b_{m+1} = \sum_{i=1}^{n} \{x_i \ \Delta H_{f,i} + \int_{298^oK}^{T_p} x_i \ C_{p,i} \ dT\} +$$

$$\sum_{i=n+1}^{1} \{x_i \ \Delta H_{j,i} + \int_{298^oK}^{T_p} x_i \ C_{p,i} \ dT\} \qquad \text{(G-4)}$$

Note that Equation (G-4) has been written in the same form as the material balance expression shown in Equation (4-1). This simplified considerably the final form of the equations to be solved.

In addition, define H_i as:

$$H_i = \Delta H_{f,i} + \int_{298^oK}^{T_p} C_{p,i} \ dT$$

This is done to avoid carrying the integral term in the derivation; and the resulting equation is:

$$b_{m+1} = \sum_{i=1}^{n} H_i x_i + \sum_{i=n+1}^{1} H_i x_i \qquad \text{(G-5)}$$

Lagrange Multiplier Formulation and Minimization

To form the augmented function, the additional constraint, Equation (G-5) is added to Equation (4-25) and this results:

$$G(X) = Q(X) + \sum_{j=1}^{m} \P_j \left(b_j - \sum_{i=1}^{1} a_{ij}\, x_i\right) +$$

$$\P_{m+1} \left(b_{m+1} - \sum_{i=1}^{1} x_i\, H_i\right)$$

Following a similar procedure to that developed in Chapter IV the resulting set of equations to be solved is as follows:

$$\sum_{j=1}^{m} r_{jk}\, \P_j + b_k' u + \sum_{i=n+1}^{1} a_{ij} x_i = b_k + \sum_{i=1}^{n} a_{ik}\, f_i(Y)$$

$$k=1 \ldots m \qquad \text{(G-7)}$$

$$\sum_{j=1}^{m} r_{jk}\, \P_j + b_k' u + \sum_{i=n+1}^{1} a_{ij} x_i = b_k + \sum_{i=1}^{n} a_{ik}\, f_i(Y)$$

$$k = m+1 \qquad \text{(G-8)}$$

$$\sum_{j=1}^{m+1} b_j \P_j = \sum_{i=1}^{n} f_i(Y) \qquad \text{(G-9)}$$

$$\sum_{j=1}^{m+1} a_{ij} \P_j = \left\{\frac{F^o}{RT}\right\}_i \qquad i=n+1\ldots 1 \qquad \text{(G-10)}$$

It should be noted that Equations (G-7) and (G-8) have the same form. However, they are shown to emphasize the difference between the a_{ik}'s. The a_{ik}'s for $k \leq m$ are the formula numbers as defined in Chapter IV. But $a_{i,m+1} = H_i$.

Comparison of Results Among Equilibrium, Restricted Equilibrium Analysis and Experimental Results

The chemical composition of the pyrolysis products resulting from the degradation of a 40 percent nylon, 60 percent phenolic resin ablative composite and computed by a restricted equilibrium analysis is presented in this section. The computations have been done for two decomposition temperatures because of the uncertainty involved in the properties to calculate the average temperatures. In addition two different energy constraints were used because of uncertainties in the heat of pyrolysis. The assumed average temperatures were 600° and 700°C and the energy constraints were -17,000 and -29,000 calories/gram-mole of polymer which correspond to -228 and -390 BTU/lb of composite. The results are presented in Table G-1 and Table G-2.

In Table G-1 a comparison of restrictive equilibrium with the experimental data of Sykes (4, 5) is given for two

TABLE G-1: Comparison of Restricted Equilibrium Analysis Compositions with the Experimental Data of Sykes (4,5) for a 40% Nylon, 60% Phenolic Resin Composite at a Temperature of 700°C and .1 atm.

