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STUDY ON OXIDES OF NITROGEN AND CARBON FORMATION IN DIESEL ENGINES - COMPUTER PROGRAM USER'S MANUAL

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NOMENCLATURE

C_p	Specific heat
D	Gas binary diffusivity
P	Pressure
R	Gas constant
T	Temperature
U	Specific internal energy
erf	Error function
ϕ	Equivalence ratio based on fuel-air mass ratio
θ	Crank angle
ρ	Density

I. INTRODUCTION

This document describes the computer program and serves as a user's manual for a numerical model on THE PREDICTION OF POLLUTANT FORMATION IN DIESEL ENGINES. The model is capable of predicting both engine performance and formation of nitric oxide and soot in a direct injected diesel engine combustion process. The program is sufficiently versatile to investigate the influence of several engine parameters, such as geometry, injection timing, compression ratio, load, swirl, etc., and thus can be considered as a tool readily accessible to the design engineers. The physical and chemical processes, the detailed mathematical analysis and the assumptions upon which the model is based are discussed in the full report on this investigation. This manual contains brief descriptions of the program subroutines, program input and output. One sample case is also given to illustrate the use of the program which is designed to facilitate program check-out.

The computer program is coded in standard FORTRAN IV, and a version is currently operational in CDC 6600 computer.

II. PROGRAM DESCRIPTIONS

The main body of the program is the routine MAIN which simulates the cycle thermodynamics of a reciprocating engine and also manipulates the major input output mechanisms of the program. The cycle thermodynamic routine is used as the skeleton and the model components, coded as separated subroutines, are linked together by CALL statements, thus forming the complete program. The flow chart is shown in Figure 1.

A brief description of the subroutines included in the program are given below.

SUBROUTINE AMIX

This subroutine estimates the rate of mixing between the "air" zone and the burning zones.

BLOCK DATA

This subroutine presents the coefficients for both the internal energy polynomial, $U(P, T, \phi)$, and the gas constant polynomial, $R(P, T, \phi)$, for lean ($\phi \leq 1.0$) and rich ($\phi > 1.0$) equilibrium combustion products. The coefficients are obtained for a specific fuel by curve-fitting the calculated results from the NASA equilibrium program (Ref. 2).

SUBROUTINE CONHT

The gross rate of convective heat transfer from the entire charge within the cylinder to the cylinder walls is computed in this subroutine. The calculation is based upon the mean charge temperature and the characteristic charge Reynolds No.

FUNCTION ERF

This subroutine estimates the error function of a given argument x, i.e.,

$$\mathrm{erf}\,(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-r^2}\, dr$$

SUBROUTINE EVAP

The model requires that the premixed air-fuel packages are tracked throughout their lifetime and this operation is handled in the subroutine EVAP. The vaporization rate of each droplet size groups and the air-fuel vapor ratio of each package are defined in Lagrangian coordinates. The onset of ignition in each air-fuel package is also monitored.

SUBROUTINE FINJN

The rate of fuel injection is calculated by calling this subroutine.

SUBROUTINE FLAMEZ

This subroutine computes quasi-steady flame structure by constructing the diffusion field around a confined burning droplet with finite space. Flame temperatures, flame zone thickness, fuel, O_2 and temperature distributions are determined. Subroutine HETNOR is called in FLAMEZ to calculate the production rate for nitric oxide during droplet burning. The nitric oxide produced during droplet burning forms the heterogeneous contribution to the total emission.

SUBROUTINE HETNOR

The nitric oxide formation rate within the flame structure defined by FLAME is determined in this subroutine by integrating the finite-rate NO conservation equation. This two-point boundary value problem is solved by a trial and error method. An initial guess of the NO concentration at the droplet surface is made. The NO production equations which are based on the Zeldovich mechanism are integrated and the calculated NO concentration at the end points is checked with the given value at the end point.

SUBROUTINE HOMNOZ (HOMNOR)

The homogeneous contribution to the total amount of NO produced (which was not included in HETNOR) at the zonal NO formation rate is determined by this subroutine. The Zeldovich chemical kinetic mechanism is also used as the basis for the calculation of the homogeneous NO formation. Subroutine HOMNOR is used for that of the "air" zone.

SUBROUTINE RADHZZ (RADHZ)

This subroutine evaluates the zonal rate of radiative heat transfer. Subroutine RADHZ is used for that of the "air" zone.

SUBROUTINE SIZED

This subroutine determines the drop-size distribution of the fuel jet by an upper-limit distribution function based upon the Weber number and the Reynolds number of the jet.

SUBROUTINE SOOTRZ(SOOTR)

This subroutine calculates the zonal soot formation rate both prior to and after ignition. It also determines the soot oxidation rate based upon the zonal pressure, temperature and equivalence ratio. Subroutine SOOTR is used for that of the "air" zone.

SUBROUTINE SPECYZ (SPECY)

Zonal equilibrium species distribution is obtained via table look up for specified independent variables P, T, and φ. Subroutine TRIPIT is called to perform the three-dimensional linear interpolation. An error message will be printed out whenever any independent variable lies outside the range of the table. Subroutine SPECY is used for that of the "air" zone.

SUBROUTINE SPRAY

This subroutine calls subroutine SIZED to determine the drop-size distribution of the fuel spray. The fuel jet is simulated by a steady jet (free and wall jets) theory. Therefore, the trajectories and over-all air-fuel ratios of fuel elements are defined in Eulerian spatial coordinates.

SUBROUTINE TAPEIN

This subroutine is called at the very beginning of MAIN to the input species distribution tables from TAPE 8.

SUBROUTINE TPROPZ (TPROP)

This is a subroutine to evaluate the thermodynamic properties of the equilibrium combustion products. The internal energy and gas constant (R) are calculated as functions of P, T, and ψ by polynomial. Expressions and coefficients of these polynomials are specified in DATA BLOCK. The partial derivatives (of U and R) with respect to P, T, and ϕ, are also computed in subroutine TPROPZ. Subroutine TPROP is used to evaluate the thermodynamic properties of the "air" zone.

SUBROUTINE TRIPIT

Subroutine TRIPIT is a three-dimensional linear interpolation routine called for in subroutines SPECY and SPECYZ.

SUBROUTINE VOLM

This subroutine gives the instantaneous volume of engine cylinder.

SUBROUTINE WETBT

This subroutine estimates wet-bulb temperature of a vaporizing fuel drop at high ambient pressures and temperatures. The Cox-Antonie equation is used to evaluate the equilibrium partial vapor pressure.

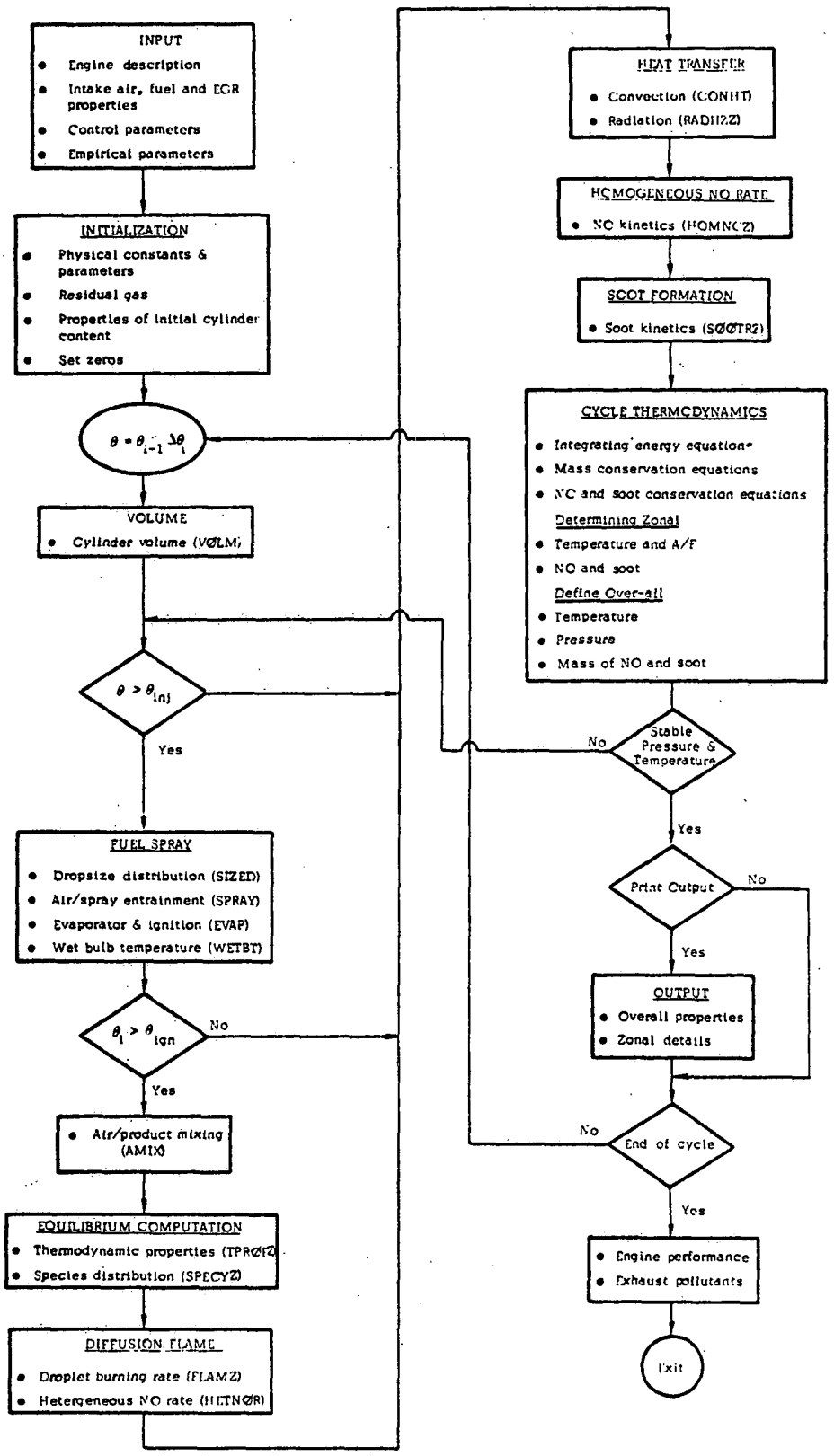
INPUT
Engine description
Intake air, fuel and EGR properties
Control parameters
Empirical parameters
INITIALIZATION
Physical constants & parameters
Residual gas
Properties of initial cylinder content
Set zeros
$\theta = \theta_{i-1} \Delta\theta_i$
VOLUME
Cylinder volume (VØLM)
$\theta > \theta_{inj}$
Yes
FUEL SPRAY
Dropsize distribution (SIZED)
Air/spray entrainment (SPRAY)
Evaporator & ignition (EVAP)
Wet bulb temperature (WETBT)
$\theta_i > \theta_{ign}$
No
Yes
Air/product mixing (AMIX)
EQUILIBRIUM COMPUTATION
Thermodynamic properties (TPRØP2)
Species distribution (SPECYZ)
DIFFUSION FLAME
Droplet burning rate (FLAMZ)
Heterogeneous NO rate (HETNØR)
HEAT TRANSFER
Convection (CONHT)
Radiation (RADIIZZ)
HOMOGENEOUS NO RATE
NO kinetics (HOMNOZ)
SOOT FORMATION
Soot kinetics (SØØTR2)
CYCLE THERMODYNAMICS
Integrating energy equation
Mass conservation equations
NO and soot conservation equations
Determining Zonal
Temperature and A/F
NO and soot
Define Over-all
Temperature
Pressure
Mass of NO and soot
Stable Pressure & Temperature
No
Yes
Print Output
No
Yes
OUTPUT
Overall properties
Zonal details
End of cycle
No
Yes
Engine performance
Exhaust pollutants
Exit

Figure 1

III. DESCRIPTION OF THE PROGRAM INPUT

The data input to the diesel engine program consists of three distinct groups:

(1) Tape Input (Species Tables): The mole fraction distributions, X_i (P, T, ψ), of the equilibrium combustion products is read in as TAPE 8 from either a magnetic tape or magnetic disc. This input is required only once for all stacked cases having the same kind of fuel. Cases using different fuels cannot be stacked.

(2) Block Data Input (Thermodynamic Properties): The internal energy, U (P, T, ϕ), and gas constant, $R(P, T, \phi)$, of the equilibrium combustion products are calculated from fitted polynomials (detail, see Ref. 1). The coefficients of these polynomials form an integral part of the program via the BLOCK DATA subroutine. The BLOCK DATA has to be revised whenever a different fuel is used.

(3) Card Input (Engine Geometry, Operating Conditions and Air-Fuel Physical Properties): Five sets of input cards are required in this group. All of them except the case identification card are input via the standard namelist format.

The five sets of cards are described below according to their input order. The definitions, format, and preset values of the variables in each set of input cards are described in functional subgroups. The order of the variables within each set of input data is arbitrary.

(a) Namelist GIVEN

This set of input cards details the common constants of engine geometry, engine operation, and fuel physical properties. The variables in the GIVEN namelist are presented in Tables 1, 2 and 3.

(b) Case Identification Card

A single card contains the case identification information in Columns 1 through 80. When no identification is desired a blank card must be provided.

(c) Namelist CPARAM

This set of card inputs provides the logic flow control parameters for the program. All the parameters in this set of data are preset to nominal values and only require to be input if it is desired to alter the preset values. These preset values apply to each individual case, therefore, all charges must be made whenever required.

When it is unnecessary to modify the parameters given in Tables 4, 5 and 6, a $CPARAM$ card starting at Column 2 must be included. It should also be noted that when NSHEL and DTHMIN are specified, the constraint:

$$(DINJ/DTHMIN) \times NSHEL \leq 100$$

must be satisfied.

(d) Namelist EPARAM

The empirical parameters, which are preset, required by the program are provided with this set of input cards. These parameters which are preset prior to each individual case need only to be input if it is desired to alter the preset values. Therefore, when the alterations are required, they must be made in every case.

If modification of the parameters listed in Table 7 is not required, a $EPARAM$ card starting at Column 2 must be included.

(e) Namelist GIVEN

The variables in this set of input are the same as that of (a). This set of inputs serve as a modification or as an addition to set (a). When neither a modification nor an addition complement is desired a $GIVEN$ card must be provided.

The order of card input is illustrated in Figure 2.

Table 1. Engine Geometry

FORTRAN SYMBOL	DESCRIPTION	FORMAT	PRESET
DE	Engine bore (cm)	F †	NA **
RFW	Crank radius (cm)	F	NA
RL	Rod length (cm)	F	NA
CR	Compression ratio	F	NA
SC	Engine clearance (cm)	F	NA
TW	Mean engine wall temperature (^{o}K)	F	NA
SCR	Supercharge (atm)	F	NA
DNØZZ	Diameter of fuel nozzle (cm)	F	NA
NNØZZ	No. of fuel nozzles	F	NA
THEVC	Closing angle of intake valve (C.A.)	F	NA
THEVØ	Opening angle of exhaust valve (C. A.)	F	NA
DBOWL	Diameter of bowl on piston head (cm)	F	NA
NSTROK	No. of strokes per power cycle	I***	4

Table 2. Engine Operation

XMAI	Mass of fresh air/powerstroke (gm)	F	NA
XMRD	Mass of residue gas/powerstroke (gm)	F	Option*
ØMEGA	Charge swirl angular velocity (rad./sec)	F	NA
THEIJ	Fuel injection time (C.A.)	F	NA
DINJ	Duration of fuel injection (C.A.)	F	NA
XMFJ	Mass of fuel injection/powerstroke (gm)	F	NA
PINJ	Fuel line pressure (atm)	F	NA
TFJ	Fuel line temperature (^{o}K)	F	NA
EGR	% of E.G.R. (base on total charge)	F	NA
RPM	Engine speed (rpm)	F	NA

† Floating point
* This value will automatically be calculated in program if not specified.
** Not applicable
*** Integer

Table 3. Fuel Properties

W	No. of C atoms in fuel molecule	F	NA
XX	No. of H atoms in fuel molecule	F	NA
FDEN	Density of fuel (gm/cm^3)	F	Option
CEN	Centan No.	F	NA
API	API Gravity at 60^oF	F	NA
XMUF	Viscosity (gm/cm-sec) at TFJ	F	NA
SURFT	Surface tension (gm/sec^2) at TFJ	F	NA
TBPF	Boiling point at 1 atm (^oK)	F	NA
TCRITF	Critical temperature (^oK)	F	NA
CPFL	Liquid specific heat (cal/gm)	F	NA
CVFV	Vapor constant volume specific heat (cal/gm)	F	NA
CPFV	Vapor constant pressure specific heat (cal/gm)	F	NA
DHFV	Latent heat at 298^oK (cal/gm)	F	NA
HFFL	Heat of formation at 298^oK (cal/gm)	F	Option*
HCØM	Heat of combustion (cal/gm)	F	Option*

* If this value is not specified it will be calculated by program.

Table 4. Pollutant Computation Control

FORTRAN SYMBOL	DESCRIPTION	FORMAT	PRESET
INØ1	Homogeneous NO rate calculation is to be performed if INØ1 ≠ 0	I	1
INØ2	Heterogeneous NO rate calculation is to be performed if INØ2 ≠ 0	I	1
ISØØT	Soot kinetic calculation is to be performed if ISØØT ≠ 0	I	1

Table 5. Numerical Stability Control

NTER	Max. No. of iterations allowed for stable solution.	I	50
NAXIL	No. of axial fuel jet stations (max. = 20)	I	20
NSHEL	No. of conical fuel jet shells (max. =4)	I	4
NSZG	No. of droplet size groups(max. =3)	I	3
NITST	No. of spatial points in droplet field intergration (max. = 50)	I	50
DTHMIN	Intergration step size (C.A.) used during fuel injection and combustion	F	1.0
DTHMED	Integration step size (C.A.) used after combustion	F	2.5
DTHMAX	Integration step size (C.A.) used before injection	F	5.0
THEMAX	Maximum crank angle to be integrated to	F	THEVC
EPSIT	Relative error bound on averaged temperature calculation	F	2.0 E-3
EPSIP	Relative error bound on pressure calculation	F	2.0 E-3

Table 6. Output Control

FORTRAN SYMBOL	DESCRIPTION	FORMAT	PRESET
NPRT	Print every NPRT intergration steps	I	2
IDTAIL	Print detailed zonal information if IDTAIL ≠ 0	I	0
IDRØPP	Print detailed droplet information if IDRØP ≠ 0 & IDTAIL ≠ 0	I	0
ISECYP	Print detailed species information of each zone if ISPECY ≠ 0 & IDTAIL ≠ 0	I	0
IRATEP	Print detailed rate information if IRATEP ≠ 0 & IDTAIL ≠ 0	I	0

Table 7.

FORTRAN SYMBOL	DESCRIPTION	FORMAT	PRESET
CA	Preconstant for rate for heat convection rate	F	0.26
CB	Reynolds No. exponent heat convection rate	F	0.75
CNOR	Multiplier of NØ rate constant	F	5.37
CVIDI	Vitiation/dilution ratio	F	0.1
CMIX	Air/product dilution coefficient	F	7.8E-3
SEFJ	Coefficient for swirl effect on jet entrainment	F	4.3
CEVAP	Crossflow effect on fuel vaporization rate	F	0.276
RHØD	ρD in droplet calculation (gm/cm-sec)	F	3.0 E-4
CPBAR	$\bar{C}_p$ in droplet calculation(cal/gm)	F	0.35
XTLYØ2	Droplet extinction limit (oxygen mass fraction)	F	0.02
HUTIM	Droplet heat-up time (sec)	F	2.0 E-4
SDEN	Density of soot particle (gm/cm^3)	F	2.0
DSOOT	Assumed mean soot particle size (cm)	F	1.0 E-4
ASOTA	Pre-constant for soot formation rate in burning zone	F	3.52
ASOTP	Pre-constant for soot formation rate in vaporizing zone	F	3.52

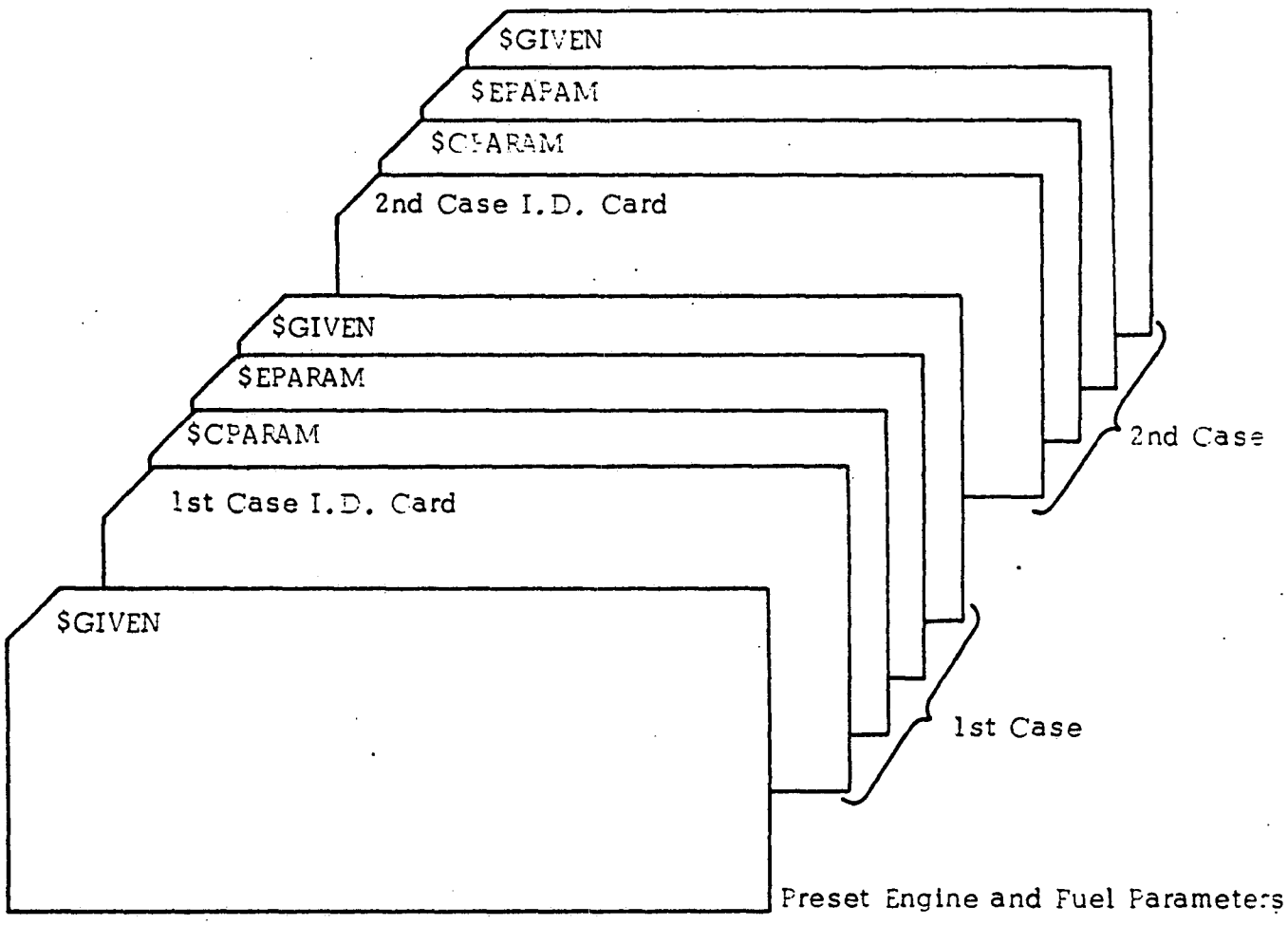

Figure 2. Input Data

IV. DESCRIPTION OF PROGRAM OUTPUT

The regular printed output of the computer program is described below. The description is presented in the order of its appearance.