Species	Restricted Equilibrium Mass Fraction for H = -29,999 cal/mole of polymer	Restricted Equilibrium Mass Fraction for H =-17,000 cal/mole of polymer	Experimental Mass Fraction
Phenol	10^{-13}	10^{-13}	0.118
Methyl Phenol	-	-	0.064
Dimethyl Phenol	-	-	0.051
Trimethyl Phenol	-	-	0.041
Benzene	10^{-17}	10^{-17}	0.003
Toluene	10^{-13}	10^{-13}	0.001
Cyclopentanone	-	-	0.029
Methane	0.025	0.024	0.010
Hydrogen	0.065	0.066	0.010
Carbon Monoxide	0.205	0.210	0.021
Carbon Dioxide	0.014	0.012	0.067
Water	0.021	0.019	0.062
NH_3	10^{-4}	10^{-4}	0.002
N_2	0.039	0.038	-
Unidentified	-	-	0.181
Carbon	0.631	0.630	0.350

energy constraints (H = -17,000 and -29,000 cal/mole of polymer) at a temperature of 700°C. The results show an order of magnitude agreement with the low molecular weight species identified by Sykes (4, 5). These are methane, hydrogen, carbon monoxide, carbon dioxide, water and ammonia. The agreement with the high molecular weight species, phenol, toluene, benzine, etc., was rather poor. The change in the energy constraint, H, from -17,000 to -29,000 cal/mole of polymer has different and opposite effects in several of the species. For example, an increase in the value of H had the effect of decreasing the amount of hydrogen, carbon and carbon monoxide, while increasing the concentrations of carbon dioxide and water. It should be noted that the mass fraction of unidentified species plus that of carbon makes up 0.521 of the total mass fraction of the experimental composition, while the restricted equilibrium predicts a mass fraction of 0.634 carbon. It should be further noticed that the mass of nitrogen makes up about four percent of the mixture. No nitrogen was reported in the experimental results (4, 5).

In Table G-2 a similar comparison is made, but the decomposition zone temperature is taken to be 600°C. Again an order of magnitude agreement is observed among the composition of the lower molecular weight species. Changing H affects the composition in the same fashion as was for the 700°C case.

TABLE G-2: Comparison of Restricted Equilibrium Analysis Compositions with the Experimental Data of Sykes (4,5) for a 40% Nylon, 60% Phenolic Resin Composite at a Temperature of 600°C and .1 atm.

Species	Restricted Equilibrium Mass Fraction for H = -29,000 cal/mole of polymer	Restricted Equilibrium Mass Fraction for H = -17,000 cal/mole of polymer	Experimental Mass Fraction
Phenol	10^{-13}	10^{-13}	0.118
Methyl Phenol	-	-	0.064
Dimethyl Phenol	-	-	0.051
Trimethyl Phenol	10^{-13}	10^{-13}	0.041
Benzene	10^{-13}	10^{-13}	0.003
Toluene	10^{-13}	10^{-13}	0.001
Cyclopentanone	-	-	0.029
Methane	0.039	0.036	0.010
Hydrogen	0.060	0.061	0.010
Carbon	0.160	0.167	0.021
Carbon Dioxide	0.027	0.024	0.067
Water	0.038	0.036	0.062
NH_3	10^{-4}	10^{-4}	0.002
N_2	.040	.040	-
Unidentified	-	-	0.181
Carbon	0.635	0.635	0.340
TOTAL	1.000	1.000	1.000

In general, restricted equilibrium provided an order of magnitude agreement for the composition of low molecular weight compound. It failed to give any agreement with the higher molecular weight component.

In table G-3 a comparison of restricted equilibrium with the general equilibrium analysis is given. It is shown that the compositions are within an order of magnitude of each other. The only mass fraction that is the same is that of nitrogen, since it is practically an inert, and that of carbon which agrees within one percent.

TABLE G-3: Comparison of Restricted Equilibrium Analysis With the General Equilibrium Analysis for a 40% Nylon, 60% Phenolic Resin Composite at 700°C and 1 atmosphere.

Species	Restricted Equilibrium Mass Fraction for H = -29,000 cal/mole of polymer	Equilibrium Composition
Phenol	10^{-13}	10^{-18}
Benzene	10^{-17}	10^{-13}
Toluene	10^{-13}	10^{-13}
Methane	0.025	0.043
Hydrogen	0.065	0.059
Carbon Monoxide	0.205	0.150
Carbon Dioxide	0.014	0.031
Water	0.021	0.043
NH_3	10^{-4}	10^{-4}
N_2	0.039	0.039
C	0.631	0.636

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1. del Valle, E. G., and R. W. Pike, "Computation of the Equilibrium Composition of Reacting Gas-Solid Mixtures with Material and Energy Balance Constraints", NASA RFL-10, NGR-19-001-016 and NGR-19-001-059 (March 1, 1979).

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APPENDIX H

EQUILIBRIUM CONVERSIONS OF CARBON-HYDROGEN-OXYGEN-NITROGEN REACTIONS

This appendix presents the equilibrium conversions at temperatures between 500°K and 3000°K for 100 chemical reactions in the C-H-O-N system.

The results presented in this appendix were used as a tool to help select the reactions of importance for the kinetics model. This is by no means an exhaustive search but it is indeed an extensive one.

Sources of these reactions were too many and varied to list them all. However, there were several sources that were extensive surveys of chemical reactions. One was a very specialized survey done by Pike (1) covering possible reactions resulting from the decomposition product of charring ablators. Another was an extensive Bibliography by Hockstein (2), and finally the work of Bahn (3). Bahn had a massive compendium of several hundred chemical reactions in the C-O-N system. Many of Bahn reactions were not analyzed because of the lack of available thermodynamic data.

The C-H-O-N system was divided into eight categories. These are carbon-hydrogen, carbon-oxygen, nitrogen-oxygen, hydrogen-oxygen, carbon-hydrogen-oxygen, carbon-hydrogen-nitrogen, hydrogen-nitrogen-oxygen and carbon-nitrogen-oxygen reactions.

A total of 47 reactions for the carbon-hydrogen reac-

tions are presented in Table H-1 with hydrocarbon reactions with up to four carbon atoms. Benzene and phenol reactions were not considered because the reactions for these components had already been selected and the kinetic data available was rather minimal.

Table H-2 presents seven carbon-oxygen reactions. Table H-3 lists 18 reactions in the nitrogen-oxygen system, except the last reaction in the table which is nitrogen dissociation. As can be seen, N_2 is a pretty stable component even at the very high temperature of 3000°K. The same can be said about the dissociation of CO (reaction 5 in Table H-2).

Table H-4 is a compendium of 11 hydrogen-oxygen reactions. In contrast to the reactions of Tables H-1 through H-3, every reaction in this table has an equilibrium conversion greater than zero at 3000°K. It is interesting to note that reactions 1 and 3 have practically the same equilibrium conversion, at leat to the number of significant digits shown; reaction 4 shows a very similar equilibrium conversion behavior as Equations 1 and 3. Reactions 9, 10, and 11 show the dissociation of hydroxyl radical, hydrogen and oxygen molecules respectively. As can be seen from the tabulation of the equilibrium conversion, there is no significant dissociation of these components until they reach a temperature of 3000°K.

Table H-5 lists 10 carbon-hydrogen-oxygen reactions. Except for the methylene radical reaction with CO, all other

TABLE H-1: EQUILIBRIUM CONVENSION AT FOUR TEMPERATURES FOR CARBON-HYDROGEN REACTIONS

	Equilibrium Conversion			
	500°K	1000°K	2000°K	3000°K
1. $CH_4 = CH_3 + H$	0.	0.	0.94	48.01
2. $CH_4 = 1/2C_2H_6 + 1/2H_2$	0.	2.83	19.56	33.11
3. $CH_4 = 1/2C_2H_4 + H_2$	0.	5.05	91.27	98.71
4. $CH_4 = 1/2C_2H_2 + 3/2H_2$	0.	1.71	99.05	100.0
5. $CH_4 = CH_2 + H_2$	0.	0.	7.39	94.42
6. $CH_4 = C_{(s)} + 2H_2$	3.0	84.77	99.92	100.00
7. $CH_3 = CH_2 + H$	0.	0.	1.27	49.37
8. $CH_2 = CH + H$	0.	0.	0.3	8.63
9. $CH = C_{(g)} + H$	0.	0.	1.58	47.46
10. $CH = C_{(s)} + H$	100.0	100.0	100.0	100.0

TABLE H-1: EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES FOR CARBON-HYDROGEN REACTIONS (CONTINUED)