(1) Printout of Program Input

The program input group (III) is printed out under namelist output format. Descriptions of these variables has been given in Section 3 under:

NAMELIST GIVEN

I.D. Card

NAMELIST CPARAM

NAMELIST EPARAM

NAMELIST GIVEN

(2) Initial Conditions

The printout of namelist INITL gives the initial conditions of the engine and the charge in it. The elements of NAMELIST INITL are described below.

SYMBOL	DESCRIPTION
THETAI	Initial C.A. for integration (or compression)
THEMAX	Maximum or final C.A.; the integration is terminated when θ = THEMAX
P	Initial pressure (atm)
T	Initial charge temperature (^{o}K)
V	Initial charge volume (cm^3)
UA	Specific internal energy of charge (cal/gm)
HA	Specific enthalpy of charge (cal/gm)
XMAØ	Total mass of initial charge

SYMBOL	DESCRIPTION
AMWA	Molecular weight of charge content
FARA	Fuel-air mass ratio of charge content
PHEA	Equivalence ratio of charge content
FARØS	Stoichiometric fuel-air ratio
XMEGR	Mass of EGR (gm)
XMAEGR	Mass of pure air contained in XMEGR (gm)
XMFEGR	Mass of fuel contained in XMEGR, (gm)
XMRD	Trapped or residual gas (gm)
XMARD	Mass of pure air contained in XMRD (gm)
XMFRD	Mass of fuel contained in XMRD (gm)
AMWF	Molecular wt. of fuel
ØXST	Stoichiometric oxygen-fuel mass ratio
XØ2A	Oxygen mole fraction in charge
FDEN	Liquid fuel density (gm/cm^3)
HHV	High heating value of fuel (cal/gm)
HCØM	Heat of combustion (cal/gm)
HFFL	Heat of formation of fuel (cal/gm)
HFJ	Enthalpy of injected fuel (cal/gm)
VC	Engine clearance volume (cm^3)
VDIS	Engine displacement (cm^3)
VFJØ	Initial velocity of fuel injection (cm/sec)

(3) Printout of Current Information at Each Specified Print Station

The program will printout averaged over-all charge properties and rate information at the specified print station controlled by NAMELIST CPARAM and every ignition step (from the onset to the end of zonal ignition). The elements of the printout are described below.

SYMBOL	DESCRIPTION
THETA	Crank Angle (in degree), zero at TDC
P	Pressure (atm)
V	Instantaneous engine (or charge) volume (cm^3)
T	Mass averaged temperature (^oK)
U	Mass averaged specific internal energy (cal/gm)
PHEE	Over-all equivalence ratio
DPDTH	Step-averaged pressure derivative, $\frac{dP}{d\theta}$ (atm/C.A.)
WP	Step-averaged work rate, $P\frac{dv}{d\theta}$ (cal/C.A.)
DFJDTH	Fuel injection rate (gm/C.A.)
SMDDTH	Step-averaged over-all dilution rate (gm/C.A.)
SMVDTH	Step-averaged over-all vitiation (air) rate (gm/C.A.)
DQRDTH	Step-averaged over-all rate of radiative heat transfer to the cylinder wall (cal/C.A.)
SVBDTH	Step-averaged over-all premixed burning rate (gm/C.A.)
SDBDTH	Step-averaged over-all droplet burning rate (gm/C.A.)
SLDDTH	Step-averaged over-all mass rate of ignition of liquid fuel (gm/C.A.)
SUMQL	Cumulated (time integrated) heat loss(convective and radiative heat transfer) to the cylinder wall. (cal.)
SUMFB	Cumulated mass of fuel burned to equilibrium products
DFBDTH	Over-all mass burning rate (gm/C.A.)
WKNET	Cumulated net work (cal), i.e., $\int_{\theta_i}^{\theta} p\frac{dv}{d\theta'}\, d\theta'$
RR	Mass averaged gas constant (cm^3 - atm/gm - ^oK)
UCHAR	Characteristics charge velocity (cm/sec)
DVDTH	Engine Volume rate (cm^3/C.A.)
DELE12	Over-all numerical error involved in integration of the system energy conservation equations, (normalized by total chemical energy released i.e. XMFJ * HCOM).

SYMBOL	DESCRIPTION
ITERPC	No. of iterations per step
XMNØE	Over-all mass of NO (gm) per power stroke
YNØE	Mass averaged NO mass fraction
XNOE	NO concentration (ppm)
SØØTE	Over-all mass of soot (gm) emission per power stroke

(4) Engine Performance and Exhaust Pollutants

The computed engine performance parameters and pollutants in the exhaust gas are printed at the end of engine cycle (i.e. θ = THEVØ) or at the end of integration (i.e. θ = THEMAX). They are:

SYMBOL	DESCRIPTION
I.M.E.P.	Indicated mean effective pressure (psi)
I.H.P.	Indicated engine horse-power (hp)
I.S.F.C.	Indicated specific fuel consumption (lb/hp-hr)
SØØT	Exhaust soot concentration (mg/m^3 at standard conditions)
NITRIC ØXIDE	Exhaust nitric oxide concentration (ppm)

V. SAMPLE CASE

The program input and output of a sample case is presented in the following pages to facilitate program checkout.

(1) INPUT

```
$GIVEN DE=13.97,RFW=7.62,FL=30.48,CP=17.0,SC=0.2032,TW=500.0,RPM=1500.,
 DPCWL=8.2,SCR=1.0,THEVC=-150.000,THEVO=140.,XMAI=2.4000,EGR=0.0,THETJ=-20,
 DINJ=17.,XMFJ=0.100,TFJ=350.,W=7.0,XX=12.0,CFN=46.7,SURFT=27.,XMUF=1.2E-2,
      API=34.5, TCRITF=567., TRPF=377.6,CPFL=0.51,CPFV=0.332,CVFV=0.32,
      CHFV=92.865,HFFL=-264.390, PINJ=231., DNOZZ=0.0254,NNOZZ=6 ,OMEGA=600.$
****** A/F=24., THETJ= 20 DEG.BTDC, MFC. SWIRL (CASE  000 ) *****
$CPARAM   THEMAX=30.0 $
$EPARAM   $
$GIVEN  $
```

(2) OUTPUT

```
$GIVEN
DE      =  0.1397E+02,
RFN     =  0.762E+01,
RL      =  0.3048E+02,
CR      =  0.17E+02,
SC      =  0.2032E+00,
TW      =  0.5E+03,
RPM     =  0.15E+04,
SCR     =  0.1E+01,
DNOZZ   =  0.2545E-01,
NNOZZ   =  6,
DBOWL   =  0.82E+01,
THEVC   = -0.15E+03,
THEVO   =  0.14E+03,
XMAT    =  0.24E+01,
EGP     =  0.0,
XMRO    =  0.0,
OMEGA   =  0.6E+03,
NSTROK  = -288230376151607813,
THEIJ   = -0.2E+02,
DINJ    =  0.17E+02,
XMFJ    =  0.1E+00,
PINJ    =  0.231E+03,
TFJ     =  0.35E+03,
W       =  0.7E+01,
XX      =  0.12E+02,
FDEN    =  0.0,
CEN     =  0.467E+02,
API     =  0.345E+02,
XMUF    =  0.12E-01,
SURFT   =  0.27E+02,
TBPF    =  0.3776E+03,
```

```
TCRITF  =  0.567E+03,
CPFL    =  0.51E+00,
CPFV    =  0.332E+00,
CVFV    =  0.32E+00,
DHFV    =  0.92365E+02,
HFFL    = -0.26439E+03,
HCOM    =  0.0,
$END
```

***** A/F=24., THFIJ= 20 DEG.BTDC, MED. SWIRL (CASE 000) *****

```
$CPARAM
INO1    =  1,
INO2    =  1,
ISOOT   =  1,
IBUG    =  0,
NTER    =  50,
NPRT    =  2,
NAXIL   =  20,
NSHEL   =  4,
NSZG    =  3,
ICROPP  =  0,
IRATEP  =  0,
ISPCYP  =  0,

IDTAIL  =  0,
NITST   =  50,
DTHMIN  =  0.1E+01,
DTHMED  =  0.25E+01,
DTHMAX  =  0.5E+01,
THEMAX  =  0.3E+02,
EPSIT   =  0.2E-02,
EPSIP   =  0.2E-02,


$END
```

```
$EPARAM
CA      =  0.26E+00,
CB      =  0.75E+00,
CNOR    =  0.537E+01,
CVIOI   =  0.1E+00,
CMIX    =  0.78E-02,
SDEN    =  0.2E+01,
DSOOT   =  0.1E-03,
ASOTA   =  0.352E+01,
ASOTP   =  0.352E+01,
HUTIM   =  0.2E-03,
DTPHY   =  0.2E-03,
SEFJ    =  0.43E+01,
CDCHG   =  0.1E+01,
CEVAP   =  0.276E+00,

AIGND   =  0.146E-03,
RHOD    =  0.3E-03,
CPBAR   =  0.35E+00,
XTLYO2  =  0.2E-01,
$END
```

```
$GIVEN
DE      =  0.1337E+02,
RFW     =  0.762E+01,
RL      =  0.3048E+02,
CR      =  0.17E+02,
SC      =  0.2032E+00,
TW      =  0.5E+03,
RPM     =  0.15E+04,
SCP     =  0.1E+01,
DNOZZ   =  0.254E-01,
NNOZZ   =  6,
DBOWL   =  0.82E+01,
THEVC   = -0.15E+03,
THEVO   =  0.14E+03,
XMAI    =  0.24E+01,
EGR     =  0.0,
XMRO    =  0.0,
OMEGA   =  0.6E+03,
NSTROK  =  4,
THEIJ   = -0.2E+02,
DINJ    =  0.17E+02,
XMFJ    =  0.1E+00,
PINJ    =  0.231E+03,
TFJ     =  0.35E+03,
W       =  0.7E+01,
XX      =  0.12E+02,
FDEN    =  0.0,
CEN     =  0.467E+02,
API     =  0.345E+02,
XMUF    =  0.12E-01,
SUPFT   =  0.27E+02,
TBPF    =  0.3776E+03,
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TCRITF  =  0.567E+03,
CPFL    =  0.51E+00,
CPFV    =  0.332E+00,
CVFV    =  0.32E+00,
DHFV    =  0.92865E+02,
HFFL    = -0.26439E+03,
HCOM    =  0.0,
$END
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$INITL
THETAI   = -0.15E+03,
THEMAX   =  0.3E+02,
P        =  0.1E+01,
T        =  0.33955427188909E+03,
V        =  0.23621320794931E+04,
UA       = -0.24477070004609E+02,
HA       = -0.11905387510382E+01,
XMAO     =  0.24530863750245E+01,
AMWA     =  0.28850043026598E+02,
FARA     =  0.10255600376831E-02,
PHEA     =  0.14677473405975E-01,
FAROS    =  0.69873063933853E-01,
XMEGR    =  0.0,
XMAEGR   =  0.0,
XMFEGR   =  0.0,
XMRO     =  0.63086375024526E-01,
XMARO    =  0.60552920023545E-01,
XMFRO    =  0.2523455000981E-02,
AMWF     =  0.96E+02,
OXST     =  0.33203066666667E+01,
XO2A     =  0.20853426216717E+00,
FDEN     =  0.85193285988741E+00,
HHV      =  0.10905555555556E+05,
HCOM     =  0.10249305555556E+05,
HFFL     = -0.26439E+03,
HFJ      = -0.23133624136 58E+03,
VC       =  0.14599813601726E+03,
VDIS     =  0.23359701762761E+04,
VFJO     =  0.20439941725328E+05,
$END
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THETA(DEG.CA)= -145.00   P(ATM)= 1.346E+00  V(CM3)= 2.319E+03  T(K)= 3.468E+02  U(CAL/GM)=-2.319E+01  PHEE= 1.468E-02
 DPDTH(ATM/CA)= 4.652E-03  WP(CAL/CA)=-2.138E-01  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DDCDTH(CAL/CA)=-4.357E-01  DDRDTH(CAL/CA)=-2.908E-05  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMGL(CAL)=-2.179E+00  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-1.069E+00  RR(CM3-ATM/GM-K)= 2.840E+00
 UCHAP(CM/SEC)= 2.147E+03  DVDTH(CM3/CA)=-9.273E+00  DELE12=-8.230E-05  ITERPC=    1
 XMNOE(GM)= 5.638E-75  YNOE= 2.289E-75  XNOE(PPM)= 2.201E-69  SOOTE(GM)= 8.160E-31

THETA(DEG.CA)= -135.00   P(ATM)= 1.151E+00  V(CM3)= 2.213E+03  T(K)= 3.642E+02  U(CAL/GM)=-2.037E+01  PHEE= 1.468E-02
 DPDTH(ATM/CA)= 1.116E-02  WP(CAL/CA)=-3.047E-01  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DDCDTH(CAL/CA)=-3.904E-01  DDRDTH(CAL/CA)=-2.769E-05  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMGL(CAL)=-6.122E+00  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-3.879E+00  RR(CM3-ATM/GM-K)= 2.840E+00
 UCHAP(CM/SEC)= 2.185E+03  DVDTH(CM3/CA)=-1.183E+01  DELE12= 1.041E-04  ITERPC=    1
 XMNOE(GM)= 6.544E-71  YNOE= 2.657E-71  XNOE(PPM)= 2.555E-65  SOOTE(GM)= 1.002E-29

THETA(DEG.CA)= -125.00   P(ATM)= 1.285E+00  V(CM3)= 2.083E+03  T(K)= 3.825E+02  U(CAL/GM)=-1.739E+01  PHEE= 1.468E-02
 DPDTH(ATM/CA)= 1.423E-02  WP(CAL/CA)=-4.132E-01  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DDCDTH(CAL/CA)=-3.257E-01  DDRDTH(CAL/CA)=-2.598E-05  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMGL(CAL)=-9.515E+00  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-7.727E+00  RR(CM3-ATM/GM-K)= 2.840E+00
 UCHAP(CM/SEC)= 2.231E+03  DVDTH(CM3/CA)=-1.425E+01  DELE12= 2.171E-04  ITERPC=    1
 XMNOE(GM)= 4.555E-67  YNOE= 1.849E-67  XNOE(PPM)= 1.778E-61  SOOTE(GM)= 2.719E-28

THETA(DEG.CA)= -115.00   P(ATM)= 1.459E+00  V(CM3)= 1.929E+03  T(K)= 4.022E+02  U(CAL/GM)=-1.411E+01  PHEE= 1.468E-02
 DPDTH(ATM/CA)= 1.853E-02  WP(CAL/CA)=-5.449E-01  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DDCDTH(CAL/CA)=-2.799E-01  DDRDTH(CAL/CA)=-2.376E-05  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMGL(CAL)=-1.236E+01  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-1.283E+01  RR(CM3-ATM/GM-K)= 2.840E+00
 UCHAP(CM/SEC)= 2.292E+03  DVDTH(CM3/CA)=-1.647E+01  DELE12= 3.266E-04  ITERPC=    1
 XMNOE(GM)= 2.595E-63  YNOE= 1.054E-63  XNOE(PPM)= 1.013E-57  SOOTE(GM)= 3.756E-27

THETA(DEG.CA)= -105.00   P(ATM)= 1.691E+00  V(CM3)= 1.755E+03  T(K)= 4.240E+02  U(CAL/GM)=-1.044E+01  PHEE= 1.468E-02
 DPDTH(ATM/CA)= 2.497E-02  WP(CAL/CA)=-7.666E-01  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DDCDTH(CAL/CA)=-2.145E-01  DDRDTH(CAL/CA)=-2.074E-05  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMGL(CAL)=-1.465E+01  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-1.947E+01  RR(CM3-ATM/GM-K)= 2.840E+00
 UCHAP(CM/SEC)= 2.333E+03  DVDTH(CM3/CA)=-1.838E+01  DELE12= 4.343E-04  ITERPC=    1
 XMNOE(GM)= 1.429E-59  YNOE= 5.861E-60  XNOE(PPM)= 5.579E-54  SOOTE(GM)= 5.061E-26

THETA(DEG.CA)=  -95.00   P(ATM)= 2.008E+00  V(CM3)= 1.563E+03  T(K)= 4.485E+02  U(CAL/GM)=-6.239E+00  PHEE= 1.468E-02
 DPDTH(ATM/CA)= 3.435E-02  WP(CAL/CA)=-9.076E-01  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DDCDTH(CAL/CA)=-1.550E-01  DDRDTH(CAL/CA)=-1.640E-05  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMGL(CAL)=-1.635E+01  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-2.802E+01  RR(CM3-ATM/GM-K)= 2.840E+00
 UCHAP(CM/SEC)= 2.379E+03  DVDTH(CM3/CA)=-1.985E+01  DELE12= 5.417E-04  ITERPC=    1
 XMNOE(GM)= 8.692E-56  YNOE= 3.529E-56  XNOE(PPM)= 3.394E-50  SOOTE(GM)= 6.950E-25

THETA(DEG.CA)=  -85.00   P(ATM)= 2.454E+00  V(CM3)= 1.359E+03  T(K)= 4.768E+02  U(CAL/GM)=-1.320E+00  PHEE= 1.468E-02
 DPDTH(ATM/CA)= 4.867E-02  WP(CAL/CA)=-1.161E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DDCDTH(CAL/CA)=-9.028E-02  DDRDTH(CAL/CA)=-9.886E-06  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMGL(CAL)=-1.742E+01  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-3.895E+01  RR(CM3-ATM/GM-K)= 2.840E+00
 UCHAP(CM/SEC)= 2.413E+03  DVDTH(CM3/CA)=-2.076E+01  DELE12= 6.501E-04  ITERPC=    1
 XMNOE(GM)= 6.494E-52  YNOE= 2.637E-52  XNOE(PPM)= 2.535E-46  SOOTE(GM)= 1.007E-23
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THETA(DEG.CA)=  -75.00   P(ATM)= 3.101E+00  V(CM3)= 1.150E+03  T(K)= 5.098E+02  U(CAL/GM)= 4.548E+00  PHEE= 1.468E-02
 DPDTH(ATM/CA)= 7.131E-02  WP(CAL/CA)=-1.493E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DQCDTH(CAL/CA)=-1.755E-02  DQRDTH(CAL/CA)= 3.082E-07  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMQL(CAL)=-1.778E+01  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-5.293E+01  RR(CM3-ATM/GM-K)= 2.840E+00
 UCHAR(CM/SEC)= 2.431E+03  DVDTH(CM3/CA)=-2.100E+01  DELE12= 7.619E-04  ITERPC=    1
 XMNOE(GM)= 6.443E-48  YNOE= 2.616E-48  XNOE(PPM)= 2.516E-42  SOOTE(GM)= 1.582E-22

THETA(DEG.CA)=  -65.00   P(ATM)= 4.079E+00  V(CM3)= 9.419E+02  T(K)= 5.492E+02  U(CAL/GM)= 1.185E+01  PHEE= 1.468E-02
 DPDTH(ATM/CA)= 1.04[illegible]E-01  WP(CAL/CA)=-1.902E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DQCDTH(CAL/CA)= 6.767E-02  DQRDTH(CAL/CA)= 1.714E-05  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMQL(CAL)=-1.733E+01  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-7.082E+01  RR(CM3-ATM/GM-K)= 2.840E+00
 UCHAR(CM/SEC)= 2.427E+03  DVDTH(CM3/CA)=-2.048E+01  DELE12= 1.298E-03  ITERPC=    2
 XMNOE(GM)= 1.099E-43  YNOE= 4.461E-44  XNOE(PPM)= 4.290E-38  SOOTE(GM)= 2.856E-21

THETA(DEG.CA)=  -55.00   P(ATM)= 5.619E+00  V(CM3)= 7.431E+02  T(K)= 5.968E+02  U(CAL/GM)= 2.072E+01  PHEE= 1.468E-02
 DPDTH(ATM/CA)= 1.732E-01  WP(CAL/CA)=-2.448E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DQCDTH(CAL/CA)= 1.729E-01  DQRDTH(CAL/CA)= 4.566E-05  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMQL(CAL)=-1.598E+01  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-9.385E+01  RR(CM3-ATM/GM-K)= 2.840E+00
 UCHAR(CM/SEC)= 2.400E+03  DVDTH(CM3/CA)=-1.914E+01  DELE12= 1.565E-03  ITERPC=    2
 XMNOE(GM)= 2.200E-39  YNOE= 8.930E-40  XNOE(PPM)= 8.588E-34  SOOTE(GM)= 5.668E-20

THETA(DEG.CA)=  -45.00   P(ATM)= 8.160E+00  V(CM3)= 5.617E+02  T(K)= 6.551E+02  U(CAL/GM)= 3.181E+01  PHEE= 1.468E-02
 DPDTH(ATM/CA)= 2.893E-01  WP(CAL/CA)=-3.158E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DQCDTH(CAL/CA)= 3.112E-01  DQRDTH(CAL/CA)= 9.542E-05  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMQL(CAL)=-1.314E+01  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-1.235E+02  RR(CM3-ATM/GM-K)= 2.840E+00
 UCHAR(CM/SEC)= 2.352E+03  DVDTH(CM3/CA)=-1.700E+01  DELE12= 1.914E-03  ITERPC=    2
 XMNOE(GM)= 5.722E-35  YNOE= 2.323E-35  XNOE(PPM)= 2.234E-29  SOOTE(GM)= 1.205E-18

THETA(DEG.CA)=  -35.00   P(ATM)= 1.253E+01  V(CM3)= 4.055E+02  T(K)= 7.262E+02  U(CAL/GM)= 4.565E+01  PHEE= 1.468E-02
 DPDTH(ATM/CA)= 5.008E-01  WP(CAL/CA)=-4.041E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DQCDTH(CAL/CA)= 5.055E-01  DQRDTH(CAL/CA)= 1.826E-04  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMQL(CAL)=-8.613E+00  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-1.616E+02  RR(CM3-ATM/GM-K)= 2.840E+00
 UCHAR(CM/SEC)= 2.288E+03  DVDTH(CM3/CA)=-1.411E+01  DELE12= 2.407E-03  ITERPC=    2
 XMNOE(GM)= 1.572E-30  YNOE= 6.382E-31  XNOE(PPM)= 6.137E-25  SOOTE(GM)= 2.651E-17

THETA(DEG.CA)=  -25.00   P(ATM)= 2.012E+01  V(CM3)= 2.816E+02  T(K)= 8.098E+02  U(CAL/GM)= 6.208E+01  PHEE= 1.468E-02
 DPDTH(ATM/CA)= 8.833E-01  WP(CAL/CA)=-4.949E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DQCDTH(CAL/CA)= 7.939E-01  DQRDTH(CAL/CA)= 3.337E-04  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMQL(CAL)=-1.465E+00  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-2.090E+02  RR(CM3-ATM/GM-K)= 2.840E+00
 UCHAR(CM/SEC)= 2.219E+03  DVDTH(CM3/CA)=-1.058E+01  DELE12= 2.699E-03  ITERPC=    1
 XMNOE(GM)= 2.455E-26  YNOE= 9.967E-27  XNOE(PPM)= 9.585E-21  SOOTE(GM)= 5.182E-16

THETA(DEG.CA)=  -19.00   P(ATM)= 2.676E+01  V(CM3)= 2.251E+02  T(K)= 8.611E+02  U(CAL/GM)= 7.206E+01  PHEE= 4.889E-02
 DPDTH(ATM/CA)= 1.207E+00  WP(CAL/CA)=-5.325E+00  DFJDTH(GM/CA)= 5.882E-03  SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DQCDTH(CAL/CA)= 1.216E+00  DQRDTH(CAL/CA)= 5.125E-04  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 4.691E+00  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-2.405E+02  RR(CM3-ATM/GM-K)= 2.840E+00
 UCHAR(CM/SEC)= 2.156E+03  DVDTH(CM3/CA)=-8.211E+00  DELE12= 3.674E-03  ITERPC=    1
 XMNOE(GM)= 3.421E-24  YNOE= 1.349E-24  XNOE(PPM)= 1.336E-18  SOOTE(GM)= 2.622E-15
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THETA(DEG.CA)=  -18.00   P(ATM)= 2.798E+01  V(CM3)= 2.171E+02  T(K)= 8.684E+02  U(CAL/GM)= 7.298E+01  PHEE= 8.311E-02
 DPDTH(ATM/CA)= 1.225E+00  WP(CAL/CA)=-5.300E+00  DFJDTH(GM/CA)= 5.882E-03  SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DQCDTH(CAL/CA)= 1.263E+00  DQRDTH(CAL/CA)= 5.354E-04  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 5.354E+00  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-2.458E+02  RR(CM3-ATM/GM-K)= 2.840E+00
 UCHAR(CM/SEC)= 2.368E+03  DVDTH(CM3/CA)=-7.802E+00  DELE12= 3.687E-03  ITERPC=    1
 XMNOE(GM)= 5.921E-24  YNOE= 2.464E-24  XNOE(PPM)= 2.312E-18  SOOTE(GM)= 3.284E-15

THETA(DEG.CA)=  -17.00   P(ATM)= 2.924E+01  V(CM3)= 2.095E+02  T(K)= 8.755E+02  U(CAL/GM)= 7.384E+01  PHEE= 1.173E-01
 DPDTH(ATM/CA)= 1.255E+00  WP(CAL/CA)=-5.256E+00  DFJDTH(GM/CA)= 5.882E-03  SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DQCDTH(CAL/CA)= 1.310E+00  DQRDTH(CAL/CA)= 5.581E-04  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 7.264E+00  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-2.510E+02  RR(CM3-ATM/GM-K)= 2.840E+00
 UCHAR(CM/SEC)= 2.562E+03  DVDTH(CM3/CA)=-7.389E+00  DELE12= 3.679E-03  ITERPC=    1
 XMNOE(GM)= 1.076E-23  YNOE= 4.368E-24  XNOE(PPM)= 4.202E-18  SOOTE(GM)= 4.078E-15

THETA(DEG.CA)=  -16.00   P(ATM)= 3.052E+01  V(CM3)= 2.023E+02  T(K)= 8.825E+02  U(CAL/GM)= 7.467E+01  PHEE= 1.515E-01
 DPDTH(ATM/CA)= 1.291E+00  WP(CAL/CA)=-5.189E+00  DFJDTH(GM/CA)= 5.882E-03  SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DQCDTH(CAL/CA)= 1.357E+00  DQRDTH(CAL/CA)= 5.808E-04  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 8.622E+00  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-2.562E+02  RR(CM3-ATM/GM-K)= 2.839E+00
 UCHAR(CM/SEC)= 2.742E+03  DVDTH(CM3/CA)=-6.972E+00  DELE12= 3.765E-03  ITERPC=    1
 XMNOE(GM)= 1.991E-23  YNOE= 8.077E-24  XNOE(PPM)= 7.782E-18  SOOTE(GM)= 5.046E-15

THETA(DEG.CA)=  -15.00   P(ATM)= 3.182E+01  V(CM3)= 1.956E+02  T(K)= 8.891E+02  U(CAL/GM)= 7.544E+01  PHEE= 1.857E-01
 DPDTH(ATM/CA)= 1.301E+00  WP(CAL/CA)=-5.098E+00  DFJDTH(GM/CA)= 5.882E-03  SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DQCDTH(CAL/CA)= 1.406E+00  DQRDTH(CAL/CA)= 6.032E-04  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 1.003E+01  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-2.613E+02  RR(CM3-ATM/GM-K)= 2.837E+00
 UCHAR(CM/SEC)= 2.910E+03  DVDTH(CM3/CA)=-6.553E+00  DELE12= 3.721E-03  ITERPC=    1
 XMNOE(GM)= 3.669E-23  YNOE= 1.487E-23  XNOE(PPM)= 1.436E-17  SOOTE(GM)= 6.222E-15

THETA(DEG.CA)=  -14.00   P(ATM)= 3.313E+01  V(CM3)= 1.892E+02  T(K)= 8.953E+02  U(CAL/GM)= 7.613E+01  PHEE= 2.200E-01
 DPDTH(ATM/CA)= 1.310E+00  WP(CAL/CA)=-4.981E+00  DFJDTH(GM/CA)= 5.882E-03  SMDDTH(GM/CA)= 0.          SMVDTH(GM/CA)= 0.
 DQCDTH(CAL/CA)= 1.455E+00  DQRDTH(CAL/CA)= 6.254E-04  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 0.          SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 1.148E+01  SUMFB(GM)= 0.          SFBDTH(GM/CA)= 0.          WKNET(CAL)=-2.663E+02  RR(CM3-ATM/GM-K)= 2.834E+00
 UCHAR(CM/SEC)= 3.068E+03  DVDTH(CM3/CA)=-6.130E+00  DELE12= 3.738E-03  ITERPC=    1
 XMNOE(GM)= 6.643E-23  YNOE= 2.689E-23  XNOE(PPM)= 2.604E-17  SOOTE(GM)= 7.611E-15

THETA(DEG.CA)=  -13.00   P(ATM)= 3.704E+01  V(CM3)= 1.833E+02  T(K)= 9.062E+02  U(CAL/GM)= 7.598E+01  PHEE= 2.542E-01
 DPDTH(ATM/CA)= 1.754E+00  WP(CAL/CA)=-5.070E+00  DFJDTH(GM/CA)= 5.882E-03  SMDDTH(GM/CA)= 3.018E-03  SMVDTH(GM/CA)= 3.018E-04
 DQCDTH(CAL/CA)= 1.503E+00  DQRDTH(CAL/CA)= 4.883E-02  SVBDTH(GM/CA)= 5.759E-03  SDBDTH(GM/CA)= 4.182E-04  SLDDTH(GM/CA)= 5.066E-03
 SUMQL(CAL)= 1.304E+01  SUMFB(GM)= 7.177E-03  SFBDTH(GM/CA)= 7.177E-03  WKNET(CAL)=-2.714E+02  RR(CM3-ATM/GM-K)= 2.842E+00
 UCHAR(CM/SEC)= 3.219E+03  DVDTH(CM3/CA)=-5.704E+00  DELE12= 1.698E-03  ITERPC=    2
 XMNOE(GM)= 2.055E-05  YNOE= 8.303E-06  XNOE(PPM)= 8.068E+00  SOOTE(GM)= 1.264E-06

THETA(DEG.CA)=  -12.00   P(ATM)= 4.227E+01  V(CM3)= 1.779E+02  T(K)= 1.064E+03  U(CAL/GM)= 7.623E+01  PHEE= 2.894E-01
 DPDTH(ATM/CA)= 2.232E+00  WP(CAL/CA)=-5.311E+00  DFJDTH(GM/CA)= 5.882E-03  SMDDTH(GM/CA)= 5.913E-03  SMVDTH(GM/CA)= 5.913E-04
 DQCDTH(CAL/CA)= 1.805E+00  DQRDTH(CAL/CA)= 1.395E-01  SVBDTH(GM/CA)= 5.820E-03  SDBDTH(GM/CA)= 8.430E-04  SLDDTH(GM/CA)= 5.945E-03
 SUMQL(CAL)= 1.498E+01  SUMFB(GM)= 1.394E-02  SFBDTH(GM/CA)= 6.663E-03  WKNET(CAL)=-2.767E+02  RR(CM3-ATM/GM-K)= 2.850E+00
 UCHAR(CM/SEC)= 3.361E+03  DVDTH(CM3/CA)=-5.276E+00  DELE12= 7.927E-04  ITERPC=    2
 XMNOE(GM)= 7.734E-05  YNOE= 3.120E-05  XNOE(PPM)= 2.997E+01  SOOTE(GM)= 5.118E-06
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THETA(DEG.CA)=  -11.00   P(ATM)= 4.639E+01  V(CM3)= 1.728E+02  T(K)= 1.130E+03  U(CAL/GM)= 7.670E+01  PHEE= 3.226E-01
 DPDTH(ATM/CA)= 2.296E+00  WP(CAL/CA)=-5.418E+00  DFJDTH(GM/CA)= 5.882E-03  SMDDTH(GM/CA)= 8.606E-03  SMVDTH(GM/CA)= 8.606E-04
 DQCDTH(CAL/CA)= 2.063E+00  DQRDTH(CAL/CA)= 2.196E-01  SVBDTH(GM/CA)= 4.623E-03  SDBDTH(GM/CA)= 1.420E-03  SLDDTH(GM/CA)= 7.142E-03
 SUMQL(CAL)= 1.726E+01  SUMFB(GM)= 1.998E-02  SFBDTH(GM/CA)= 6.043E-03  WKNET(CAL)=-2.821E+02  RR(CM3-ATM/GM-K)= 2.857E+00
 UCHAR(CM/SEC)= 3.498E+03  DVDTH(CM3/CA)=-4.845E+00  DELE12= 6.577E-04  ITERPC=    2
 XMNOE(GM)= 1.700E-04  YNOE= 6.846E-05  XNOE(PPM)= 6.554E+01  SOOTE(GM)= 1.174E-05

THETA(DEG.CA)=  -10.00   P(ATM)= 5.017E+01  V(CM3)= 1.681E+02  T(K)= 1.195E+03  U(CAL/GM)= 7.703E+01  PHEE= 3.568E-01
 DPDTH(ATM/CA)= 2.443E+00  WP(CAL/CA)=-5.397E+00  DFJDTH(GM/CA)= 5.882E-03  SMDDTH(GM/CA)= 1.113E-02  SMVDTH(GM/CA)= 1.113E-03
 DQCDTH(CAL/CA)= 2.285E+00  DQRDTH(CAL/CA)= 2.879E-01  SVBDTH(GM/CA)= 2.351E-03  SDBDTH(GM/CA)= 2.471E-03  SLDDTH(GM/CA)= 9.414E-03
 SUMQL(CAL)= 1.983E+01  SUMFB(GM)= 2.471E-02  SFBDTH(GM/CA)= 4.822E-03  WKNET(CAL)=-2.875E+02  RR(CM3-ATM/GM-K)= 2.861E+00
 UCHAR(CM/SEC)= 3.629E+03  DVDTH(CM3/CA)=-4.412E+00  DELE12= 4.726E-04  ITERPC=    2
 XMNOE(GM)= 3.323E-04  YNOE= 1.336E-04  XNOE(PPM)= 1.277E+02  SOOTE(GM)= 2.255E-05

THETA(DEG.CA)=   -9.00   P(ATM)= 5.317E+01  V(CM3)= 1.640E+02  T(K)= 1.222E+03  U(CAL/GM)= 7.752E+01  PHEE= 3.910E-01
 DPDTH(ATM/CA)= 2.513E+00  WP(CAL/CA)=-5.236E+00  DFJDTH(GM/CA)= 5.882E-03  SMDDTH(GM/CA)= 1.293E-02  SMVDTH(GM/CA)= 1.293E-03
 DQCDTH(CAL/CA)= 2.478E+00  DQRDTH(CAL/CA)= 3.442E-01  SVBDTH(GM/CA)= 3.794E-04  SDBDTH(GM/CA)= 2.866E-03  SLDDTH(GM/CA)= 5.503E-03
 SUMQL(CAL)= 2.266E+01  SUMFB(GM)= 2.795E-02  SFBDTH(GM/CA)= 3.245E-03  WKNET(CAL)=-2.927E+02  RR(CM3-ATM/GM-K)= 2.864E+00
 UCHAR(CM/SEC)= 3.755E+03  DVDTH(CM3/CA)=-3.977E+00  DELE12= 1.088E-03  ITERPC=    2
 XMNOE(GM)= 5.820E-04  YNOE= 2.336E-04  XNOE(PPM)= 2.231E+02  SOOTE(GM)= 3.754E-05

THETA(DEG.CA)=   -8.00   P(ATM)= 5.623E+01  V(CM3)= 1.602E+02  T(K)= 1.260E+03  U(CAL/GM)= 7.786E+01  PHEE= 4.252E-01
 DPDTH(ATM/CA)= 2.470E+00  WP(CAL/CA)=-4.968E+00  DFJDTH(GM/CA)= 5.882E-03  SMDDTH(GM/CA)= 1.482E-02  SMVDTH(GM/CA)= 1.482E-03
 DQCDTH(CAL/CA)= 2.618E+00  DQRDTH(CAL/CA)= 3.921E-01  SVBDTH(GM/CA)= 3.901E-04  SDBDTH(GM/CA)= 3.185E-03  SLDDTH(GM/CA)= 5.492E-03
 SUMQL(CAL)= 2.567E+01  SUMFB(GM)= 3.153E-02  SFBDTH(GM/CA)= 3.575E-03  WKNET(CAL)=-2.977E+02  RR(CM3-ATM/GM-K)= 2.857E+00
 UCHAR(CM/SEC)= 3.876E+03  DVDTH(CM3/CA)=-3.540E+00  DELE12= 1.866E-03  ITERPC=    2
 XMNOE(GM)= 8.605E-04  YNOE= 3.449E-04  XNOE(PPM)= 3.290E+02  SOOTE(GM)= 5.518E-05

THETA(DEG.CA)=   -7.00   P(ATM)= 5.930E+01  V(CM3)= 1.569E+02  T(K)= 1.297E+03  U(CAL/GM)= 7.799E+01  PHEE= 4.595E-01
 DPDTH(ATM/CA)= 2.478E+00  WP(CAL/CA)=-4.635E+00  DFJDTH(GM/CA)= 5.882E-03  SMDDTH(GM/CA)= 1.682E-02  SMVDTH(GM/CA)= 1.682E-03
 DQCDTH(CAL/CA)= 2.760E+00  DQRDTH(CAL/CA)= 4.432E-01  SVBDTH(GM/CA)= 4.006E-04  SDBDTH(GM/CA)= 3.305E-03  SLDDTH(GM/CA)= 5.432E-03
 SUMQL(CAL)= 2.987E+01  SUMFB(GM)= 3.523E-02  SFBDTH(GM/CA)= 3.706E-03  WKNET(CAL)=-3.024E+02  RR(CM3-ATM/GM-K)= 2.870E+00
 UCHAR(CM/SEC)= 3.994E+03  DVDTH(CM3/CA)=-3.101E+00  DELE12= 2.492E-03  ITERPC=    2
 XMNOE(GM)= 1.179E-03  YNOE= 4.718E-04  XNOE(PPM)= 4.495E+02  SOOTE(GM)= 7.510E-05

THETA(DEG.CA)=   -6.00   P(ATM)= 6.237E+01  V(CM3)= 1.546E+02  T(K)= 1.336E+03  U(CAL/GM)= 7.792E+01  PHEE= 4.937E-01
 DPDTH(ATM/CA)= 2.458E+00  WP(CAL/CA)=-4.234E+00  DFJDTH(GM/CA)= 5.882E-03  SMDDTH(GM/CA)= 1.890E-02  SMVDTH(GM/CA)= 1.890E-03
 DQCDTH(CAL/CA)= 2.960E+00  DQRDTH(CAL/CA)= 4.969E-01  SVBDTH(GM/CA)= 4.108E-04  SDBDTH(GM/CA)= 3.504E-03  SLDDTH(GM/CA)= 5.472E-03
 SUMQL(CAL)= 3.227E+01  SUMFB(GM)= 3.915E-02  SFBDTH(GM/CA)= 3.915E-03  WKNET(CAL)=-3.066E+02  RR(CM3-ATM/GM-K)= 2.873E+00
 UCHAR(CM/SEC)= 4.107E+03  DVDTH(CM3/CA)=-2.661E+00  DELE12= 3.279E-03  ITERPC=    2
 XMNOE(GM)= 1.532E-03  YNOE= 6.123E-04  XNOE(PPM)= 5.827E+02  SOOTE(GM)= 9.702E-05

THETA(DEG.CA)=   -5.00   P(ATM)= 6.535E+01  V(CM3)= 1.516E+02  T(K)= 1.374E+03  U(CAL/GM)= 7.751E+01  PHEE= 5.279E-01
 DPDTH(ATM/CA)= 2.414E+00  WP(CAL/CA)=-3.764E+00  DFJDTH(GM/CA)= 5.882E-03  SMDDTH(GM/CA)= 2.105E-02  SMVDTH(GM/CA)= 2.105E-03
 DQCDTH(CAL/CA)= 3.039E+00  DQRDTH(CAL/CA)= 5.518E-01  SVBDTH(GM/CA)= 4.207E-04  SDBDTH(GM/CA)= 3.651E-03  SLDDTH(GM/CA)= 5.462E-03
 SUMQL(CAL)= 3.596E+01  SUMFB(GM)= 4.322E-02  SFBDTH(GM/CA)= 4.072E-03  WKNET(CAL)=-3.103E+02  RR(CM3-ATM/GM-K)= 2.876E+00
 UCHAR(CM/SEC)= 4.219E+03  DVDTH(CM3/CA)=-2.219E+00  DELE12= 3.874E-03  ITERPC=    2
 XMNOE(GM)= 1.866E-03  YNOE= 7.444E-04  XNOE(PPM)= 7.076E+02  SOOTE(GM)= 1.200E-04
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THETA(DEG.CA)=   -4.00   P(ATM)= 6.827E+01  V(CM3)= 1.436E+02  T(K)= 1.413E+03  U(CAL/GM)= 7.687E+01  PHEE= 5.621E-01
 DPDTH(ATM/CA)= 2.338E+00  WP(CAL/CA)=-3.223E+00  DFJDTH(GM/CA)= 5.882E-03  SMDDTH(GM/CA)= 2.324E-02  SMVDTH(GM/CA)= 2.324E-03
 DDCDTH(CAL/CA)= 3.175E+00  DQRDTH(CAL/CA)= 6.080E-01  SVBDTH(GM/CA)= 4.306E-04  SDBDTH(GM/CA)= 3.743E-03  SLDDTH(GM/CA)= 5.452E-03
 SUMQL(CAL)= 3.964E+01  SUMF3(GM)= 4.739E-02  SFBDTH(GM/CA)= 4.173E-03  WKNET(CAL)=-3.136E+02  RR(CM3-ATM/GM-K)= 2.879E+00
 UCHAR(CM/SEC)= 4.325E+03  DVDTH(CM3/CA)=-1.777E+00  DELE12= 4.578E-03  ITERPC=    2
 XMNOE(GM)= 2.271E-03  YNOE= 9.048E-04  XNOE(PPM)= 8.591E+02  SOOTE(GM)= 1.444E-04

THETA(DEG.CA)=   -3.00   P(ATM)= 7.107E+01  V(CM3)= 1.480E+02  T(K)= 1.451E+03  U(CAL/GM)= 7.587E+01  PHEE= 5.963E-01
 DPDTH(ATM/CA)= 2.706E+00  WP(CAL/CA)=-2.615E+00  DFJDTH(GM/CA)= 5.882E-03  SMDDTH(GM/CA)= 2.544E-02  SMVDTH(GM/CA)= 2.544E-03
 DDCDTH(CAL/CA)= 3.306E+00  DQRDTH(CAL/CA)= 6.652E-01  SVBDTH(GM/CA)= 4.388E-04  SDBDTH(GM/CA)= 3.863E-03  SLDDTH(GM/CA)= 5.444E-03
 SUMQL(CAL)= 4.361E+01  SUMF3(GM)= 5.169E-02  SFBDTH(GM/CA)= 4.301E-03  WKNET(CAL)=-3.162E+02  RR(CM3-ATM/GM-K)= 2.882E+00
 UCHAR(CM/SEC)= 4.429E+03  DVDTH(CM3/CA)=-1.333E+00  DELE12= 5.170E-03  ITERPC=    2
 XMNOE(GM)= 2.702E-03  YNOE= 1.074E-03  XNOE(PPM)= 1.019E+03  SOOTE(GM)= 1.702E-04

THETA(DEG.CA)=   -2.00   P(ATM)= 7.377E+01  V(CM3)= 1.469E+02  T(K)= 1.490E+03  U(CAL/GM)= 7.535E+01  PHEE= 5.963E-01
 DPDTH(ATM/CA)= 1.994E+00  WP(CAL/CA)=-1.941E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 2.767E-02  SMVDTH(GM/CA)= 2.767E-03
 DDCDTH(CAL/CA)= 3.433E+00  DQRDTH(CAL/CA)= 7.234E-01  SVBDTH(GM/CA)= 4.472E-04  SDBDTH(GM/CA)= 4.073E-03  SLDDTH(GM/CA)= 5.435E-03
 SUMQL(CAL)= 4.777E+01  SUMF3(GM)= 5.621E-02  SFBDTH(GM/CA)= 4.521E-03  WKNET(CAL)=-3.181E+02  RR(CM3-ATM/GM-K)= 2.886E+00
 UCHAR(CM/SEC)= 4.531E+03  DVDTH(CM3/CA)=-8.892E-01  DELE12= 6.031E-03  ITERPC=    2
 XMNOE(GM)= 3.100E-03  YNOE= 1.230E-03  XNOE(PPM)= 1.166E+03  SOOTE(GM)= 1.968E-04

THETA(DEG.CA)=   -1.00   P(ATM)= 7.622E+01  V(CM3)= 1.462E+02  T(K)= 1.528E+03  U(CAL/GM)= 7.513E+01  PHEE= 5.963E-01
 DPDTH(ATM/CA)= 1.720E+00  WP(CAL/CA)=-1.205E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 2.923E-02  SMVDTH(GM/CA)= 2.923E-03
 DDCDTH(CAL/CA)= 3.555E+00  DQRDTH(CAL/CA)= 7.838E-01  SVBDTH(GM/CA)= 4.551E-04  SDBDTH(GM/CA)= 4.103E-03  SLDDTH(GM/CA)= 5.427E-03
 SUMQL(CAL)= 5.211E+01  SUMF3(GM)= 6.377E-02  SFBDTH(GM/CA)= 4.558E-03  WKNET(CAL)=-3.193E+02  RR(CM3-ATM/GM-K)= 2.890E+00
 UCHAR(CM/SEC)= 4.530E+03  DVDTH(CM3/CA)=-4.447E-01  DELE12= 8.554E-03  ITERPC=    1
 XMNOE(GM)= 3.471E-03  YNOE= 1.375E-03  XNOE(PPM)= 1.301E+03  SOOTE(GM)= 2.221E-04

THETA(DEG.CA)=    1.00   P(ATM)= 7.844E+01  V(CM3)= 1.462E+02  T(K)= 1.567E+03  U(CAL/GM)= 7.372E+01  PHEE= 5.963E-01
 DPDTH(ATM/CA)= 9.328E-01  WP(CAL/CA)= 4.225E-01  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 3.070E-02  SMVDTH(GM/CA)= 3.070E-03
 DDCDTH(CAL/CA)= 3.726E+00  DQRDTH(CAL/CA)= 8.413E-01  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 2.790E-03  SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 6.116E+01  SUMF3(GM)= 6.635E-02  SFBDTH(GM/CA)= 2.790E-03  WKNET(CAL)=-3.193E+02  RR(CM3-ATM/GM-K)= 2.894E+00
 UCHAR(CM/SEC)= 4.530E+03  DVDTH(CM3/CA)= 4.447E-01  DELE12= 6.360E-03  ITERPC=    1
 XMNOE(GM)= 4.140E-03  YNOE= 1.637E-03  XNOE(PPM)= 1.546E+03  SOOTE(GM)= 2.622E-04

THETA(DEG.CA)=    3.00   P(ATM)= 7.916E+01  V(CM3)= 1.480E+02  T(K)= 1.597E+03  U(CAL/GM)= 6.540E+01  PHEE= 5.963E-01
 DPDTH(ATM/CA)= 2.201E-01  WP(CAL/CA)= 2.129E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 3.168E-02  SMVDTH(GM/CA)= 3.168E-03
 DDCDTH(CAL/CA)= 3.803E+00  DQRDTH(CAL/CA)= 8.667E-01  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 2.377E-03  SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 7.346E+01  SUMF3(GM)= 7.174E-02  SFBDTH(GM/CA)= 2.377E-03  WKNET(CAL)=-3.159E+02  RR(CM3-ATM/GM-K)= 2.895E+00
 UCHAR(CM/SEC)= 4.530E+03  DVDTH(CM3/CA)= 1.333E+00  DELE12= 5.444E-03  ITERPC=    1
 XMNOE(GM)= 4.625E-03  YNOE= 1.825E-03  XNOE(PPM)= 1.723E+03  SOOTE(GM)= 2.873E-04

THETA(DEG.CA)=    4.00   P(ATM)= 7.901E+01  V(CM3)= 1.496E+02  T(K)= 1.609E+03  U(CAL/GM)= 6.218E+01  PHEE= 5.963E-01
 DPDTH(ATM/CA)=-1.239E-01  WP(CAL/CA)= 2.979E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 3.199E-02  SMVDTH(GM/CA)= 3.199E-03
 DDCDTH(CAL/CA)= 3.823E+00  DQRDTH(CAL/CA)= 9.719E-01  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 2.234E-03  SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 7.515E+01  SUMF3(GM)= 7.398E-02  SFBDTH(GM/CA)= 2.234E-03  WKNET(CAL)=-3.129E+02  RR(CM3-ATM/GM-K)= 2.895E+00
 UCHAR(CM/SEC)= 4.531E+03  DVDTH(CM3/CA)= 1.777E+00  DELE12= 4.877E-03  ITERPC=    1
 XMNOE(GM)= 4.812E-03  YNOE= 1.897E-03  XNOE(PPM)= 1.790E+03  SOOTE(GM)= 2.964E-04
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THETA(DEG.CA)=    5.00   P(ATM)= 7.856E+01  V(CM3)= 1.516E+02  T(K)= 1.619E+03  U(CAL/GM)= 5.877E+01  PHEE= 5.963E-01
 DPDTH(ATM/CA)=-4.459E-01  WP(CAL/CA)= 3.812E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 3.218E-02  SMVDTH(GM/CA)= 3.218E-03
 DQCDTH(CAL/CA)= 3.830E+00  DQRDTH(CAL/CA)= 8.724E-01  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 2.089E-03  SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 7.935E+01  SUMFB(GM)= 7.607E-02  SFBDTH(GM/CA)= 2.089E-03  WKNET(CAL)=-3.091E+02  RR(CM3-ATM/GM-K)= 2.896E+00
 UCHAR(CM/SEC)= 4.531E+03  DVDTH(CM3/CA)= 2.219E+00  DELE12= 4.657E-03  ITERPC=    1
 XMNOE(GM)= 4.974E-03  YNOE= 1.959E-03  XNOE(PPM)= 1.848E+03  SOOTE(GM)= 3.039E-04

THETA(DEG.CA)=    7.00   P(ATM)= 7.675E+01  V(CM3)= 1.569E+02  T(K)= 1.635E+03  U(CAL/GM)= 5.109E+01  PHEE= 5.963E-01
 DPDTH(ATM/CA)=-1.023E+00  WP(CAL/CA)= 5.392E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 3.218E-02  SMVDTH(GM/CA)= 3.218E-03
 DQCDTH(CAL/CA)= 3.813E+00  DQRDTH(CAL/CA)= 8.653E-01  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 1.821E-03  SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 8.923E+01  SUMFB(GM)= 7.993E-02  SFBDTH(GM/CA)= 1.821E-03  WKNET(CAL)=-2.991E+02  RR(CM3-ATM/GM-K)= 2.897E+00
 UCHAR(CM/SEC)= 4.533E+03  DVDTH(CM3/CA)= 3.101E+00  DELE12= 4.372E-03  ITERPC=    1
 XMNOE(GM)= 5.239E-03  YNOE= 2.060E-03  XNOE(PPM)= 1.944E+03  SOOTE(GM)= 3.154E-04

THETA(DEG.CA)=    9.00   P(ATM)= 7.393E+01  V(CM3)= 1.640E+02  T(K)= 1.643E+03  U(CAL/GM)= 4.233E+01  PHEE= 5.963E-01
 DPDTH(ATM/CA)=-1.505E+00  WP(CAL/CA)= 6.799E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 3.172E-02  SMVDTH(GM/CA)= 3.172E-03
 DQCDTH(CAL/CA)= 3.754E+00  DQRDTH(CAL/CA)= 8.453E-01  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 1.586E-03  SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 9.847E+01  SUMFB(GM)= 8.312E-02  SFBDTH(GM/CA)= 1.586E-03  WKNET(CAL)=-2.862E+02  RR(CM3-ATM/GM-K)= 2.897E+00
 UCHAR(CM/SEC)= 4.534E+03  DVDTH(CM3/CA)= 3.977E+00  DELE12= 4.099E-03  ITERPC=    1
 XMNOE(GM)= 5.452E-03  YNOE= 2.141E-03  XNOE(PPM)= 2.020E+03  SOOTE(GM)= 3.225E-04

THETA(DEG.CA)=   11.00   P(ATM)= 7.032E+01  V(CM3)= 1.728E+02  T(K)= 1.646E+03  U(CAL/GM)= 3.256E+01  PHEE= 5.963E-01
 DPDTH(ATM/CA)=-1.876E+00  WP(CAL/CA)= 7.987E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 3.088E-02  SMVDTH(GM/CA)= 3.088E-03
 DQCDTH(CAL/CA)= 3.661E+00  DQRDTH(CAL/CA)= 8.132E-01  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 1.328E-03  SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 1.075E+02  SUMFB(GM)= 8.590E-02  SFBDTH(GM/CA)= 1.328E-03  WKNET(CAL)=-2.708E+02  RR(CM3-ATM/GM-K)= 2.896E+00
 UCHAR(CM/SEC)= 4.537E+03  DVDTH(CM3/CA)= 4.845E+00  DELE12= 3.491E-03  ITERPC=    1
 XMNOE(GM)= 5.615E-03  YNOE= 2.203E-03  XNOE(PPM)= 2.078E+03  SOOTE(GM)= 3.261E-04

THETA(DEG.CA)=   12.00   P(ATM)= 6.828E+01  V(CM3)= 1.779E+02  T(K)= 1.644E+03  U(CAL/GM)= 2.746E+01  PHEE= 5.963E-01
 DPDTH(ATM/CA)=-2.058E+00  WP(CAL/CA)= 8.492E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 3.035E-02  SMVDTH(GM/CA)= 3.035E-03
 DQCDTH(CAL/CA)= 3.604E+00  DQRDTH(CAL/CA)= 7.940E-01  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 1.210E-03  SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 1.119E+02  SUMFB(GM)= 8.711E-02  SFBDTH(GM/CA)= 1.210E-03  WKNET(CAL)=-2.623E+02  RR(CM3-ATM/GM-K)= 2.896E+00
 UCHAR(CM/SEC)= 4.538E+03  DVDTH(CM3/CA)= 5.276E+00  DELE12= 3.315E-03  ITERPC=    1
 XMNOE(GM)= 5.694E-03  YNOE= 2.229E-03  XNOE(PPM)= 2.103E+03  SOOTE(GM)= 3.272E-04

THETA(DEG.CA)=   13.00   P(ATM)= 6.613E+01  V(CM3)= 1.833E+02  T(K)= 1.641E+03  U(CAL/GM)= 2.214E+01  PHEE= 5.963E-01
 DPDTH(ATM/CA)=-2.117E+00  WP(CAL/CA)= 8.936E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 2.975E-02  SMVDTH(GM/CA)= 2.975E-03
 DQCDTH(CAL/CA)= 3.541E+00  DQRDTH(CAL/CA)= 7.725E-01  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 1.105E-03  SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 1.162E+02  SUMFB(GM)= 8.822E-02  SFBDTH(GM/CA)= 1.105E-03  WKNET(CAL)=-2.534E+02  RR(CM3-ATM/GM-K)= 2.895E+00
 UCHAR(CM/SEC)= 4.540E+03  DVDTH(CM3/CA)= 5.704E+00  DELE12= 2.936E-03  ITERPC=    1
 XMNOE(GM)= 5.742E-03  YNOE= 2.251E-03  XNOE(PPM)= 2.124E+03  SOOTE(GM)= 3.277E-04

THETA(DEG.CA)=   15.00   P(ATM)= 6.168E+01  V(CM3)= 1.956E+02  T(K)= 1.633E+03  U(CAL/GM)= 1.139E+01  PHEE= 5.963E-01
 DPDTH(ATM/CA)=-2.235E+00  WP(CAL/CA)= 9.644E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 2.840E-02  SMVDTH(GM/CA)= 2.840E-03
 DQCDTH(CAL/CA)= 3.402E+00  DQRDTH(CAL/CA)= 7.257E-01  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 9.021E-04  SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 1.246E+02  SUMFB(GM)= 9.012E-02  SFBDTH(GM/CA)= 9.021E-04  WKNET(CAL)=-2.344E+02  RR(CM3-ATM/GM-K)= 2.894E+00
 UCHAR(CM/SEC)= 4.544E+03  DVDTH(CM3/CA)= 6.553E+00  DELE12= 2.708E-03  ITERPC=    1
 XMNOE(GM)= 5.826E-03  YNOE= 2.282E-03  XNOE(PPM)= 2.154E+03  SOOTE(GM)= 3.280E-04
```