		Equilibrium Conversion(5)			
		500°K	1000°K	2000°K	3000°K
11.	$C_2H_6 = 2CH_3$	0.	0.	22.03	100.0
12.	$C_2H_6 = C_2H_4 + H_2$	0.	50.52	99.99	100.0
13.	$C_2H_6 = CH_4 + 1/2C_2H_4$	53.62	98.63	99.87	100.0
14.	$C_2H_6 = CH_2 + CH_4$	0.	0.01	52.51	99.52
15.	$C_2H_4 = C_2H_2 + H_2$	0.	4.51	99.77	100.0
16.	$C_2H_4 = 2C + 2H_2$	100.0	100.0	100.0	100.0
17.	$C_2H_2 = 2C + H_2$	100.0	100.0	99.96	99.21
18.	$C_2H_2 = C_2H + H$	0.0	0.0	0.15	18.75
19.	$C_2H = C_2 + H$	0.0	0.0	0.01	1.56
20.	$C_2H_3 = C_2H_2 + H$	0.0	1.29	96.07	100.0

TABLE H-1 : EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES FOR CARBON-HYDROGEN REACTIONS (CONTINUED)

	Equilibrium Conversion			
	500°K	1000°K	2000°K	3000°K
21. $C_3H_6 = C_2H_3 + CH_3$	0.	0.	11.37	98.31
22. $C_3H_6 = C_3H_5 + H$	0.	0.	72.37	100.0
23. $C_3H_5 = C_3H_4 + H$	0.	0.	2.07	30.88
24. $C_3H_4 = 3C + 2H_2$	100.0	100.0	100.0	100.0
25. $C_3H_8 = C_3H_6 + H_2$	0.01	87.15	100.0	100.0
26. $C_3H_8 = CH_4 + C_2H_4$	19.61	99.90	100.0	100.0
27. $C_6H_6 = 3C_2H_2$	0.	0.	99.48	100.0
28. $C_3H_6 + CH_3 = CH_4 + C_3H_5$	0.01	0.04	0.87	2.30
29. $CH_4 + C_4H_5 = CH_3 + C_4H_6$	0.0	0.42	5.69	12.66
30. $C_2H_4 + CH_4 = C_3H_6 + H_2$	0.38	6.63	24.34	25.27

TABLE H-1 : EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES FOR CARBON-HYDROGEN REACTIONS (CONTINUED)

	Equilibrium Conversion			
	500°K	1000°K	2000°K	3000°K
31. $CH_3 + H_2 = CH_4 + H$	13.37	13.61	14.73	16.50
32. $CH_2 + H = CH + H_2$	0.	1.54	18.69	35.24
33. $C_{(g)} + H_2 = CH + H$	0.	0.58	9.27	22.56
34. $C_{(s)} + H_2 = CH + H$	0.	0.	0.	0.20
35. $CH + C_{(s)} = C_2 + H$	0.	0.01	3.80	16.77
36. $C_2 + H = CH + C_{(g)}$	0.	0.	0.15	1.81
37. $C_2H + H = C_2 + H$	0.	0.11	2.91	9.02
38. $C_2H_2 + H_2 = C_2H_3 + H$	0.	0.	0.04	0.75
39. $C_2H_2 + H = C_2H + H_2$	1.90	22.33	47.83	54.87
40. $C_2H_3 + CH_4 = C_2H_4 + CH_3$	33.37	33.38	33.55	45.55

TABLE H-1 : EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES FOR CARBON-HYDROGEN REACTIONS (CONTINUED)

	Equilibrium Conversion			
	500°K	1000°K	2000°K	3000°K
41. $C_3H_5 + H_2 = C_3H_6 + H$	0.	0.	0.2	0.52
42. $I\text{-}C_4H_8 = 2C_2H_4$	0.29	93.90	100.0	100.0
43. $N\text{-}C_4H_{10} = C_3H_6 + CH_4$	69.67	100.0	100.0	100.0
44. $N\text{-}C_4H_{10} = 2C_4H_4 + H_2$	0.01	99.27	100.0	100.0
45. $N\text{-}C_4H_{10} = C_2H_6 + C_2H_4$	5.13	99.72	100.0	100.0
46. $I\text{-}C_4H_{10} = C_3H_6 + CH_4$	60.90	100.0	100.0	100.0