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THETA(DEG.CA)=   17.00   P(ATM)= 5.716E+01  V(CM3)= 2.095E+02  T(K)= 1.620E+03  U(CAL/GM)= 4.303E-01  PHEE= 5.963E-01
 DPDTH(ATM/CA)=-2.253E+00  WP(CAL/CA)= 1.013E+01  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 2.693E-02  SMVDTH(GM/CA)= 2.693E-03
 DQCDTH(CAL/CA)= 3.252E+00  DQRDTH(CAL/CA)= 6.767E-01  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 7.084E-04  SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 1.325E+02  SUMF3(GM)= 9.163E-02  SFBDTH(GM/CA)= 7.084E-04  WKNET(CAL)=-2.144E+02  RR(CM3-ATM/GM-K)= 2.894E+00
 UCHAR(CM/SEC)= 4.544E+03  DVDTH(CM3/CA)= 7.389E+00  DELE12= 2.617E-03  ITERPC=    1
 XMNOE(GM)= 5.884E-03  YNOE= 2.303E-03  XNOE(PPM)= 2.175E+03  SOOTE(GM)= 3.275E-04

THETA(DEG.CA)=   19.00   P(ATM)= 5.270E+01  V(CM3)= 2.251E+02  T(K)= 1.605E+03  U(CAL/GM)=-1.072E+01  PHEE= 5.963E-01
 DPDTH(ATM/CA)=-2.206E+00  WP(CAL/CA)= 1.043E+01  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 2.540E-02  SMVDTH(GM/CA)= 2.540E-03
 DQCDTH(CAL/CA)= 3.098E+00  DQRDTH(CAL/CA)= 6.287E-01  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 5.497E-04  SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 1.401E+02  SUMF3(GM)= 9.280E-02  SFBDTH(GM/CA)= 5.497E-04  WKNET(CAL)=-1.936E+02  RR(CM3-ATM/GM-K)= 2.892E+00
 UCHAR(CM/SEC)= 4.552E+03  DVDTH(CM3/CA)= 8.211E+00  DELE12= 2.329E-03  ITERPC=    1
 XMNOE(GM)= 5.921E-03  YNOE= 2.317E-03  XNOE(PPM)= 2.188E+03  SOOTE(GM)= 3.268E-04

THETA(DEG.CA)=   21.00   P(ATM)= 4.841E+01  V(CM3)= 2.424E+02  T(K)= 1.597E+03  U(CAL/GM)=-2.185E+01  PHEE= 5.963E-01
 DPDTH(ATM/CA)=-2.106E+00  WP(CAL/CA)= 1.056E+01  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 2.388E-02  SMVDTH(GM/CA)= 2.388E-03
 DQCDTH(CAL/CA)= 2.944E+00  DQRDTH(CAL/CA)= 5.822E-01  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 4.291E-04  SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 1.472E+02  SUMF3(GM)= 9.372E-02  SFBDTH(GM/CA)= 4.291E-04  WKNET(CAL)=-1.726E+02  RR(CM3-ATM/GM-K)= 2.891E+00
 UCHAR(CM/SEC)= 4.557E+03  DVDTH(CM3/CA)= 9.017E+00  DELE12= 2.036E-03  ITERPC=    1
 XMNOE(GM)= 5.944E-03  YNOE= 2.325E-03  XNOE(PPM)= 2.197E+03  SOOTE(GM)= 3.260E-04

THETA(DEG.CA)=   23.00   P(ATM)= 4.440E+01  V(CM3)= 2.612E+02  T(K)= 1.569E+03  U(CAL/GM)=-3.271E+01  PHEE= 5.963E-01
 DPDTH(ATM/CA)=-1.970E+00  WP(CAL/CA)= 1.056E+01  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 2.239E-02  SMVDTH(GM/CA)= 2.239E-03
 DQCDTH(CAL/CA)= 2.794E+00  DQRDTH(CAL/CA)= 5.391E-01  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 3.429E-04  SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 1.540E+02  SUMF3(GM)= 9.445E-02  SFBDTH(GM/CA)= 3.429E-04  WKNET(CAL)=-1.514E+02  RR(CM3-ATM/GM-K)= 2.890E+00
 UCHAR(CM/SEC)= 4.562E+03  DVDTH(CM3/CA)= 9.807E+00  DELE12= 2.093E-03  ITERPC=    1
 XMNOE(GM)= 5.955E-03  YNOE= 2.329E-03  XNOE(PPM)= 2.202E+03  SOOTE(GM)= 3.253E-04

THETA(DEG.CA)=   25.00   P(ATM)= 4.062E+01  V(CM3)= 2.816E+02  T(K)= 1.549E+03  U(CAL/GM)=-4.368E+01  PHEE= 5.963E-01
 DPDTH(ATM/CA)=-1.834E+00  WP(CAL/CA)= 1.045E+01  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 2.097E-02  SMVDTH(GM/CA)= 2.097E-03
 DQCDTH(CAL/CA)= 2.650E+00  DQRDTH(CAL/CA)= 4.984E-01  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 2.879E-04  SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 1.634E+02  SUMF3(GM)= 9.504E-02  SFBDTH(GM/CA)= 2.879E-04  WKNET(CAL)=-1.305E+02  RR(CM3-ATM/GM-K)= 2.887E+00
 UCHAR(CM/SEC)= 4.568E+03  DVDTH(CM3/CA)= 1.058E+01  DELE12= 1.336E-03  ITERPC=    1
 XMNOE(GM)= 5.961E-03  YNOE= 2.330E-03  XNOE(PPM)= 2.205E+03  SOOTE(GM)= 3.246E-04

THETA(DEG.CA)=   30.00   P(ATM)= 3.252E+01  V(CM3)= 3.391E+02  T(K)= 1.494E+03  U(CAL/GM)=-6.948E+01  PHEE= 5.963E-01
 DPDTH(ATM/CA)=-1.521E+00  WP(CAL/CA)= 9.961E+00  DFJDTH(GM/CA)= 0.          SMDDTH(GM/CA)= 1.837E-02  SMVDTH(GM/CA)= 1.837E-03
 DQCDTH(CAL/CA)= 2.414E+00  DQRDTH(CAL/CA)= 4.187E-01  SVBDTH(GM/CA)= 0.          SDBDTH(GM/CA)= 2.466E-04  SLDDTH(GM/CA)= 0.
 SUMQL(CAL)= 1.751E+02  SUMF3(GM)= 9.633E-02  SFBDTH(GM/CA)= 2.466E-04  WKNET(CAL)=-7.989E+01  RR(CM3-ATM/GM-K)= 2.894E+00
 UCHAR(CM/SEC)= 4.579E+03  DVDTH(CM3/CA)= 1.242E+01  DELE12= 5.082E-04  ITERPC=    1
 XMNOE(GM)= 5.964E-03  YNOE= 2.330E-03  XNOE(PPM)= 2.207E+03  SOOTE(GM)= 3.219E-04

   ----- INDICATED ENGINE PERFORMACE AND ENGINE EMISSION -----

                 I.M.E.P.(PSI)=   7.463E+01
                 I.H.P.(HP)=   2.015E+01
                 I.S.F.C.(LB/HP-HR)=   4.924E-01
                 SOOT(MG/M3STP)=   1.454E+02
                 NITRIC OXIDE(PPM)=   2.207E+03
```

VI. PROGRAM STATISTICS

The computer program is coded in standard FORTRAN IV, and the version is currently compiled and optimized in FTN (FORTRAN Extended) mode and ran on a CDC 6600 computer. The computer statistics (based on the sample case presented in preceding section) are shown in the Table below.

Compilation Time	71 sec.
Run Time	128 sec.
Core Used	120 K (octal)
Tape Required	1 (7 track)
Compilation I/O Time	98 sec.
Run I/O Time	6 sec.

VII. REFERENCES

1. Kau, C.J., Tyson, T.J. and Heap, M.P. "Study of the Oxides of Nitrogen and Carbon Formation in Diesel Engines". Final Report Phase II and III, Ultrasystems, Inc., June, 1975.

2. Gordon, S. and McBride, B.J. "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouguet Detonation", NASA SP-273, NASA Lewis Research Center, 1971.

APPENDIX: FORTRAN LISTING OF DIESEL ENGINE PROGRAM

The subroutines follow the main program are listed in alphabetical order.

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*DECK MAIN
      PROGRAM MAIN(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE8)
C     SINGLE-CYLINDERED DIESEL ENGINE ENGINE ANALYSIS
C CYCLE THERMODYNAMICS MODIFIED (12/2/74,CJK)
C CYCLE THERMODYNAMICS MODIFIED (12/5/74,CJK)
C EQUILIBRIUM COMPOSITION CALCULATIONS MODIFIED (1/30/75,CJK)
C VITIATION ADDED AND IGNITION DELAY MODIFIED (2/12/75,CJK)
C Q-S THIN FLAME IN FINITE SPACE FOR HET. NO RATE INCLUDED (3/27/75,CJK)
C NUMERICAL SCHEME REFINED (4/30/75,CJK)
C ENTIRE PROGRAM CLEANED AND STORED IN A PERMANENT FILE (5/12/75,CJK)
C VERSION B ..... IMPROVE COMPUTATIONAL EFFICIENCY BY 20 PERCENT (6/1/75,CJK)
      DIMENSION IDD(8)
      DIMENSION DTBDTH(100),DNODTH(100),DMSDTH(100),DAPDTH(100),
     1 DPHDTH(100),XFIDTH(100),XAIDTH(100), QBM(100),DMDDTH(100),
     2 DMVDTH(100),DCMDTH(100),BTABM(100),GBM(100),AAM(100),BBM(100),
     3 YNO(100),YS(100),XMNO(100)
      DIMENSION TBMO(100),DTBDTO(100),XMNOO(100),DNODTO(100),XMSOTO(100)
     2          ,DMSDTO(100),XMFBMO(100),XMPAMO(100)
     3          ,XFIDTO(100),XAIDTO(100),DIO(100,5),XKKO(100,5)
     4          ,QBMO(100),DMDDTO(100),DMVDTO(100),DLBDTO(100)
      COMMON/INTEGR/ INO1,INO2,ISOOT,IWETBT,NPRT,IDTAIL,NTER,NAXIL,
     1               NSHEL,NSZG,NITST,IBUG,II,III
      COMMON/SPECYI/  XH2(100),XH2O(100),XCO(100),XCO2(100),XN2(100),
     1                XNO(100),XOH(100),XH(100),XO(100),XN(100),XO2(100)
     2                ,XCH4(100),XNONEQ(100)
      COMMON/PRATEI/ DNODT1(100),DNODT2(100),DMSDT1(100),DMSDT2(100),
     1               DRMDTH(100),DLBDTH(100),XMDF(100)
      COMMON/TPROPI/ P,TBM(100),UBM(100),HBM(100),VBM(100),CPBM(100),
     1               AMWBM(100),RBM(100),PHE(100),AFR(100),XMFBM(100),
     2               XMPAM(100)
      COMMON /AIRP/ XMAI,XMFJ,XMEGR,XMRD,XMAO,XMARD,XMAEGR,XMFRD,XMFEGR,
     1              AMWA,AFRA,FARA,PHEA
      COMMON/FUELP/W,XX,YFL,ZFL,YSTOA,ZSTOA,API,FDEN,FAROS,AMWF,SURFT
     1            ,XMUF,CEN,OXST,HCOM
      COMMON/DROPC/ HUTIM,DTPHY,XTLYO2,CPBAR,RHOD,TCRITF,XL298,
     1              XMBM(100),DVBDTH(100),DLDDTH(100),XMFLI(100),
     2              DI(100,3),DMFLI(100,3),DMLDT(100,3),XNDI(100,3),
     3              XKK(100,3)
      COMMON /SHEAT/ HFCO2,HFH2O,DHVH2O,HFH2OG ,CPFL,CPFV,DHFV,HHV,TBPF
     1               ,HFJ,TFJ,HFFL,UFFL
      COMMON /SOOTP/ SDEN,DSOOT, ASOTP,ASOTA,XMSOOT(100)
      COMMON/RANGS/ TRANG1,TRANG2,PRANG1,PRANG2,PHERG1,PHERG2
      COMMON /PDRVI/ PUPP,PUPT,PRPF,PUPF,PRPT,PRPP
      COMMON/PDRVIZ/ PUPPBM(100),PUPTBM(100),PRPFBM(100),PUPFBM(100),
     1               PRPTBM(100),PRPPBM(100)
      COMMON/CONVF/ XJ,ATD,DTR,XK,SIG,R,RU,DTDTH,DTHDT,DTRDT,PI
      COMMON/SCA/ THEMAX,THEIJ,THEIG,DINJ,THENB,THEVO,THEVC,DTINJ,
     1            DTHMIN,DTHMED,DTHMAX,DTHETA,DT
      COMMON/ENGEO/ DE,RFW,RL,VC,SC,S,USI,CR,RPM,TW,DNOZZ,NNOZZ,DBOWL,
     1              VFJO
      COMMON/SPTAB/ NPTB,NTTB,NPHTB,PTB(7),TTB(13),PHETB(11),
     *              XH2TB(7,13,11),XH2OTB(7,13,11),XCOTB(7,13,11),
     1              XCO2TB(7,13,11),XN2TB(7,13,11),XNOTB(7,13,11),
     2              XOHTB(7,13,11),XHTB(7,13,11),XOTB(7,13,11),
     3              XNTB(7,13,11),XO2TB(7,13,11),XCH4TB(7,13,11)
      NAMELIST /GIVEN/ DE,RFW,RL,CR,SC,TW,RPM    ,SCR,DNOZZ,NNOZZ,DBOWL,
     1                 THEVC,THEVO,XMAI    ,EGR     ,XMRD,OMEGA,NSTROK,
     2                 THEIJ,DINJ,XMFJ,PINJ,TFJ,
     3                 W,XX,FDEN,CEN,API,XMUF,SURFT,
     4                 TBPF,TCRITF,CPFL,CPFV,CVFV,DHFV,HFFL,HCOM
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      NAMELIST/CPARAM/ IN01,IN02,ISOOT,IBUG        ,NTER,NPRT,MAXIL,NSHEL
     1                ,NSZG,IDROPP,IRATEP,ISPCYP,IWETBT,IDTAIL,NITST
     2                ,DTHMIN,DTHMED,DTHMAX,THEMAX
     3                ,EPSIT,EPSIP,EPSINO,EPSIST
      NAMELIST/EPARAM/ CA,CB,CNOR,      CVIDI,CMIX,SDEN,DSOOT,ASOTA,ASOTP
     1                 ,HUTIM,DTPHY,SEFJ      ,COCHG,CEVAP,CBURN,AIGND
     2                 ,RHOD,CPGAR,XTLYO2
      NAMELIST /INITL/ THETAI,THEMAX,P,T,V,UA,HA,XMAO,AMWA ,FARA,PHEA,
     1                 FAROS,XMEGR,XMAEGR,XMFEGR,XMRD,XMARD,XMFRD,AMWF,
     2                 OXST,XO2A,FDEN,HHV,HCOM,HFFL,HFJ,VC,VDIS,VFJO
C   CONSTANTS
C UNIVERSAL GAS CONSTANTS IN CM3-ATM/G-MOLE-K
      R=82.054
C UNIVERSAL GAS CONSTANTS IN CAL/G-MOLE-K
      RU=1.987
C  THERMAL CONDUCTIVITY CAL/CM-SEC-K
      XK= 3.4165E-4
C S-B CONSTANT IN CAL/SEC-CM2-K4
      STG= 1.3538E-12
C HEAT OF FORMATION (CAL/MOLE) OF CO2, H2O AT 298 K
      HFCO2=-94.05E3
      HFH2O=-68.3 E3
      DHVH2O= 10.5E3
      HFH2OG= HFH2O+ DHVH2O
C  CONVERSION FACTORS
      PI= 3.141592654
      XJ= 4.18674E7
      ATD= 1.01325E6
      DTR= 3.14159/180.
      RORU= R/RU
      ATDXJ= ATD/XJ
C INPUT EQUILIBRIUM COMPOSITION TABLES FROM TAPE8
      CALL TAPEIN
C SPECIES TABLE RANGES
      PRANG1= PTB(1)
      PRANG2= PTB(NPTB)
      TRANG1= TTB(1)
      TRANG2= TTB(NTTB)
      PHERG1= PHETB(1)
      PHERG2= PHETB(NPHTB)
C PRE-SET ENGINE PARAMETERS AND FUELING PROPERTIES
      HFFL= 0.0
      XMRD= 0.0
      FDEN= 0.0
      HCOM= 0.0
      READ (5,GIVEN)
      WRITE(6,GIVEN)
    1 CONTINUE
C PRE-SET CONTROL PARAMETERS
C  INTEGERS
      IN01= 1
      IN02= 1
      ISOOT= 1
      NPRT= 2
      IDTAIL= 0
      IRATEP= 0
      IDROPP= 0
      ISPCYP= 0
      NTER= 50
      NSZG= 3
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```
      NSHEL= 4
      NAXIL= 20
      NITST= 50
      IBUG= 0
      IWETBT= 0
      ICRITA= 0
      NSTROK= 4
C INTEGRATION STEP SIZE  (IN DEGREE C.A.)
      DTHMIN= 1.0
      DTHMED= 2.5
      DTHMAX= 5.0
      THEMAX= THEVO
C RELATIVE ERROR BOUNDS
      EPSIT= 2.0E-3
      EPSIP= 2.0E-3
      EPSINO= 1.0
      EPSIST= 1.0
C PRE-SET EMPIRICAL CONSTANTS
C AIR/PRODUCT MIXING
      CMIX=7.8E-3
      CVIDI= 0.1
C HETEROGENEOUS BRUNING RATE
      CBURN=  0.0
      XTLYO2= 0.02
C VAPORIZATION
      CEVAP= 0.276
      HUTIM= 2.0E-4
C IGNITION DELAY
      AIGND= 1.460E-4
C EMPIRICAL PARAMETERS ACCOUNT FOR SWIRL EFFECT ON SPRAY GROWTH
      SEFJ= 4.3
C NOZZLE DISCHARGE
      CDCHG= 1.0
C IGNITION DELAY
      DTPHY= 2.0E-4
C HEAT CONVECTION
      CA= 0.26
      CB= 0.75
C DROPLET
      RHOD= 3.0E-4
      CPBAR= 0.35
C NO KINETICS
      CNOR= 5.37
C SOOT KINETICS
      SDEN=2.0
      DSOOT=1.0E-4
      ASOTA= 3.52
      ASOTP= 3.52
C COEFFICIENTS FOR VAPOR PRESSURE (COX-ANTONIE EQ.)
      A= 4.091
      B= 1324.77
      C= 53.74
      PHEFG= 0.0
      WRITE(6,107)
C INPUT CASE IDENTIFICATION
      READ (5,99)(IDD(I),I=1,8)
      IF (EOF(5)) 999,34
   34 CONTINUE
      WRITE(6,99)(IDD(I),I=1,8)
C MODIFICATION OF CONTROL PARAMETERS THROUGH  NAMELIST INPUT
```

```
      READ (5,CPARAM)
      WRITE(6,CPARAM)
C MODIFICATION OF EMPIRICAL PARAMETERS THROUGH  NAMELIST INPUT
      READ (5,EPARAM)
      WRITE(6,EPARAM)
C MODIFICATION OF ENGINE PARAMETERS AND FUELING PROPERTIES THROUGH INPUT
      READ (5,GIVEN)
      WRITE(6,GIVEN)
      DTROT= RPM* 3.14159/30.
      DTHDT=6.0*RPM
      DTDTH=1.0/DTHDT
C MEAN SWIRL AND MEAN PISTON VELOCITIES
      USI= 0.25*DE*OMEGA
      UPBAR= RFW*RPM/15.
C  FUEL COMPOSITION C(W)H(XX)
C  THEORETICAL (O),(N) COMPOSITION FOR STOICHIOMETRIC BURNING O(YSTOA)N(ZSTOA
      YSTOA= 2.0*W+0.5*XX
      ZSTOA= 3.764*YSTOA
C  FUEL SPECIFICATION
C  MOLECULAR WEIGHTS OF FRESH AIR,FUEL AND THEORETICAL COMBUSTION PRODUCTS
      AMWAI=28.967
      AMWF= W*12.0+XX
      XL298= DHFV
      RFG=RU/AMWF
C  CALCULATE STOICHIOMETRIC F/A RATIO REFERENCE TO PURE AIR
      FAROS=AMWF/((W+0.25*XX)*(32.0+3.764*28.0))
      OXST= 0.232/FAROS
C  DENSITY OF LIQUID FUEL (GM/CM3)
      IF (FDEN.LE.0.0)
     1FDEN= 141.5/(API+131.5)*1.939*32.179/0.06243* 1.0E-3
C  FUEL INJECTION VELOCITY
      IDINJ= DINJ+ 0.5
      DINJ= IDINJ
      THEEIJ= THEIJ+DINJ
      DTINJ= DINJ*DTDTH
      XJF= XMFJ/DTINJ/NNOZZ
      ANOZZ= 0.25*PI*DNOZZ*DNOZZ
      VFJO= XJF/(FDEN*ANOZZ*CDCHG)
C NO. OF BURNING ZONES TO BE TREATED
      NXXX=(DINJ+0.001*DTHMIN)/DTHMIN
      NSS= NSHEL*NXXX
      XMFJ95= 0.95*XMFJ
      XMFJ99= 0.99*XMFJ
      IF (HCOM.NE.0.0) GO TO 39
C API FORMULA FOR HIGH HEATING VALUE OF FUEL
      HHV= (18650.+40.*(API-10.))/1.8*AMWF
C  HEAT OF COMBUSTION OR L.H.V.
      HCOM= HHV -0.5*XX*DHVH2O
C------ CONVERT ALL THE HEATS TO CAL/GM
      HHV=HHV/AMWF
      HCOM=HCOM/AMWF
   39 CONTINUE
C HEAT OF FORMATION (CAL/GM) OF FUEL AT 298 K
      IF (HFFL.NE.0.0) GO TO 40
      HFFL= HCOM*AMWF+ W*HFCO2+ 0.5*XX*HFH2OG
      HFFL= HFFL/AMWF
   40 CONTINUE
C I.E. OF LIQUID FUEL AT B.P.
      UFFL= HFFL- ATDXJ/FDEN
      UFLBP= CPFL*(TBPF-298.0) +UFFL
```

```
      UFJ=(TFJ-TBPF)*CPFL+UFLBP
      HFJ= UFJ+ PINJ/FDEN*ATDXJ
C CRITICAL FUEL PROPERTIES
      UFCRIT= (TCRITF-TBPF)*CPFL+ UFLBP
C  ENGINE DISPLACEMENT AND CLEARANCE VOLUME
      VDIS= 0.5*3.14159*DE*DE*RFW
      VC= VDIS/(CR-1.0)
      FARORD= XMFJ/XMAI
      AFRORD= 1.0/FARORD
      EGR1=1.0-EGR
      XMEGR=EGR*XMAI/EGR1
      XMAEGR= XMEGR/(1.0+FARORD)
      XMFEGR= FARORD*XMAEGR
      PE= 1.0
      P1= SCR
      THETAI= THEVC
      CALL VOLM(THETAI,DSDTH,DVDTH,V1)
      WP= P1*DVDTH*ATDXJ
      IF (XMRD.GT.0.0) GO TO 4
C EVALUATE RESIDUAL GAS VIA A SIMPLIFIED OTTO CYCLE (OPTION)
      V2= V1/CR
      G12= 1.35
      G34= 1.273
      CV1= 0.251
      XMRD1= 0.0
      DO 5 ITER=1, 20
      XMAO= XMRD+XMAI+XMEGR
      T1= P1*V1*AMWAI/XMAO/R
      T2= T1*(CR)**(G12-1.0)
C ASSUMMING 25 PER CENT HEAT LOSS
      T3= T2+ HCOM/CV1/(AFRORD+1.0)*0.75
      P3= (XMAO+XMFJ)*R*T3/AMWAI/V2
      P4= P3*(CR)**(-G34)
      V4P= V1*((P4/PE)**(1./G34))
      RSD= V2/V4P
      XMRD= RSD*(XMAO+XMFJ)
      IF (ABS(XMRD-XMRD1).LT.0.01*XMRD) GO TO 4
      XMRD1= XMRD
    5 CONTINUE
      WRITE(6,117)
      STOP
    4 CONTINUE
      XMAO= XMRD+ XMAI+ XMEGR
      XMARD= XMRD/(1.0+FARORD)
      XMFRD= FARORD*XMARD
C EQUIVALENCE RATIO FOR ≠AIR≠ (I.E. INTAKE PURE AIR  + EGR + RESIDUES )
      FARA= (XMFEGR+XMFRD)/ (XMAI+XMARD+XMAEGR)
      AFRA= 1.0/FARA
      PHEA= FARA/FARDS
C  INITIALIZATION
      TIM=1.0E-15
      BTAA=1.0
      GA=1.0
      XMA=XMAO
      XMFA= XMA/(1.0+AFRA)
      XMPAA= XMA/(1.0+FARA)
      T1= P1*V1*AMWAI/XMAO/R
      P=P1
      V=V1
      T=T1
```

```
      TA= T1
      RHO= XMAO/V
      CALL TPROP(TA,P,VXA,CVA,CPA,UA,HA,AMWA,GAMA,RA,PHEA)
      CALL SPECY(P,TA,PHEA,AMWA,XH2A,XH2OA,XCOA,XCO2A,XN2A,XNOA,XOHA,
     1 XHA,XOA,XNA,XO2A,XCH4A)
      YO2A= XO2A*32./AMWA
      YNOA= XNOA*(30./AMWA)
      XMNOA= XMA*YNOA
      XNOANE= XNOA
      XMNOAO= XMNOA
      YSA= 0.0
      XMSOTA= 0.0
      XMSTAO= XMSOTA
      SUMM= XMAO
      EO= XMAO*UA
      DTHETA= DTHMAX
C PRINT INITIAL CONDITIONS
      WRITE(6,INITL)
      WRITE(6,98)
C   SET ZERO
      GFG=0.0
      BTAFG=0.0
      XMFL=0.0
      XMFG=0.0
      XMD  = 0.0
      XMV  = 0.0
      XMFV = 0.0
      XMFLD= 0.0
      XMFDB= 0.0
      XMFLB= 0.0
      XMFPB= 0.0
      XMAPB= 0.0
      XMAFA= 0.0
      SUMFJ= 0.0
      SUMFB= 0.0
      SUMWK= 0.0
      SUMQL= 0.0
      WKNET= 0.0
      SUMBM= 0.0
      DPDTH= 0.0
      DTIDTH= 0.0
      TFL= 0.0
      HFV= 0.0
      UFL= 0.0
      TFG= 0.0
      UFG= 0.0
      TFLB= 0.0
      UFLB= 0.0
      HFDS= 0.0
      TFGO= 0.0
      II= 0
      III= 0
      IPRT= 0
      IIOLD= 0
      KOUNT= 0
      IGEND= 0
      INEWP= 0
C   START THE INTEGRATION
    2 CONTINUE
      XMAA= XMA
```