TABLE H-2 : EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES FOR THE CARBON-OXYGEN REACTIONS

	Equilibrium Conversion			
	500°K	1000°K	2000°K	3000°K
1. $C_{(g)} + O_2 = CO_2$	100.	100.	100.	100.
2. $C_{(g)} + 1/2O_2 = CO$	100.	100.	100.	100.
3. $CO_2 = CO + O$	0.	0.	0.	19.0
4. $C_{(s)} + CO_2 = 2CO$	0.	54.96	100.0	100.0
5. $CO = C_{(g)} + O$	0.	0.	0.	0.
6. $CO_2 = C_{(g)} + 2O$	0.	0.	0.	0.
7. $CO_2 + O = CO + O_2$	8.32	39.36	59.44	63.14

TABLE H-3 : EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES FOR THE NITROGEN-OXYGEN REACTIONS

		Equilibrium Conversion(%)			
		500°K	1000°K	2000°K	3000°K
1.	$NO = N + O$	0.	0.	0.	0.04
2.	$N_2 + O_2 = 2NO$	0.	0.	0.98	5.73
3.	$2NO = N_2O + O$	0.	0.	0.03	1.50
4.	$2NO_2 = 2NO + O_2$	4.91	93.99	99.79	100.0
5.	$N_2O = N_2 + O$	0.	14.55	99.91	100.0
6.	$NO_2 = NO + O$	0.	0.	39.26	99.47
7.	$N_2O = NO + N$	0.	0.	3.81	100.0
8.	$NO + O_2 = NO_2 + O$	0.	0.	0.02	1.18
9.	$NO + N = N_2 + O$	0.	0.	0.01	0.4
10.	$2NO = NO_2 + N$	0.	0.	0.	0.

TABLE H-3 : EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES FOR NITROGEN-OXYGEN REACTIONS (CONTINUED)

	Equilibrium Conversion			
	500°K	1000°K	2000°K	3000°K
11. $NO_2 + N_2 = NO + N_2O$	0.	0.04	1.88	7.62
12. $N_2 + O = 2N + 1/2O_2$	0.	0.	0.	0.
13. $N_2 + O_2 = NO_2 + N$	0.	0.	0.	0.
14. $NO + O = N + O_2$	0.	0.	0.00	3.7
15. $N_2 + O_2 + N_2O + O$	0.	0.	0.	0.01
16. $NO + N_2 = N_2O + N$	0.	0.	0.	0.
17. $N_2O + O_2 = 2NO + O$	0.	0.	0.	0.
18. $N_2 = 2N$	0.	0.	0.	0.

TABLE H-4 : EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES FOR THE HYDROGEN-OXYGEN REACTIONS

	Equilibrium Conversion(%)			
	500°K	1000°K	2000°K	3000°K
1. $H_2O = OH + H$	0.01	2.20	15.94	27.33
2. $H_2O = O + H_2$	0.	0.	0.	7.19
3. $H_2O + O = 2OH$	0.	2.20	15.94	27.33
4. $H_2 + O_2 = 2OH$	0.03	2.26	16.79	27.93
5. $O + H_2 = OH + H$	37.06	48.31	54.25	56.29
6. $O + OH = H_2 + OH$	100.0	100.0	100.0	97.1
7. $H_2O + H = H_2 + OH$	0.37	4.57	24.26	36.87
8. $H + O_2 = OH + O$	0.18	6.11	32.73	47.96
9. $OH = O + H$	0.	0.	0.17	12.11
10. $H_2 = 2H$	0.	0.	0.01	7.82
11. $O_2 = 2O$	0.	0.	0.	5.71