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C  INTEGRATION STEP SIZE CONTROL
      IF (THETAI.GE.THEIJ) DTHETA= DTHMIN
      IF ((THETAI.LT.THEIJ) .AND. ((THETAI+DTHETA).GT.THEIJ)) DTHETA=
     1 THEIJ-THETAI
      IF (SUMFB.GT.XMFJ95 ) DTHETA= DTHMED
      IF ((THETAI+DTHETA).GT.THEVO) DTHETA= THEVO-THETAI
      DTHET2= 0.5*DTHETA
      DT= DTHETA*DTDTH
      DT2= 0.5*DT
C CHARACTERISTIC VELOCITIES
      UP =DSDTH*DTHDT
      XXX= USI*USI+UP *UP
      UT= SQRT(XXX)
      XXXX= (XMAO*XXX+SUMFJ*VFJO*VFJO)/(XMAO+ SUMFJ)
      UCHAR= SQRT(XXXX)
C CHARATERISTIC RENOLDS NO.
      XMU = 1.25E-5*(T **1.5)/(T +110.)
      REPBAR= RHO*UPBAR*DE/XMU
      REI= RHO*UT*DE/XMU
      REJ= RHO*UCHAR*DE/XMU
C***  TOTAL CONVECTIVE H,T,
      CALL CONHT(REPBAR ,T,DQCDTH,CA,CB)
      SMAPB= 0.0
      SVBDTH= 0.0
      DFGDTH= 0.0
      DFVDTH= 0.0
      DFJDTH= 0.0
      SLDDTH= 0.0
      APBDTH= 0.0
      XMSDTU= 0.0
      IF (THETAI.LT. THEIJ) GO TO 80
      IF (IBUG.NE.0) IPRT=0
      IF ((THETAI-DTHETA).GE.THEIJ) GO TO 3
C ESTIMATE SPRAY TRAJECTORIES
      DELP= PINJ- P
      CALL SPRAY(RHOA,OMEGA,DELP,SEFJ,CDCHG)
C INITIAL FUEL PROPERTIES
      CALL WETBT(P,TA,AMWA,AMWF,A,B,C,TFL,DHFVP)
      UFL= UFFL+ CPFL*(TFL-298.)
      TFG= TFL
      HFL= UFL+ P/FDEN*ATDXJ
      HFV= HFL+ DHFVP
      UFG= HFV- RFG*TFG
      TFLB= TFL
      UFLB= UFL
      TFGO= TFG
      IF (ICRITA.EQ.0) GO TO 17
      HFDS= UFCRIT
      TFDS= TCRITF
      GO TO 3
   17 CONTINUE
      HFDS= HFL
      TFDS= TFL
    3 CONTINUE
C RATE OF FUEL INECCTION
      IF (THETAI.LT.THEEIJ)
     1CALL FINJN(THETAI,DFJDTH,XMFJ)
      IIOLD= II
C ESTIMATE THE VAPORIZATION OF FUEL SPRAY
      IF (KOUNT.GT. NSS ) GO TO 25
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      IPRT=0
      CALL EVAP(P,T,TA,TFL,CPA,OMEGA,TIM,RHOA,XXXX,XMAFA,KOUNT,CEVAP,
     1 AIGND,XMSOTU)
      XMAA= XMA-XMAFA
      DFGDTH=(XXXX-XMFG)/DTHETA
      IF (XMAA.LT.0.0) XMAA=0.0
      IF (XMAA.LE.0.0) KOUNT=NSS
      IF (II.LE.0) GO TO 25
      IGEND= IGEND+ 1
      IF(IIOLD.EQ.II) GO TO 25
C   INITIAL CONDITIONS FOR NEW  ZONE
      IGEND= 0
      IIOLD1= IIOLD+ 1
      DO 21 I=IIOLD1,II
      AMWBM(I )= AMWA
      XMAPBI= XMBM(I)
      DAPDTH(I)= XMAPBI/DTHETA
      XO2(I)= XO2A
      XNONEQ(I )= XNOANE
      YNO(I)= YNOA
      XMNO(I )= XMAPBI*YNO(I)
      TBM(I)= TA
      UBM(I)= UA
      HBM(I)= HA
      CPBM(I)= CPA
      RBM(I)= RA
      AFR(I )= AFRA
      PHE(I)= PHEA
      ETAA= 1.0/(1.0+AFRA)
      ALPA= 1.0- ETAA
      XMFBM(I)= XMBM(I)*ETAA
      XMPAM(I)= XMBM(I)*ALPA
      XMFLI(I)= DLDDTH(I)*DTHETA
      BTABM(I )= BTAA*(XMBM(I )/XMA)
      GBM(I )= GA*(XMBM(I )/XMA)**0.6666667
      BTAA= BTAA- BTABM(I)
      GA= GA-GBM(I)
      YS(I)= XMSOOT(I)/XMBM(I)
      SMAPB= SMAPB+ XMBM(I)
      SLDDTH= SLDDTH+ DLDDTH(I)
      SVBDTH= SVBDTH+ DVBDTH(I)
      IF (IBUG.EQ.0) GO TO 21
      WRITE(6,111) I,AFR(I),XMFG,PHE(I),TBM(I),UBM(I),RBM(I),CPBM(I)
     1 ,DVBDTH(I),XMFLI(I)
      WRITE(6,112)
      DO 20 L=1,NSZG
      WRITE(6,109) L, DI(I ,L),XNDI(I ,L),DMFLI(I ,L)
   20 CONTINUE
   21 CONTINUE
      SUMBM= SUMBM+ SMAPB
      XMA= XMA- SMAPB
      IF (XMA.LT.0.0) XMA=0.0
      XMAA= XMAA- SMAPB
      IF (XMAA.LT.0.0) XMAA=0.0
      IF (XMAA.LE.0.0) KOUNT= NSS
      XMFA= XMA*ETAA
      XMPAA= XMA*ALPA
      XMNOA= XMA*YNOA
      XMSOTA= XMA*YSA
      APBDTH= SMAPB/DTHETA
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   25 CONTINUE
      DFVDTH= DFGDTH+ SVBDTH
   80 CONTINUE
      ITERPC= 0
      PO= P
      TO= T
      TAO= TA
      TFGO= TFG
      TFLO= TFL
      WPO= WP
      HAO= HA
      HFGO= HFG
      HFDSO= HFDS
      DPDTHO= DPDTH
      DTDTHO= DTIDTH
      XMDO  = XMD
      XMVO  = XMV
      XMFVO = XMFV
      XMFAO= XMFA
      XMAPBO= XMAPB
      XMPAAO= XMPAA
      XMFLDO= XMFLD
      XMFPBO= XMFPB
      XMFDBO= XMFDB
      XMNOAO= XMNOA
      XMSTAO= XMSOTA
      SUMFJO= SUMFJ
      IF (II.LE.0) GO TO 63
      DO 62 I=1,II
      TBMO(I)= TBM(I)
      XMNOO(I)= XMNO(I)
      XMSOTO(I)= XMSOOT(I)
      XMFBMO(I)= XMFBM(I)
      XMPAMO(I)= XMPAM(I)
      DO 82 L=1,NSZG
      DIO(I,L)= DI(I,L)
      IF (DI(I,L).LE.0.0) XNDI(I,L)= 0.0
   82 CONTINUE
      IF (I.GT.IIOLD) GO TO 62
      DAPDTH(I)= 0.0
      DVBDTH(I)= 0.0
      DLDDTH(I)= 0.0
   62 CONTINUE
   63 CONTINUE
C IF NO NEW SYSTEM IS CREATED ,SPARE THE FIRST ITERATION
      IF ((                THETAI.GT.THEVC .AND. THETAI.LT.THEIJ) .OR.
     1 (IGEND.GT.3)) GO TO 49
   61 CONTINUE
      SUM1= 0.0
      SUM2= 0.0
      SUM3= 0.0
      SUM4= 0.0
      SUM5= 0.0
      DTLDTH= 0.0
      SDBDTH= 0.0
      SMDDTH= 0.0
      SMVDTH= 0.0
      XFADTH= 0.0
      XAADTH= 0.0
      DORDTH= 0.0
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      IF (II .LE.0) GO TO 79
C BURNING SYSTEMS
C   MIXING RATE OF AIR-BURNING SYSTEM
      CALL AMIX(XMAA,SUMBM,UCHAR,BTABM,AFR,DMDDTH,DMVDTH,CMIX,CVIDI)
      DO 18 I=1,II
      SMDDTH= SMDDTH+ DMDDTH(I)
      SMVDTH= SMVDTH+ DMVDTH(I)
   18 CONTINUE
      ETAA= 1.0/(1.0+AFRA)
      ALPA= 1.0- ETAA
      XAADTH=        - ALPA*SMDDTH
      XFADTH=        - ETAA*SMDDTH
C  EQUILIBRIUM CALCULATION
      CALL TPROPZ
C SPECIES DISTRIBUTION
      CALL SPECYZ
      DO 55 I=1,II
      VBM(I)= V*BTABM(I)
   55 CONTINUE
C  DIFFUSION BURNING RATE OF THE SYSTEM
C ESTIMATE HETEROGENEOUS NO PRODUCTION RATE
      CALL FLAMEZ(TFDS,TFL,CPFL,CNOR)
C ESTIMATE HOMOGENEOUS NO PRODUCTION RATE
      CALL HOMNOZ(CNOR)
C ESTIMATE SOOT FORMATION RATE
      CALL SOOTPZ(T,V)
C   RATE OF RADIATIVE H.T. FOR EACH BURNED SYSTEM
      CALL RADHZZ
      DO 71 I=1,II
      SDBDTH= SDBDTH+ DLBDTH(I)
      ETABM= 1.0/(1.0+AFR(I))
      ALPBM= 1.0-ETABM
      XFIDTH(I)=       (DLBDTH(I)+ DVBDTH(I)+ ETAA*DMDDTH(I)- ETABM*DMVDT
     1H(I))
      XAIDTH(I)=       (ALPA*DMDDTH(I)- ALPBM*DMVDTH(I))
      XFADTH= XFADTH+  ETABM*DMVDTH(I)
      XAADTH= XAADTH+  ALPBM*DMVDTH(I)
      DNODTH(I)= (DNODT1(I)+DNODT2(I))*DTDTH + YNOA*DMDDTH(I)
     1            - YNO(I)*DMVDTH(I)
C NET PRODUCTION RATE
      DMSDT= DMSDT1(I)- DMSDT2(I)
      DMSDTH(I)= DMSDT*DTDTH+ YSA*DMDDTH(I)- YS(I)*DMVDTH(I)
      DQRDTH=DQRDTH+DRMDTH(I)
      DCMDTH(I)= GBM(I)*DQCDTH
      Q2I= (UFLB-UFL)*DLDDTH(I)+ (HFDS-UFLB)*DLDDTH(I)
      QBM(I)= DRMDTH(I)+ DCMDTH(I)+ Q2I
      DPHDTH(I)= (XMPAM(I)*XFIDTH(I)-XMFBM(I)*XAIDTH(I))/(FAROS*XMPAM(I)
     1 **2)
      XX1= ( HA-HBM(I))*DMDDTH(I)+(HFDS-HBM(I))*DLBDTH(I)
     1     +(HFG-HBM(I))*DVBDTH(I)
      XXA= XMBM(I)*(RBM(I)*TBM(I)/P-PUPPBM(I)-TBM(I)*PRPPBM(I))
      XXB= XMBM(I)*(PUPFBM(I)+TBM(I)*PRPFBM(I))
      XXC= XMBM(I)*(PUPTBM(I)+TBM(I)*PRPTBM(I)+RBM(I))
      BBM(I)= (XX1-XXB*DPHDTH(I)-QBM(I))/XXC
      AAM(I)= XXA/XXC
      SUM1= SUM1+ RBM(I)*TBM(I)*(DMDDTH(I)+DLBDTH(I)+DVBDTH(I)-DMVDTH(I)
     1 )
      SUM2= SUM2+ XMBM(I)*TBM(I)*PRPFBM(I)*DPHDTH(I)
      SUM3= SUM3+ BBM(I)*XMBM(I)*(RBM(I)+TBM(I)*PRPTBM(I))
      SUM4= SUM4+ XMBM(I)*TBM(I)*PRPPBM(I)
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      SUM5= SUM5+ AAM(I)*XMBM(I)*(RBM(I)+TBM(I)*PRPTBM(I))
   71 CONTINUE
   79 CONTINUE
C LIQUID FUEL SYSTEM (VAPORING)
      IF (XMFL.LE.0.0 .OR. IWETBT.EQ.0) GO TO 27
C THE TEMPERATURE OF VAPORIZING LIQUID FUEL IS ASSUMED TO BE THE STABLE
C WET-BULB TEMPERATURE
      CALL WETBT(P,TA,AMWA,AMWF,A,B,C,TFL,DHFVP)
      UFL= UFFL+ CPFL*(TFL-298.)
      HFL= UFL+ P/FDEN*ATDXJ
      DTLDTH= (TFL-TFLO)/DTHETA
C LIQUID FUEL SYSTEM (BURNING)
      TFLB= TFL
      UFLB= UFL
      IF (ICRITA.NE.0) GO TO 27
      HFDS= HFL
      TFDS= TFL
   27 CONTINUE
C   FUEL GAS   SYSTEM
      AAFG= 0.0
      BBFG= 0.0
      DRFDTH=0.0
      IF (XMFG.LE.0.0) GO TO 28
      VFG=V*BTAFG
      CALL  RADHZ(TFG,   XMFG,VFG,DRFDTH)
      DQRDTH= DQRDTH+ DRFDTH
      DCFDTH= GFG*DQCDTH
      HFG= UFG+RFG*TFG
C***** ASSUMING  THE LIQUID FUEL IS VAPORIZED TO THE LOCALL FUEL GAS TEMP.
      HFV= HFG
      QFG= DRFDTH+DCFDTH
      XX1= (HFV-HFG)*DFVDTH- QFG
      XX2=XMFG*(CVFV+RFG)
      AAFG= (RFG*TFG)/P/(CVFV+RFG)
      BBFG= XX1/XX2
      SUM1= SUM1+ RFG*TFG*DFGDTH
      SUM3= SUM3+ BBFG*XMFG*RFG
      SUM5= SUM5+ AAFG*XMFG*RFG
   28 CONTINUE
C   AIR SYSTEM
      AAA= 0.0
      BBA= 0.0
      DRADTH=0.0
      IF (XMA.LE.0.0) GO TO 26
      CALL TPROP(TA,P,VXA,CVA,CPA,UA,HA,AMWA,GAMA,RA,PHEA)
      CALL SPECY(P,TA,PHEA,AMWA,XH2A,XH2OA,XCOA,XCO2A,XN2A,XNOA,XOHA,
     1 XHA,XOA,XNA,XO2A,XCH4A)
      VA=V*BTAA
      RHOA= XMA/VA
      CALL RADHZ(TA,   XMFA,VA,DRADTH)
      DQRDTH= DQRDTH+ DRADTH
      DCADTH=GA*DQCDTH
      QEVDTH= (HFV-UFL)*DFVDTH- (UFJ-UFL)*DFJDTH+ XMFL*CPFL*DTLDTH
      QA= DRADTH+DCADTH+QEVDTH- (HFJ-UFJ)*DFJDTH
      XX1= (RA*TA/P-PUPP-TA*PRPP)*XMA
      XX2= (PUPT+RA+TA*PRPT)*XMA
      XX3= XMA*(PUPF+TA*PRPF)
      XX4= 0.0
      SNODTH= 0.0
      SMSDTH= 0.0
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      IF (II    .LE.0) GO TO 38
      DO 37 I=1,II
      XX4= XX4+ (HBM(I)-HA)*DMVDTH(I)
      SNODTH= SNODTH+ YNO(I)*DMVDTH(I)
      SMSDTH= SMSDTH+ YS(I)*DMVDTH(I)
   37 CONTINUE
   38 CONTINUE
      PHADTH= (XMPAA*XFADTH- XMFA*XAADTH)/(FAROS*XMPAA*XMPAA)
      AAA= XX1/XX2
      BBA= (-XX3*PHADTH+XX4-QA)/XX2
      SUM1= SUM1+ RA*TA*(SMVDTH-SMDDTH)
      SUM2= SUM2+ XMA*TA*PRPF*PHADTH
      SUM3= SUM3+ BBA*XMA*(RA+TA*PRPT)
      SUM4= SUM4+ XMA*TA*PRPP
      SUM5= SUM5+ AAA*XMA*(RA+TA*PRPT)
      DNODTA= 0.0
      IF (INO1.EQ.0) GO TO 26
      CALL HOMNOR(P,TA,XNOA,XN2A,XO2A,XNOANE,CNOR,XNODTA)
      YNODTA= XNODTA*(30./AMWA)
      DNODTA= XMA*YNODTA
   26 CONTINUE
      ANODTH= DNODTA*DTDTH+ SNODTH- YNOA*SMDDTH
      YO2A= XO2A*32./AMWA
      DMSDTA=0.0
      IF (XMAA.LE.0.0 .OR. ISOOT.EQ.0) GO TO 32
      VAA= XMAA*VA/XMA
      IDIGI= 3
      CALL SOOTR(P,TA,AFRA,YO2A,V,T,IDIGI,XMSDTA,VAA,DMSDTA,AMSDT1
     1  ,AMSDT2)
   32 CONTINUE
      AMSDTH= DMSDTA*DTDTH+ SMSDTH- YSA*SMDDTH
C PRESSURE DERIVATIVE
      WP= P*DVDTH*ATDXJ
      DPDTH= (-WP+SUM1+SUM2+SUM3)/(V*ATDXJ-SUM4-SUM5)
      IF (DPDTH.GT.20.) WRITE(6,109) ITERPC,WP,V,ATDXJ,
     1                        SUM1,SUM2,SUM3,SUM4,SUM5
C  TEMPERATURE DERIVATIVES
      DTADTH= AAA*DPDTH+ BBA
      TFGDTH= AAFG*DPDTH+ BBFG
      IF (II    .LE.0) GO TO 6
      DO 7 I=1,II
      DTBDTH(I)= AAM(I)*DPDTH+ BBM(I)
    7 CONTINUE
    6 CONTINUE
      IF (ITERPC.NE.0) GO TO 50
C..... PREDICTORS... PREDICTORS
   49 CONTINUE
      DTADTO= DTADTH
      ANODTO= ANODTH
      AMSDTO= AMSDTH
      TFGDTO= TFGDTH
      IF (II.LE.0) GO TO 54
      DO 53 I=1,II
      DBMO(I)= DBM(I)
      DMDDTO(I)= DMDDTH(I)
      DMVDTO(I)= DMVDTH(I)
      DLBDTO(I)= DLBDTH(I)
      DTBDTO(I)= DTBDTH(I)
      DNODTO(I)= DNODTH(I)
      DMSDTO(I)= DMSDTH(I)
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      XFIDTO(I)= XFIDTH(I)
      XAIDTO(I)= XAIDTH(I)
      DO 83 L=1,NSZG
      XKKO(I,L)= XKK(I,L)
   83 CONTINUE
   53 CONTINUE
   54 CONTINUE
      SMDDTO= SMDDTH
      SMVDTO= SMVDTH
      SDBDTO= SDBDTH
      XAADTO= XAADTH
      XFADTO= XFADTH
      DFJDTO= DFJDTH
      DFVDTO= DFVDTH
      SLDDTO= SLDDTH
      SVBDTO= SVBDTH
      APBDTO= APBDTH
      DQCDTO= DQCDTH
      DQRDTO= DQRDTH
      THETAI=THETAI+DTHETA
      CALL VOLM(THETAI,DSDTH,DVDTH,V)
C..... CORRECTORS... CORECTORS
   50 CONTINUE
C MASS CONSERVATION
      SUMFJ= SUMFJO+ (DFJDTH+DFJDTO)*DTHET2
      XMFV = XMFVO + (DFVDTH+DFVDTO)*DTHET2
      XMFLD= XMFLDO+ (SLDDTH+SLDDTO)*DTHET2
      XMFPB= XMFPBO+ (SVBDTH+SVBDTO)*DTHET2
      XMAPB= XMAPBO+ (APBDTH+APBDTO)*DTHET2
      XMD  = XMDO  + (SMDDTH+SMDDTO)*DTHET2
      XMV  = XMVO  + (SMVDTH+SMVDTO)*DTHET2
      XMFDB= XMFDBO+ (SDBDTH+SDBDTO)*DTHET2
      XMFA = XMFAO + (XFADTH+XFADTO)*DTHET2
      XMPAA= XMPAAO+ (XAADTH+XAADTO)*DTHET2
      AFRA= XMPAA/XMFA
      FARA= 1.0/AFRA
      PHEA= FARA/FAROS
      SUMBM=0.0
      XMFLB= 0.0
      IF (II.LE.0) GO TO 8
      DO 9 I=1,II
      XMFBM(I)= XMFBMO(I)+ (XFIDTH(I)+XFIDTO(I))*DTHET2
      XMPAM(I)= XMPAMO(I)+ (XAIDTH(I)+XAIDTO(I))*DTHET2
      XMBM(I )= XMPAM(I)+XMFBM(I )
      AFR(I)= XMPAM(I)/XMFBM(I)
      PHE(I)= 1.0/(AFR(I)*FAROS)
      SUMBM= SUMBM+ XMBM(I)
      XMFLI(I)= 0.0
      DO 81 L=1,NSZG
      D2= DIO(I,L)*DIO(I,L)- (XKK(I,L)+XKKO(I,L))*DT2
      IF (D2.LT.1.0E-16) D2= 0.0
      DI(I,L)= SQRT(D2)
      DMFLI(I,L)= XNDI(I,L)*(0.5235987757 *FDEN*DI(I,L)**3)
      XMFLI(I)= XMFLI(I)+ DMFLI(I,L)
   81 CONTINUE
      XMFLB= XMFLB+ XMFLI(I)
    9 CONTINUE
    8 CONTINUE
      XMA  = XMAO +XMV-XMD-XMAPB
      XMFL= SUMFJ-XMFV-XMFLD
```

```
      XMFLB= XMFLD- XMFDB
      XMFG = XMFV- XMFPB
      IF (XMA.LT.(1.0E-5*XMAO)) XMA= 0.0
      IF (XMFL.LT.0.0) XMFL= 0.0
      IF (XMFG.LT.(1.0E-5*XMFJ)) XMFG= 0.0
      GA= 0.0
      GFG= 0.0
      BTAA= 0.0
      BTAFG= 0.0
      IF (II.LE.0) GO TO 29
      DO 30 I=1, II
      BTABM(I)=0.0
      GBM(I)= 0.0
   30 CONTINUE
   29 CONTINUE
      SUMR=0.0
      SUMG=0.0
      SUMU=0.0
      SUMRT=0.0
      IF(XMA.LE.0.0) GO TO 31
      TA= TAO+ (DTADTO+DTADTH)*DTHET2
      XMNOA= XMNOAO+ (ANODTO+ANODTH)*DTHET2
      IF (XMNOA.LT.0.0) XMNOA= 0.0
      XMSOTA= XMSTAO+ (AMSDTO+AMSDTH)*DTHET2
      IF (TA.LT.TRANG1 .OR. TA.GT.TRANG2) WRITE(6,108) THETAI,TA,PHEA,P,
     1 DTADTH,DTADTO,TAO
      IF (PHEA.LT.PHERG1 .OR. PHEA.GT.PHERG2) WRITE(6,108) THETAI,TA,P,
     1 PHEA,XMFA,XMPAA
      YNOA= XMNOA/XMA
      XNOANE=  (AMWA/30.)*YNOA
      YSA= 0.0
      IF (XMAA.GT.0.0) YSA= XMSOTA/XMAA
      BTAA=XMA*RA*TA
      GA=  (TA-TW)*(BTAA **(.6666667))
      SUMG= SUMG+ GA
      SUMR= SUMR+ XMA*RA
      SUMU= SUMU+ XMA*UA
      SUMRT= SUMRT+ BTAA
   31 CONTINUE
      IF (XMFG.LE.0.0) GO TO 33
      TFG= TFGO+ (TFGDTO+TFGDTH)*DTHET2
      UFG= UFLBP+ (TFG-TBPF)*CVFV
      IF (TFG.LT.0.0) WRITE(6,100) TFG,TFGDTH,AAFG,BBFG,DPDTH,DFVDTH
     1                              ,XMFG
      BTAFG=XMFG*RFG*TFG
      GFG= (TFG-TW)*(BTAFG**(.6666667))
      SUMG= SUMG+ GFG
      SUMR= SUMR+ XMFG*RFG
      SUMU= SUMU+ XMFG*UFG
      SUMRT= SUMRT+ BTAFG
   33 CONTINUE
      SUMU= SUMU+ XMFL*UFL+ XMFLB*UFLB
      IF (II.LT.1) GO TO 73
      DO 72 I=1,II
      IF (I.GT.IIOLD) GO TO 67
      TBM(I)= TBMO(I)+ (DTBDTO(I)+DTBDTH(I))*DTHET2
      GO TO 73
   67 CONTINUE
C REFINE THE TEMPERTURRE CALCULATION FOR NEWLY IGNITED SYSTEMS
      QBMAVX= 0.5*(QBM(I)+QBMO(I))
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      DMDAVX= 0.5*(DMDDTH(I)+DMDDTO(I))
      DMVAVX= 0.5*(DMVDTH(I)+DMVDTO(I))
      DLBAVX= 0.5*(DLBDTH(I)+DLBDTO(I))
      XXX1= HAO*(DAPDTH(I)+DMDAVX    -DMVAVX    )+ HFDSO*DLBAVX
     1     + HFGO*DVBDTH(I)- QBMAVX
      XXX2=  XXX1*DTHETA/XMBM(I)
      RHP= RBM(I)
      THP= TBM(I)
      DO 68 ITER=1,NTER
      UBMII= XXX2- RHP*THP
      CALL TPROP(THP,P,VXHP,CVHP,CPHP,UHP,HHP     ,AWMHP,GAMHP,
     1 RHP,PHE(I))
      XXX= UBMII- UHP
      IF (ABS(XXX/UBMII)     .LT.0.002) GO TO 69
      THP=THP+XXX/CVHP
   68 CONTINUE
      WRITE(6,97) I, ITERPC,THP,UBMII,UHP
      STOP
   69 CONTINUE
      TBM(I)= THP
   70 CONTINUE
      XMNO(I)= XMNOO(I)+ (DNODTO(I)+DNODTH(I))*DTHET2
      IF (XMNO(I).LT.0.0) XMNO(I)= 0.0
      XMSOOT(I)= XMSOTO(I)+ (DMSDTO(I)+DMSDTH(I))*DTHET2
      IF (TBM(I).LT.TRANG1 .OR. TBM(I).GT.TRANG2) WRITE(6,109) I,THETAI,
     1TBM(I),PHE(I),DTBDTH(I),DTBDTO(I),TBMO(I),DPDTH
     2  ,DLBDTH(I),DVBDTH(I),DMDDTH(I),DMVDTH(I)
      IF (PHE(I).LT.PHERG1 .OR. PHE(I).GT.PHERG2) WRITE(6,109) I,THETAI,
     1 TBM(I),PHE(I)
      YNO(I)= XMNO(I)/XMBM(I)
      XNONEO(I)= (AMWBM(I)/30.)*YNO(I)
      YS(I)= XMSOOT(I)/XMBM(I)
      BTABM(I)=                XMBM(I)* RBM(I)*  TBM(I)
      GBM(I) = BTABM(I)**(.6666667)*(TBM(I)-TW)
      SUMG=SUMG+GBM(I)
      SUMU= SUMU+ XMBM(I)*UBM(I)
      SUMRT= SUMRT+BTABM(I)
      SUMR= SUMR+XMBM(I)*RBM(I)
   72 CONTINUE
   73 CONTINUE
      IF (XMA.LE.0.0) GO TO 35
      BTAA=BTAA/SUMRT
      GA= GA/SUMG
   35 CONTINUE
      IF (XMFG.LE.0.0) GO TO 36
      BTAFG= BTAFG/SUMRT
      GFG= GFG/SUMG
   36 CONTINUE
      IF (II.LT.1) GO TO 74
      DO  75 I=1,II
      IF (XMFBM(I).LE.0.0) GO TO 75
      BTABM(I)= BTABM(I)/SUMRT
      GBM(I)=  GBM(I)/SUMG
   75 CONTINUE
   74 CONTINUE
      SUMM= XMA+ XMFG+ SUMBM
      SUMCKM= XMA+ XMFL+ XMFLB+ XMFG+ SUMBM
      CHK= ABS(SUMCKM-SUMFJ-XMAO)
      IF (CHK.GT. 1.0E-5*XMAO) WRITE(6,118) SUMCKM,CHK
     1                         ,XMA,XMFL,XMFLB,XMFG,SUMBM
```

```
C GROSS CYLINDER PROPERTIES
C AVERAGED DENSITY AND INTERNAL ENERGY
      RHO= SUMM/V
      U=SUMU/SUMCKM
C AVERAGED GAS CONSTANTS IN CM3-ATM/GM-K
      RR =(SUMR/SUMM)*RORU
C   AVERAGED PRESSURE
      P= SUMRT/V*RORU
C   AVERAGED TEMPERATURE
      T= P*V/(SUMM*RR)
C OVER-ALL POLLUTANTS
      XMNOE= XMNOA
      SOOTE= XMSOTA+ XMSOTU
      IF (II.LE.0) GO TO 60
      DO 59 I=1,II
      SOOTE= SOOTE+ XMSOOT(I)
      XMNOE= XMNOE+ XMNO(I)
   59 CONTINUE
   60 CONTINUE
      IF (ITERPC.EQ.0) GO TO 64
C  ACCURACY CHECK
      CHKT= T-TX
      IF (ABS(CHKT) .GT. EPSIT*TO) GO TO 57
      CHKP= P-PX
      IF (ABS(CHKP) .GT. EPSIP*PO) GO TO 57
      CHKNO= XMNOE- XMNOEX
      IF (XMNOE.GT.5.0E-4 .AND. ABS(CHKNO).GT.EPSINO*XMNOE) GO TO 57
      CHKSOT= SOOTE- SOOTEX
      IF (SOOTE.GT.1.0E-5 .AND. ABS(CHKSOT).GT.EPSIST*SOOTE) GO TO 57
      GO TO 58
   57 CONTINUE
C CALCULATION DOES NOT PASS THE ACCURACY CHECK
      IF (ITERPC.LT.NTER) GO TO 64
      WRITE(6,120) THETAI,P,TA,TFG,DTADTH,TFGDTH,DPDTH
      WRITE(6,119) ITERPC,TAO     ,TA,XMNOAO        ,XMNOA
      WRITE(6,119) ITERPC,TFGO      ,TFG
      IF (II.LE.0) GO TO 66
      DO 65 I=1,II
      WRITE(6,119) I, TBMO(I)          ,TBM(I),XMNOO(I)           ,XMNO(I)
     1,DTBDTO(I),DTBDTH(I),DNODT1(I),DNODT2(I)
   65 CONTINUE
   66 CONTINUE
      STOP
   64 CONTINUE
      PX= P
      TX= T
      XMNOEX= XMNOE
      SOOTEX= SOOTE
      ITERPC= ITERPC+ 1
      GO TO 61
   58 CONTINUE
      SUMFB= XMFPB+ XMFDB
      IF (SUMFB.GT.XMFJ99) KOUNT= NSS+1
      SUMWK=SUMWK+ ABS(WP)*DTHETA
      SUMQL= SUMQL+ (DQCDTH+ DQCDTO+ DQRDTH+ DQRDTO)*DTHET2
      WKNET= WKNET+ (WP+WPO)*DTHET2
C DETAILED OUTPUT STEP SIZE CONTROL
      IF ((DPDTH*DPDTHO) .LT. 0.0) GO TO 10
      DTIDTH=(T-TO)/DTHETA
      IF ((DTIDTH*DTDTHO) .LT. 0.0) GO TO 10
```