TABLE H-5: EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES FOR THE CARBON-HYDROGEN-OXYGEN REACTIONS

		Equilibrium Conversion			
		500°K	1000°K	2000°K	3000°K
1.	$CO_2 + H = CO + OH$	0.	3.86	40.53	61.22
2.	$CH_3 + O_2 = CH + 2OH$	0.	0.	2.24	65.59
3.	$CO_2 + H_2 = CO + H_2O$	7.86	45.49	68.12	73.00
4.	$CH_2 + CO = C_2H_2 + O$	0.	0.	0.02	0.23
5.	$C_2H + H_2O = C_2H_2 + OH$	5.05	14.33	25.88	32.44
6.	$C_2H_3 + H_2O = C_2H_4 + OH$	0.01	1.35	7.49	13.66
7.	$CH_2 + O = CO + H_2$	100.	100.	100.	100.
8.	$CH_4 + O = CH_3 + OH$	79.23	95.59	100.	100.
9.	$CH_3 + H_2O = CH_4 + OH$	0.	0.71	5.24	10.36
10.	$C + H_2O = CO + H_2$	0.	84.45	100.0	100.0

reactions show a measurable degree of conversion.

Table H-6, the last table of this appendix, is a compendium of carbon-hydrogen-oxygen, hydrogen-nitrogen-oxygen and carbon-nitrogen-oxygen reactions. A total of 8 reactions are presented in this table.

TABLE H-6 : EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES FOR THE CARBON-HYDROGEN-NITROGEN, HYDROGEN-NITROGEN-OXYGEN AND CARBON-NITROGEN-OXYGEN REACTIONS

	Equilibrium Conversion			
	500°K	1000°K	2000°K	3000°K
1. $C + 1/2N_2 = C_2N_2$	0.	0.	0.	0.01
2. $HCN = H + CN$	0.	0.	0.	9.59
3. $NH_3 + C = HCN + H_2$	0.	12.12	99.92	100.0
4. $NH_3 = 1/2N_2 + 3/2H_2$	83.26	99.96	100.0	100.0
5. $N_2 + OH = N_2O + H$	0.	0.	0.0	0.1
6. $NO + OH = NO_2 + H$	0.	0.	0.36	1.20
7. $NO + CO_2 = NO_2 + CO$	0.	0.	0.21	1.88
8. $NO + CO = CO_2 + N$	0.	0.	0.06	1.86

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VITA

Eduardo Gonzalez del Valle was born in [redacted], on [redacted]. He completed his primary and secondary education at the Jesuit run, Colegio de Belen, where he graduated June 16, 1960. Because of the communist take-over of Cuba, he was forced to leave his native country for the U. S. A. In the summer of 1960 he became Junior Counselor at Kingswood Camp, located in Pike, New Hampshire, which he had attended as a summer camper since 1956. The following year he became a Senior Counselor and was appointed instructor of swimming, boating and canoeing.

From September 1960 to June 1962, he attended Villanova University where he won for two consecutive years the Johnson Foundation Scholarship Award. Because of the family's financial difficulties, he moved to Miami where his parents lived. There he enrolled at the University of Miami for the school year 1962-1963, while working parttime. There he was awarded a diploma for "Outstanding Academic Achievement". In September 1963 he transferred to Louisiana State University where he received his Bachelor of Science Degree in Chemical Engineering in June 1965.

In his senior year, he received the Monsanto Chemical Company Scholarship Award.

As an undergraduate he was Editor of a Spanish news-paper called "Liborito". Also member and later Chairman of

a subcommittee of the Student Government Association. He became a member of the following honorary societies: Tau Beta Pi and Phi Kappa Phi.

On June 12, 1965, he married the former Margarita [redacted]. They have three children.

After graduation in 1965, he went to work for Kaiser Aluminum in Baton Rouge. The following year he started full time graduate work at LSU in February, 1966, and left in February, 1970. While in Graduate School he became member of the following honorary societies: Phi Lambda Upsilum and Sigma Xi.

In March 1970, he joined the Mathematics, Computer and Systems Department of Exxon Corporation in Florham Park, New Jersey. In August, 1973, he was transferred by Exxon to its refinery in Aruba, Netherlands Antilles, where he presently resides.

With his Dissertation, he will have a total of 24 publications.

EXAMINATION AND THESIS REPORT

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Title of Thesis: In Depth Response of Ablative Composites

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Date of Examination:

April 26, 1974