```
      IF (II.EQ.1) GO TO 10
      IXX=IPRT/NPRT
      IXX=IXX*NPRT
      IF ( IPRT.NE.IXX ) GO TO 77
   10 CONTINUE
C PRINT OUTPUT
C  OVER ALL ENERGY BALANCE
      E1= SUMU-EO
      E2= HFJ*SUMFJ- WKNET- SUMQL
      DELE12= (E1- E2)/(XMFJ*HCOM)
C AVERAGED POLLUTANT FORMATION
      SUMMW= XMA*AMWA+ XMFG*AMWF
      SUMPAE= XMPAA
      SUMPFE= XMFA+ XMFL+ XMFLB+ XMFG
      IF (II.LE.0) GO TO 23
      DO 16 I= 1,II
      SUMMW= SUMMW+ XMBM(I)*AMWBM(I)
      SUMPAE= SUMPAE+ XMPAM(I)
      SUMPFE= SUMPFE+ XMFBM(I)
   16 CONTINUE
   23 CONTINUE
      PHEE= SUMPFE/SUMPAE/FAROS
      AMWE= SUMMW/SUMM
      YNOE= XMNOE/SUMM
      XNOE= (AMWE/30.)*YNOE*1.0E6
C GROSS OUTPUT
      WPB    = 0.5*(WP     + WPO    )
      DPDTHB= 0.5*(DPDTH + DPDTHO)
      DFJDTB= 0.5*(DFJDTH+ DFJDTO)
      DQCDTB= 0.5*(DQCDTH+ DQCDTO)
      DQRDTB= 0.5*(DQRDTH+ DQRDTO)
      SMDDTB= 0.5*(SMDDTH+ SMDDTO)
      SMVDTB= 0.5*(SMVDTH+ SMVDTO)
      SVBDTB= 0.5*(SVBDTH+ SVBDTO)
      SDBDTB= 0.5*(SDBDTH+ SDBDTO)
      SLDDTB= 0.5*(SLDDTH+ SLDDTO)
      SFBDTB= SVBDTB+ SDBDTB
      WRITE(6,101) THETAI,P,V,T,U,PHEE,
     1             DPDTHB,WPB,DFJDTB,SMDDTB,SMVDTB,
     2             DQCDTB,DQRDTB,SVBDTB,SDBDTB,SLDDTB,
     2             SUMQL,SUMFB,SFBDTB,WKNET,RR,
     4             UCHAR,DVDTH,DELE12,ITERPC,
     5             XMNOE,YNOE,XNOE,SOOTE
      INEWP= INEWP+ 1
      IF (( (INEWP/7)*7.EQ.INEWP) .AND. (IDTAIL.EQ.0)) WRITE(6,98)
      IF (IDTAIL.EQ.0) GO TO 77
C  DETAIL OUTPUT
      WRITE(6,102)
      XXXXX=  XMFA+ XMPAA
      WRITE(6,105)XMA,TA,UA,PHEA,BTAA,XMNOA, XNOANE,XMSOTA,XXXXX,XMPAA,
     1            XMFA
      IF(THETAI.LT. THEIJ) GO TO 77
      WRITE(6,104)XMFG,TFG,UFG,PHEFG,BTAFG
      WRITE(6,103) XMFL ,TFL ,UFL
      WRITE(6,103) XMFLB,TFLB,UFLB
      IF (II.LT. 1) GO TO 77
      DO 78 I=1,II
      WRITE(6,106) I,XMBM(I),TBM(I),UBM(I),PHE(I),BTABM(I),XMDF(I),
     1 XNONEQ(I),XMSOOT(I),XMFLI(I),XMPAM(I),XMFBM(I)
   78 CONTINUE
```

```
      IF (ISPCYP.EQ.0) GO TO 12
      WRITE(6,110)
      IF (XMA.GT.0.0) WRITE(6,109) II,XH2A,XH2OA,XCOA,XCO2A,XN2A,XNOA,
     1                                XOHA,XHA,XOA,XNA,XO2A,XCH4A
      DO 11 I=1,II
      WRITE(6,109) I,XH2(I),XH2O(I),XCO(I),XCO2(I),XN2(I),XNO(I),XOH(I),
     1          XH(I),XO(I),XN(I),XO2(I),XCH4(I)
   11 CONTINUE
   12 CONTINUE
      IF (IRATEP.EQ.0) GO TO 51
      WRITE(6,114)
      DO 14 I= 1,II
      WRITE(6,109) I,DTBDTH(I),DMDDTH(I),DMVDTH(I),DVBDTH(I),DLBDTH(I)
     1 ,DNODTH(I),DNODT1(I),DNODT2(I),DMSDTH(I),DMSDT1(I),DMSDT2(I)
   14 CONTINUE
   51 CONTINUE
      IF (IDROPP.EQ.0) GO TO 77
      WRITE(6,115)(L,L=1,NSZG)
      DO 15 I=1,II
      WRITE(6,109) I,(DI(I,L),XNDI(I,L),DMFLI(I,L),DMLDT(I,L),L=1,NSZG)
   15 CONTINUE
   77 CONTINUE
      IF (IGEND.GE.3) KOUNT= NSS
      IF (KOUNT.EQ. NSS) KOUNT= KOUNT+1
      IPRT=IPRT+1
      IF (THETAI.LT. THEMAX) GO TO 2
C INDICATED ENGINE PERFORMANCE
      VDIS1= 6.10236E-2*VDIS
      XIMEP= 37.05576*SUMWK/VDIS1/2
      XIHP= XIMEP*VDIS1*RPM/(396000.*NSTROK/2.)
      XISFC= 60.*XMFJ*RPM/(XIHP*NSTROK/2.)/453.59
C SOOT CONCENTRATION (MG/M3STP)
      PSTP= 1.0
      TSTP= 300.
      VSTP= (P*V/T)*(TSTP/PSTP)
      XISOOT= SOOTE*1.0E3/(VSTP*1.0E-5)
      WRITE(6,116) XIMEP,XIHP,XISFC,XISOOT,XNOE
C PROCEDE TO THE NEXT CASE
      GO TO 1
C  FORMAT STATEMENTS
   97 FORMAT (1X,*ITERATION DOES NOT CONVERGE TO THE CORRECT TEMP*/
     1 2I5,1P7E10.3/)
   98 FORMAT(1H1)
   99 FORMAT(8A10)
  100 FORMAT(8E10.3)
  101 FORMAT(//1X,*THETA(DEG.CA)=*,F8.2, 3X,*P(ATM)=*,1PE10.3,2X,*V(CM3)
     1=*,E10.3,2X,*T(K)=*,E10.3,2X,*U(CAL/GM)=*,E10.3,2X,*PHEE=*,E10.3/
     22X,*DPDTH(ATM/CA)=*,E10.3,2X,*WP(CAL/CA)=*,E10.3,2X,*DFJDTH(GM/CA)
     3=*,E10.3,2X,*SMDDTH(GM/CA)=*,E10.3,2X,*SMVDTH(GM/CA)=*,E10.3/
     42X,*DQCDTH(CAL/CA)=*,E10.3,2X,*DQRDTH(CAL/CA)=*,E10.3,2X,*SVBDTH(G
     5M/CA)=*,E10.3,2X,*SDBDTH(GM/CA)=*,E10.3,2X,*SLDDTH(GM/CA)=*,
     6 E10.3/2X,*SUMQL(CAL)=*,E10.3,2X,*SUMFB(GM)=*,E10.3,2X,*SFBDTH(GM/
     7CA)=*,E10.3,2X,*WKNET(CAL)=*,E10.3,2X,*RR(CM3-ATM/GM-K)=*,E10.3/
     82X,*UCHAR(CM/SEC)=*,E10.3,2X,*DVDTH(CM3/CA)=*,E10.3,
     92X,*DELF12=*,E10.3,2X,*ITERPC=*,I5/
     *2X,*XMNOE(GM)=*,E10.3,2X,*YNOE=*,E10.3,2X,*XNOE(PPM)=*,E10.3,2X,
     1 *SOOTE(GM)=*,E10.3)
  102 FORMAT(/1X,*SYSTEM*,3X,*MASS(GM)*,4X,*T(K)*,8X,*UI(CAL/GM)*,2X,
     1 *PHE*,10X,* BETA*,7X,*XMDF(GM)*,4X,*XNONEQ*,5X,*XMSOOT(GM)*,2X,
     2 *XMFLI(GM)*,2X,*AIR(GM)*,1X,*FUEL(GM)*)
```

```
103 FORMAT(1X,*L.FUEL*,1P9E12.3,0P2F7.4)
104 FORMAT(1X,*G.FUEL*,1P9E12.3,0P2F7.4)
105 FORMAT(1X,* AIR   *,1P9E12.3,0P2F7.4)
106 FORMAT(1X,I4,2X,1P9E12.3,0P2F7.4)
107 FORMAT(1H1)
108 FORMAT( 5X,1P11E11.3)
109 FORMAT(1X,I5,1P12E10.2)
110 FORMAT(//50X,*MOLF FRACTIONS*//1X,*SYSTEM*,4X,*H2*,8X,*H2O*,7X,*CO
   1*,8X,*CO2*,7X,*N2*,8X,*NO*,8X,*OH*,8X,*H*, 9X,*O*, 9X,*N*,9X,*O2*,
   2 9X,*CH4*)
111 FORMAT(1X,*FORMATION OF A NEW SYSTEM*,I5,1P10E10.3)
112 FORMAT(/5X,*L*,3X,*D(CM)*,3X,*NO. DROPS*,2X,*MASS(GM)*)
114 FORMAT(/1X,* RATE INFORMATION*/1X,*SYSTEM  DTBDTH*,3X,*DMDDTH*,4X,
   1 *DMVDTH*,4X,*DVBDTH*,4X,*DLBDTH*  ,4X,*DNODTH*,4X,*DNODT1*,4X,
   2 *DNODT2*,4X, *DMSTTH*,4X,*DMSDT1*,4X,*DMSDT2*)
115 FORMAT(/20X,*DROPLET  STATISTICS*//* SYSTEM*,3(I3,37X))
116 FORMAT(//1X,*   ----- INDICATED ENGINE PERFORMACE AND ENGINE EMISS
   *ION -----*  .                                //20X,*I.M.E.P.(PSI)=*
   1 ,1PE12.3/20X,*I.H.P.(HP)=*,E12.3/20X,*I.S.F.C.(LB/HP-HR)=*,E12.3
   2 /20X,*SOOT(MG/M3STP)=*,E12.3/20X,*NITRIC OXIDE(PPM)=*,E12.3)
117 FORMAT(1X,* RESIDUAL GAS CALCULATION DOES NOT CONVERGE */)
118 FORMAT(/*  ERROR..... MASS CONSERVATION DOES NOT SATISFIED.....*,
   1 1P7E10.3/)
119 FORMAT(2X,I5,1P4(2X,2E10.3))
120 FORMAT(/1X,* ERROR IN ITERATION   *,1P10E10.3)
999 CALL EXIT
    END
```

```
*DECK AMIX
      SUBROUTINE AMIX(XMAA,SUMBM,UCHAR,BTABM,AFR,DMDOTH,DMVOTH,CMIX,
     1 CVIDI)
C THIS ROUTINE ESTIMATES THE RATE OF MIXING BETWEEN AIR AND BURNING ZONES
      DIMENSION DMDOTH(100),BTABM(100),AFR(100),DMVOTH(100)
      COMMON/INTEGR/ IN01,IN02,ISOCT,IWETBT,NPRT,IDTAIL,NTER,NAXIL,
     1                NSHEL,NSZG,NTTST,IPUG,II,III
      COMMON/ENGEO/ DE,REW,RL,VC,SC,S,USI,CR,RPM,TW,DNOZZ,NNOZZ,DBOWL,
     1              VFJC
      RE= 0.5*DE
      AP= 3.14159*RE*RE
      V= VC+ AP*S
      XLBAR= V/AP
      XLCHAR= (RE*XLBAR)/2.0/(RE+XLBAR)
      CCMIX= CMIX*UCHAR/XLCHAR/RPM
      IF (XMAA.LT.0.0) XMAA=0.0
      XXX=XMAA*SUMBM/(SUMBM+XMAA)
      DMADTH=CCMIX*XXX
      SUMBTA= 0.0
      DO 1 I=1,II
      SUMBTA= SUMBTA+ BTABM(I)
    1 CONTINUE
      DO 2 I=1,II
      DMDOTH(I)= (BTABM(I)/SUMBTA)*DMADTH
      DMVOTH(I)= CVIDI*DMDOTH(I)
    2 CONTINUE
      RETURN
      END
```

```
*DECK BDATA
      BLOCK DATA
C     POLYNOMIAL COEFFICIENTS FOR THERMODYNAMICC DATA OF C(N)H(1.7N) COMBUSTI
C     PRODUCTS  U(P,T,PHE) IN CAL/GM-OF AIR AND R(P,T,PHE) IN CAL/GM-OF-AIR-K
C       P IS IN ATM, T IS IN K, PHE IS EQUIVALENCE RATIO
C*****   H/C=1.71
      COMMON /HPCOE/ AA1(6),BB1(6),DD1(11),RR1(8), AA2(6),BB2(6),DD2(11)
     1               ,RR2(8)
C LEAN PRODUCTS
      DATA AA1
     1 / -5.5492336E+01,  7.8374758E-02,  1.6734745E-04, -1.1376329E-07,
     2    4.0737814E-11, -5.4383649E-15 /
      DATA BB1
     1 /  7.3465276E+02,  3.7817476E-02, -1.0774602E-04,  6.1112624E-08,
     2   -1.4435963E-11,  9.9489198E-16 /
      DATA DD1
     1 /  1.3700202E+01, -1.1017390E+00, -5.7155909E-01, -2.6780469E+01,
     2    7.2448177E+00,  1.3090986E+00,  5.0189713E-01, -5.2147343E-01,
     3    5.3444392E-02, -2.6396627E+00,  1.6068921E+00 /
      DATA RR1
     1 /  6.8789266E-02,  4.3293620E-03, -9.8361298E-01,  6.6435220E+00,
     2    1.1172543E-01,  2.3055506E+00, -2.5753610E+01, -4.0113958E-01/
C RICH PRODUCTS
      DATA AA2
     1 / -8.5550595E+02,  2.5318868E-01, -1.6176604E-05, -1.0563951E-07,
     2    7.2508183E-11, -1.2100101E-14 /
      DATA BB2
     1 / -1.1796443E+02,  6.5986551E-01, -1.1692944E-03,  7.1490345E-07,
     2   -1.8777443E-10,  1.7905013E-14 /
      DATA DD2
     1 /  9.7714237E+00,  4.3547107E+00, -7.2560124E-02, -9.6828140E+00,
     2   -1.5763997E+01,  2.3124308E-01, -6.4445759E+00,  7.2392234E+00,
     3    5.2083600E-03,  2.2071211E+01, -2.5775327E+01 /
      DATA RR2
     1 /  4.3246505E-02,  1.2509687E-02,  2.3144593E-01, -3.8400357E-01,
     2   -3.3850784E-03, -4.0003995E+00,  2.9256778E-01, -1.7973466E-02/
      END
```

```
*DECK CCNHT
      SUBROUTINE CCNHT(REI,TI,DQCDTH,CA,CB)
C THIS ROUTINE ESTIMATES OVER-ALL CONVECTIVE HEAT TRANSFER TO AN UNIFORM
C TEMPERTURED CYLINDER WALL BASED ON MASS AVERAGED GAS TEMPERATURE
      COMMON/CONVE/ XJ,ATD,DTR,XK,SIG,R,RU,DTDTH,DTHDT,DTRDT
      COMMON/ENGEO/ DE,RFW,RL,VC,SC,S,USI,CE,RFM,TW,DNOZZ,NNOZZ,DBOWL,
     1              VFJO
      XLI=S+SC
      HW=CA *XK*(REI**CB)/DE
      AH= 0.7853981635*DE*DE
      AP=AH
      ASLVI= 3.14159*DE*XLI
      AI= AH+AP+ASLVI
      QCG= HW*AI*(TI-TW )
      DQCDTH=QCG*DTDTH
      RETURN
      END



*DECK ERF
      FUNCTION ERF(Z)
C ERROR FUNCTION EVALUATION
      X=Z
      A=1.0
      IF(X.LT.0.)A=-1.0
      X=A*X
      XI=-(X**2)
      T=1.0/(1.+.3275911*X)
      EMIX2=EXP(XI)
      ERF=A*(1.-EMIX2*T*(.254829592+T*(-.284496736+T*(1.421413741+T*(-1.
     1453152027+T*1.061405429)))))
      RETURN
      END
```

```
*DECK EVAP
      SUBROUTINE EVAP(P,T,TA,TL,CP,OMEGA,TIM,RHOA,XMFG,XMAFA,KOUNT,CEVAP
     1,AIGND,XMSOTU)
C THIS ROUTINE CALCULATES THE VAPORIZATION OF FUEL DROPLETS IN A SPRAY
C AND ALSO ESTIMATES THE IGNITION OF EACH SUBSYSTEM
      COMMON/INTEGR/ INO1,INC2,ISOCT,IWETBT,NPRT,IDTAIL,NTER,NAXIL,
     1                NSHEL,NSZG,NITST,IBUG,II,III
      COMMON/CONVF/ XJ,ATD,DTR,XK,SIG,R,RU,DTDTH,DTHDT,DTRDT,PI
      COMMON/SCA/ THEMAX,THEIJ,THEIG,DINJ,THENB,THEVC,THEVC,DTINJ,
     1            DTHMIN,DTHMED,DTHMAX,DTHETA,DT
      COMMON /AIRP/ XMAI,XMFJ,XMEGR,XMRD,XMAO,XMARD,XMAEGR,XMFRD,XMFEGR,
     1              AMWA,AFRA,FARA,PHEA
      COMMON/FUELP/W,XX,YFL,ZFL,YSTOA,ZSTOA,API,FDEN,FAROS,AMWF,SURFT
     1            ,XMUF,DEN,DXST,HCOM
      COMMON /SHEAT/ HFCO2,HFH2O,DHVH2O,HFH2OG ,CPFL,CPFV,DHFV,HHV,TBPF
     1               ,HFJ,TFJ,HFFL,UFFL
      COMMON /SOOTP/ SDEN,DSOOT, ASOTP,ASOTA,XMSOOT(100)
      COMMON/ENGEO/ DE,RFW,RL,VO,SC,S,USI,CR,RPM,TW,DNOZZ,NNOZZ,DBOWL,
     1              VFJO
      COMMON/DROPO/ HUTIM,DTPHY,XTLYO2,CPBAR,PHOD,TCRITF,XL298,
     1              XMBM(100),DVBDTH(100),DLDDTH(100),XMFLI(100),
     2              DI(100,3),DMFLI(100,3),DMLDT(100,3),XNDI(100,3),
     3              XKK(100,3)
      COMMON/JETP/ DJF,XS(20),YS(20,4),VS(20,4),RHOF(20,4),AFT(20,4),
     1             PTIM(20,4),ETAI(20,5),DYS(20,4), GDSZ(3),SZBAR(3),
     2             C(25,4,3),XSS(25,4),YSS(25,4),DYSS(25,4),TAFV(25,4),
     3             AFV(25,4),XMFVS(25,4),XMSOT(25,4),TO(25,4),PO(25,4),
     4             IDIG(25,4)
      PR= 1.0
      PR3= PR**0.333333
      DEN69= DEN**0.69
      RBOWL= 0.5*DBOWL
      DMFIJT= DJF*DT
      XMUA= 1.25E-5*(TA**1.5)/(TA+110.)
      XL= XL298*((TCRITF-TL)/(TCRITF-298.))**0.38
      IF (TIM.GT.DTINJ) GO TO 24
C ISSUING A NEW SUBSYSTEM
      III= III+1
      DO 22 J=1, NSHEL
      TAFV(III,J)= TA
      AFV(III,J)=1.0E10
      XMSOT(III,J)=0.0
      IDIG(III,J)=0
      TO(III,J)= T
      PO(III,J)= P
      DO 23 L=1, NSZG
      D(III,J,L)= SZBAR(L)
   23 CONTINUE
   22 CONTINUE
   24 CONTINUE
      XMFG1= 0.0
      XMAFA1= 0.0
      XMSOT1= 0.0
      DO 1 I=1,III
      TIMI= TIM-(I-1)*DT
      DO 2 J=1,NSHEL
      IF(IDIG(I,J).GE.3) GO TO 2
C LOCATE THE NEW COORDINATES FOR EACH ELEMENT
      DO 11 ID=2,NAXIL
      IF(TIMI.GE.PTIM(ID-1,J) .AND. TIMI.LT. PTIM(ID,J)) GO TO 12
```

```
   11 CONTINUE
      WRITE(6,100) I,J
      GO TO 7
   12 CONTINUE
      IDM1= ID-1
      DPT= PTIM(ID,J) - PTIM(IDM1,J)
      DPT1=(PTIM(ID,J)-TIMI)/DPT
      DPT2=(TIMI-PTIM(IDM1,J))/DPT
      XSS(I,J)=  XS(IDM1)  *DPT1 + XS(ID)  *DPT2
       YSS(I,J)=   YS(IDM1,J)*DPT1 +  YS(ID,J)*DPT2
      DYSS(I,J)=  DYS(IDM1,J)*DPT1 + DYS(ID,J)*DPT2
      RHOFT=   RHOF(IDM1,J)*DPT1+RHOF(ID,J)*DPT2
      AFTI=      AFT(IDM1,J)*DPT1+ AFT(ID,J)*DPT2
      VSSIJ=  VS(IDM1,J)*DPT1 + VS(ID,J)*DPT2
      VSSIJ= VSSIJ*VFJO
      XMFVS(I,J)= 0.0
      IF (TIMI.LT. HUTIM) GO TO 17
C  VAPORIZATION FUNCTION
      DO 3 L=1,NSZG
      IF (D(I,J,L).LE.0.0) GO TO 18
      XXX1= 1.0+ CPBAR*(TA-TL)/XL
      XKKO= 2.0*PI*RHOD*ALOG(XXX1)
      RSS= XSS(I,J)
      IF (RSS.GT.RBOWL) RSS= RBOWL
      USII= RSS*OMEGA
      RED= RHOA*USII*D(I,J,L)/XMUA
      CREV= 1.0+ CEVAP*SQRT(RED)*PR3
      XKKK= CREV*XKKO
      DD2DT= -4.0*XKKK/PI/FDEN
      DT1= DT
      IF ((TIMI-DT).LT.HUTIM) DT1= TIMI- HUTIM
      D2=  D(I,J,L)**2 + DD2DT*DT1
      IF (D2.LT.0.0) D2=0.0
      D(I,J,L)= SQRT(D2)
   18 DXXX= GDSZ(L)*(1.0-(D(I,J,L)/SZBAR(L))**3)
      XMFVS(I,J)= XMFVS(I,J)+ DXXX
    3 CONTINUE
      SAVEAF= AFTI/XMFVS(I,J)
      AFV(I,J)= SAVEAF
      TAFV(I,J)= (TL+AFV(I,J)*TA)/(1.0+AFV(I,J))
C SOOT FORMATION
      AFVJ= AFV(I,J)
      TAFVJ= TAFV(I,J)
      VIJ= 2.0*PI*YSS(I,J)*DYSS(I,J)*VSSIJ*DT
      IDIGJ= 0
      VOV= VIJ/VC
      CALL SOOTR(P,TAFVJ,AFVJ,YC2,VC,T ,IDIGJ,XMSOT(I,J),VIJ,DMSDT,
     1 DMSDT1,DMSDT2)
      XMSOT(I,J)= XMSOT(I,J)+ DMSDT*DT
C SELF-IGNITION CRITERIA (AFTER SHIPINSKI,ET.AL.)
      PXX= 0.5*(P+PO(I,J))
      TXX= 0.5*(T +TO(I,J))
      DIG= AIGND   *EXP(4645./TXX)/(CEN69*(PXX**0.396))
      IF (DIG.LE.TIMI) GO TO 7
   17 CONTINUE
C UNBURNED FUEL VAPOR
      XMFG1= XMFG1+ XMFVS(I,J)*DMFIJT
      XMAFA1= XMAFA1+ AFTI*DMFIJT
      XMSOT1= XMSOT1+ XMSOT(I,J)
      GO TO 2
```

```
    7 CONTINUE
C COLLECTING THE BURNING SYSTEMS (I.E. DEFINING BURNING RATE)
      IDIG(I,J)=3
      II= II+1
      KOUNT= KOUNT+1
      XMSOOT(II)= XMSOT(I,J)*NNOZZ
      XMBM(II)= NNOZZ*AFTI*DMFIJT
      DVBDTH(II)= NNOZZ*XMFVS(I,J)*DMFIJT/DTHETA
      XMFLI(II)= 0.0
      DO 10 K= 1,NSZG
      DI(II,K)= D(I,J,K)
      DMFLI(II,K)= 0.0
      XNDI(II,K)= 0.0
      IF (DI(II,K).LE.0.0) GO TO 10
      DMFLI(II,K)= NNOZZ*(DI(II,K)/SZBAR(K))**3*GDSZ(K)*DMFIJT
      XNDI(II,K)= 6.0*DMFLI(II,K)/(FDEN*PI*(DI(II,K)**3))
      XMFLI(II)= XMFLI(II)+ DMFLI(II,K)
   10 CONTINUE
      DLDDTH(II)= XMFLI(II)/DTHETA
      IF (IDTAIL.NE.0)  WRITE(6,101)
     1            I,J ,AFV(I,J),XMFVS(I,J),XMBM(II),TIMI,DIG,XMSOT(I,J)
    2 CONTINUE
    1 CONTINUE
      XMFG= NNOZZ*XMFG1
      XMAFA= NNOZZ*XMAFA1
      XMSOTU= NNOZZ*XMSOT1
      TIM= TIM+DT
      IF (IBUG.EQ.0 ) RETURN
      DO 15 J=1,NSHEL
      WRITE(6,99)
      WRITE(6,102)    ( XSS(III-I+1,J),I=1,III)
      WRITE(6,103)    ( YSS(III-I+1,J),I=1,III)
      WRITE(6,108)    (DYSS(III-I+1,J),I=1,III)
      WRITE(6,104)   (XMFVS(III-I+1,J),I=1,III)
      WRITE(6,105)    ( AFV(III-I+1,J),I=1,III)
      WRITE(6,106)    (TAFV(III-I+1,J),I=1,III)
   15 CONTINUE
      WRITE(6,99)
   99 FORMAT(/)
  100 FORMAT(1X,* I=*,I3,*  J=*,I3,*  ELEMENT IMPINGES A NEGHBOR JET*)
  101 FORMAT (1X,*----- SYSTEM *,2I3,*  IS BURNNED *,1P6E12.3)
  102 FORMAT(1X,*  X   *,1P10E12.3)
  103 FORMAT(1X,*  Y   *,1P10E12.3)
  104 FORMAT(1X,*XMFV *,1P10E12.3)
  105 FORMAT(1X,*A/FV *,1P10E12.3)
  106 FORMAT(1X,*TAVF *,1P10E12.3)
  108 FORMAT(1X,* DY   *,1P10E12.3)
      RETURN
      END
```

```
*DECK FINJN
      SUBROUTINE FINJN(THETAI,DFJDTH,XMFJ)
C THIS ROUTINE GIVES CONSTANT FUEL INJECTION RATE
C   ASSUMING  CONSTANT INJECTION RATE
      COMMON/SCA/ THEMAX,THEIJ,THEIG,DINJ,THENB,THEVO,THEVC,DTINJ,
     1            DTHMIN,DTHMED,DTHMAX,DTHETA,DT
      DFJDTH=0.0
      IF((THETAI.LT.THEIJ).OR.(THETAI.GE.(THEIJ+DINJ))) RETURN
      DFJDTH= XMFJ/DINJ
      RETURN
      END
```

```
*DECK FLAMEZ
      SUBROUTINE FLAMEZ(TL,TLC,CPL,CNOP)
C COMPUTATION OF QUASI-STEADY THIN FLAME STRUCTURE (WITHIN A FINITE SPACE)
      COMMON/INTEGR/ INO1,INC2,ISOCT,IWETBT,NPRT,IOTAIL,NTER,NAXIL,
     1               NSHEL,NSZG,NITST,IBUG,II,III
      COMMON/CONVF/ XJ,ATD,DTR,XK,SIG,R,RU,DTDTH,DTHDT,DTRDT,PI
      COMMON/SPECYI/  XH2(100),XH2C(100),XCC(100),XCO2(100),XN2(100),
     1                XNO(100),XOH(100),XH(100),XC(100),XN(100),XO2(100)
     2                ,XCH4(100),XNONEQ(100)
      COMMON/PRATEI/ DNODT1(100),DNODT2(100),DMSDT1(100),DMSDT2(100),
     1               DRMDTH(100),DLBDTH(100),XMDF(100)
      COMMON/TPROPI/ P,TBM(100),UBM(100),HBM(100),VBM(100),CPBM(100),
     1               AMWBM(100),RBM(100),PHE(100),AFR(100),XMFBM(100),
     2               XMPAM(100)
      COMMON/SCA/ THEMAX,THEIJ,THEIG,DINJ,THENB,THEVO,THEVC,DTINJ,
     1            DTHMIN,DTHMED,DTHMAX,DTHETA,DT
      COMMON/DROPC/ HUTIM,DTPHY,XTLYO2,CPBAR,RHOD,TCRITF,XL298,
     1              XMBM(100),DVBDTH(100),DLDDTH(100),XMFLI(100),
     2              DI(100,3),DMFLI(100,3),DMLDT(100,3),XNDI(100,3),
     3              XKK(100,3)
      COMMON/FUELP/W,XX,YFX,ZFL,YSTOA,ZSTOA,API,FDEN,FAPOS,AMWF,SURFT
     1            ,XMUF,CEN,OXST,HCOM
      COMMON/FLAMES/ AMWMP,RMAX,YN2L,TF,RF,XMDCT,RL,R8,TDF(50),YFDF(50),
     1               YO2DF(50),YN2DF(50),YNCDF(50),WDCT(50),RDF(50)
      CCP= HCOM/CPBAR
      NITST1= NITST- 1
      NITST2= NITST/5
      NITST3= NITST2+ 2
      DO 20 I=1,II
      XMDF(I)= 0.0
      DLBDTH(I)= 0.0
      DNODT2(I)= 0.0
      DO 19 L=1,NSZG
      XKK(I,L)= 0.0
      DMLDT(I,L)= 0.0
   19 CONTINUE
      DLBDT= 0.0
      DMLDTI= 0.0
      IF (XMFLI(I).LE.0.0) GO TO 20
      YO28= XO2(I)*32./AMWBM(I)
      YN28= XN2(I)*28./AMWBM(I)
      YNO8= XNONEQ(I)*30./AMWBM(I)
      T8= TBM(I)
      AMWMP= AMWBM(I)*P
      YO28J= YO28/OXST
      XXXMDF= 12.56637062*AMWMP/82.054
C DROPLET SPACING
      SUMNDI= 0.0
      DO 9 L=1,NSZG
      IF (DI(I,L).GT.0.0) SUMNDI= SUMNDI+ XNDI(I,L)
    9 CONTINUE
      VMAX= VBM(I)/SUMNDI
      RMAX= (0.23873*VMAX)**0.333333
      DO 10 L=1,NSZG
      IF (DI(I,L).LE.0.0) GO TO 10
      RL= 0.5*DI(I,L)
      IF (YO28.LT.XTLYO2) GO TO 12
      IF ((TCRITF-TL).LE.1.0E-6) GO TO 15
C SUBCRITICAL ASSUMPTION
      XL= XL298*((TCRITF-TL )/(TCRITF-298.))**0.38
```

```
      GO TO 16
C CRITICAL UNION SKIN ASSUMPTION
   15 XL= CPL*(TL-TLO)
   16 CPLXL= CPBAR/XL
      B2= CPLXL*(T8-TL+ QCP*YO28J)
      ALOG2= ALOG(1.0+B2)
      YFL= 1.0-(1.0+YO28J)/(1.0+B2)
      ALOG4= ALOG(1.0+YFL/(1.0-YFL))
      AAA= ALOG2/ALOG4
C FLAME TEMPERATURE
      TF= (T8+TL*YO28J/YFL+QCP*YO28J     )/(1.0+YO28J/YFL)
      TFT8= TF/T8
      XLHS= RMAX**3
      DR8= -0.05*(RMAX-RL)
      R8= RMAX-DR8
      DO 1 ITER=1,50
      R8= R8+ DR8
      IF (RR.LE.RL) GO TO 12
      RORMR= R8/(R8-RL)
      XMDOT= RL*RORMR*ALOG2
      XXX= RORMR*AAA
      RFRL= XXX/(XXX-1.0)
      RF= RL*RFRL
      XXXX= XMDOT/RF
      IF (XXXX.GT.200.) XXXX=200.
      ERF= EXP(-XXXX)
      XXXX= XMDOT/R8
      IF (XXXX.GT.200.) XXXX= 200.
      ER8= EXP(-XXXX)
      DRI= (RMAX-RF)/30.
      RI= RF- DRI
      SUM=0.0
      DO 2 IR=1,30
      RI= RI+DRI
      ER= EXP(-XMDOT/RI)
      XITGD= (ERF-ER)*RI*RI/((ERF-ER)+TFT8*(ER-ER8))
      IF (XITGD.LT.0.0) XITGD=0.0
      SUM= SUM+ XITGD
    2 CONTINUE
      XRHS= 3.0*SUM*DRI
      CHK= (XLHS-XRHS)/XLHS
      IF (ITER.EQ.1) GO TO 4
      IF (ABS(CHK).LT.0.01) GO TO 3
      CHKX= CHK1*CHK
      IF (CHKX.LT.0.0) GO TO 5
    4 CONTINUE
      CHK1= CHK
      GO TO 1
    5 CONTINUE
      R8= R8- DR8
      DR8= 0.5*DR8
    1 CONTINUE
      WRITE(6,101) P,T8,TL,TLO,YO28,RL,RMAX
      WRITE(6,100) ITER,XLHS,XRHS,CHK,RF,TF,R8,RI
      STOP
C IN TRANSIENT O-S DIFFUSION FLAME CAN NOT BE ESTABLISHED
   12 CONTINUE
      XL= XL298*((TCRITF-TLC)/(TCRITF-298.))**0.38
      XXX= 1.0+ CPBAR*(T8-TLC)/XL
      QMLOTI= 12.56637062*RHOD*RL*ALOG(XXX)
```

```
      GO TO 11
    3 CONTINUE
C BURNING RATE
      DMLDTI= 12.56637062*RHOD*XMDOT
      IF (INO2.EQ.0) GO TO 11
C MASS FRACTION OF N2 ON SURFACE
      WXX4= W+ 0.25*XX
      XXX1= 44.0*(W+WXX4*XCO2(I)/XC2(I))
      XXX2= 18.0*(0.5*XX+WXX4*XH2O(I)/XC2(I))
      XXX3= 28.0*(WXX4*XN2(I)/XC2(I))
      XXX= (XXX1+XXX2)/XXX3
      YN2L= (1.0-YFL)/(1.0+XXX)
      XXXX= XMDOT/RL
      IF (XXXX.GT.200.) XXXX=200.
      ERL= EXP(-XXXX)
      ERLF= ERL- ERF
      ERL8= ERL- ER8
      ERF8= ERF- ER8
      TFMTLE= (TF-TL)/ERLF
      YFLE= YFL/ERLF
      TFMT8E= (TF-T8)/ERF8
      YO28E= YO28/ERF8
      YN2L8E= (YN2L-YN28)/ERL8
C COMPUTATION OF DISTRIBUTIONS AROUND A BURNING DROPLET
      DRI= (RF-RL)/NITST2
      RI= RL-DRI
      DO 8 IR=1,NITST
      IF (IR.EQ.NITST3) DRI= (R8-RF)/(NITST1-NITST2)
      RI= RI+DRI
      RDF(IR)= RI
      XXXX= XMDOT/RI
      IF (XXXX.GT.200.) XXXX= 200.
      ER= EXP(-XXXX)
      IF (RI.GT.RF) GO TO 6
C TEMPERATURE DISTRIBUTION --- FUEL SIDE
      TDF(IR)= TF+ TFMTLE*(ERF-ER)
      YFDF(IR)= YFLE*(ER-ERF)
      YO2DF(IR)= 0.0
      GO TO 7
C TEMPERATURE DISTRIBUTION --- OXIDANT SIDE
    6 CONTINUE
      TDF(IR)= T8+ TFMT8E*(ER-ER8)
      YO2DF(IR)= YO28E*(ERF-ER)
      YFDF(IR)= 0.0
C N2 DISTRIBUTION
    7 CONTINUE
      YN2DF(IR)= YN28+ YN2L8E*(ER-ER8)
    8 CONTINUE
C CALCULATE HETERGENOUUCTION RATE AROUND A BURNING DROPLET
      IF (DMLDTI.LT.1.0E-15) GO TO 11
      CALL HETNOR(P,YNO8,AMWBM(I),RHOD,NITST,CNOR,DNODTI)
      DNCDT2(I)= DNCDT2(I)+ DNCDTI*XNDI(I,L)
C MASS INVOLVED IN HETEROGENEOUS FORMATION
      XMDFI= 0.0
      DO 14 IR=NITST3,NITST
      RI= 0.5*(RDF(IR)+ RDF(IR-1))
      RI2= RI*RI
      DRI= RDF(IR)- RDF(IR-1)
      TDFAV= 0.5*(TDF(IR)+ TDF(IR-1))
      XMDFI= XMDFI+ RI2*DRI/TDFAV
```

```
   14 CONTINUE
      XMDF(I)= XMDF(I)+ XNDI(I,L)*XXXMDF*XMCFI
   11 CONTINUE
      DMLDT(I,L)= DMLDTI
      XKK(I,L)= (0.6366197723/FDEN/RL)*DMLDTI
      DLBDT= DLBDT+ DMLDTI*XNDI(I,L)
   10 CONTINUE
C OVER-ALL DIFFUSIVE ZONAL BURNING RATE
      DLBDTH(I)= DLBDT*DTDTH
      IF (DLBDTH(I)*DTHETA.GT.XMFLI(I)) DLBDTH(I)= XMFLI(I)/DTHETA
   20 CONTINUE
  100 FORMAT(1X,I5,1P12E10.3)
  101 FORMAT(//1X,*.... ERROR IN FLAME  ITERATION ...*,1P7E10.3)
      RETURN
      END
```

```
*DECK HETNOR
      SUBROUTINE HETNOR(P,YNO8 ,AMW,RHOD,NITST,CNOR,DNODTI)
C HETERGENOUS NO FORMATION RATE
      DIMENSION  Y1(50),Y2(50),WDOT1(50),XK2(50),XK3(50),SAVE1(51),
     1 SAVE2(51),WDOTAV(50)
      COMMON/FLAMES/ AMWMP,RMAX,YN2L,TF,RF,XMDOT,RL,R8,TDF(50),YFDF(50)
     1                YO2DF(50),YN2DF(50),YNODF(50),WDOT(50),RDF(50)
      NITST1= NITST- 1
      DO 7 I=1,NITST
      WDOT1(I)=0.0
      XK2(I)= 0.0
      XK3(I)= 0.0
      IF (YO2DF(I).LE.0.0) GO TO 7
C RATE CONSTANTS
      RT=1.987*TDF(I)
      XKF1=       1.36E14*EXP(-75400./RT)
      XKB1=       3.12E13*EXP(-400./RT)
      XKF2= 1.33E10*TDF(I)*EXP(-7080./RT)
      XKB2= 3.2E9*TDF(I)*EXP(-39100./RT)
      XKEQ3= 5.0*EXP(-58300./RT)
      XK1= CNOR*5.095E-4*(XKF1*XKEQ3)
      WDOT1(I)= XK1*((AMWMP/TDF(I))**1.5)*YN2DF(I)*SQRT(YO2DF(I))
      XK2(I)= 0.9955*(XKB1*XKB2/(XKF1*XKF2))/(YN2DF(I)*YO2DF(I))
      XK3(I)= 1.1428*(XKB1/XKF2)/YO2DF(I)
    7 CONTINUE
C INTEGRATING NO CONSERVATION EQUATION
      DY1= 2.0E-4
      IF (YNO8.GT.2.0E-3) DY1= 0.1*YNO8
      Y1(1)= 2.0E-4- DY1
      WDOT(1)= 0.0
      ITER= 0
      ILOW= 0
      IUPR= 0
      CHKUPR= 1.0E10
      CHKLOW=-1.0E10
    2 CONTINUE
      Y1(1)=  Y1(1)+ DY1
    6 CONTINUE
C INITIAL CONDITIONS
      IF (ITER.GE.NITST) GO TO 4
      Y2(1)= XMDOT*Y1(1)
      YNODF(1)=Y1(1)
      DO 1 I=1,NITST1
      RI= 0.5*(RDF(I+1)+RDF(I))
      DRI= RDF(I+1)-RDF(I)
      RI2= RI*RI
      Y1(I+1)= Y1(I)+ (Y2(I)/RI2)*DRI
      IF (Y1(I+1).LT.-1.0E-20) Y1(I+1)= -1.0E-20
      IF (Y1(I+1).GT.1.0) Y1(I+1)= 1.0
      YNODF(I+1)= Y1(I+1)
C PRODUCTION RATES
      CORR1= 1.0- XK2(I+1)*(YNODF(I+1)*YNODF(I+1))
      CORR2= 1.0+ XK3(I+1)*YNODF(I+1)
      CORR= CORR1/CORR2
      WDOT(I+1)= WDOT1(I+1)*CORR
      WDOTAV(I)= 0.5*(WDOT(I)+WDOT(I+1))
      Y2(I+1)= Y2(I)+((XMDOT*Y2(I)/RI2)-(RI2*WDOTAV(I)/RHOD))*DRI
    1 CONTINUE
      ITER= ITER+ 1
      SAVE1(ITER)= Y1(1)
```

```
      SAVE2(ITER)= Y1(NITST)
      CHK= Y1(NITST)- YNO8
      ABSCHK= ABS(CHK)
      IF (((ABSCHK.LT.1.0E-6).AND.(Y1(NITST).GE.0.0)) .OR.
     1   (ABSCHK.LT.0.005*YNO8)) GO TO 3
C  IMPROVING INITIAL GUESS
      IF (ILOW.EQ.0 .AND. CHK.LT.0.0) GO TO 14
      IF (IUPR.EQ.0 .AND. CHK.GT.0.0) GO TO 15
      IF (CHK.LT.0.0 .AND. CHK.GE.CHKLOW) GO TO 14
      IF (CHK.GT.0.0 .AND. CHK.LE.CHKUPR) GO TO 15
      GO TO 16
   14 CONTINUE
      ILOW= 1
      Y1OLOW= Y1(1)
      Y18LOW= SAVE2(ITER)
      CHKLOW= CHK
      GO TO 17
   15 CONTINUE
      IUPR= 1
      Y1OUPR= Y1(1)
      CHKUPR= CHK
   17 CONTINUE
      IUPLO= ILOW*IUPR
      IF (IUPLO.LE.0) GO TO 16
      Y1(1)= (Y1OLOW*CHKUPR- Y1OUPR*CHKLOW)/(CHKUPR-CHKLOW)
      IF (Y18LOW.LE.0.0) Y1(1)= 0.5*(Y1OLOW+ Y1OUPR)
      GO TO 6
   16 CONTINUE
      IF (ITER.EQ.1) GO TO 2
      ITER1= ITER-1
      IF (ABS(SAVE2(ITER)-SAVE2(ITER1)) .LE. 1.0E-20) GO TO 2
      IF (ABS(SAVE1(ITER)-SAVE1(ITER1)) .LT. 1.0E-20) GO TO 4
      DDY1= (SAVE2(ITER)-SAVE2(ITER1))/(SAVE1(ITER)-SAVE1(ITER1))
      Y1(1)= Y1(1)- CHK/DDY1
      GO TO 6
    4 CONTINUE
      WRITE(6,101) ITER,   P,AMW,RHOD  ,YNO8,XMDOT,RL,RF,R8,RMAX
      DO 8 I=1,NITST
      WRITE(6,100) I,RDF(I),TDF(I),YFDF(I),YO2DF(I),YN2DF(I),WDOT1(I)
     1        WDOT(I),YNODF(I),Y2(I),SAVE1(I),SAVE2(I)
    8 CONTINUE
      STOP
    3 CONTINUE
C OVER-ALL NO PRODUCTION  PER DROPLET
      DNODTI=0.0
      DO 5 I=1,NITST1
      RI= 0.5*(RDF(I+1)+RDF(I))
      DRI= RDF(I+1)-RDF(I)
      DNODTI= DNODTI+ WDOTAV(I)*RI*RI*DRI
    5 CONTINUE
      DNODTI= 12.56637062*DNODTI
  100 FORMAT(1X,I5,1P12E10.3)
  101 FORMAT(//1X,  *.. ERROR IN HETNOR ITERATION ..* , I3,1P9E10.3)
      RETURN
      END
```

```
*DECK HOMNOR
      SUBROUTINE HOMNOR(P,T,XNC,XN2,XO2,XNONEQ,CNOR,XNODT1)
C THIS ROUTINE CALCULATES HOMOGENEOUS NO PRODUCTION RATE
      RT= 1.987*T
C RATE CONSTANTS
      XKF1=       1.36E14*EXP(-75400./RT)
      XKB1=       3.12E13*EXP(-400./RT)
      XKF2= 1.33E10*T*EXP(-7080./RT)
      XKB2= 3.2E9*T      *EXP(-39100./RT)
      XKEQ3= 5.0*EXP(-58300./RT)
      XK1= CNOR*0.220782*(XKF1*XKEQ3)
      XK2 = (XKB1*XKB2/(XKF1*XKF2))
      XK3= XKB1/XKF2
      CORR1= 1.0- XK2*(XNONEQ*XNONEQ/(XN2*XO2))
      CORR2= 1.0+ XK3*(XNONEQ/XO2)
      CORR= CORR1/CORR2
      XNODT1= XK1*XN2*SQRT(XO2*P/T)*CORR
      RETURN
      END
```

```
*DECK HOMNOZ
      SUBROUTINE HOMNOZ(CNOR)
C THIS ROUTINE CALCULATES HOMOGENEOUS NO PRODUCTION RATE
      COMMON/INTEGR/ INO1,INO2,ISOCT,IWETBT,NPRT,ICTAIL,NTER,NAXIL,
     1               NSHEL,NSZG,NITST,IBUG,II,III
      COMMON/SPECYI/  XH2(100),XH2O(100),XCO(100),XCO2(100),XN2(100),
     1                XNO(100),XOH(100),XH(100),XO(100),XN(100),XO2(100)
     2                ,XCH4(100),XNONEQ(100)
      COMMON/PRATEI/ DNODT1(100),DNODT2(100),DMSDT1(100),DMSDT2(100),
     1               DRMDTH(100),DLBDTH(100),XMDF(100)
      COMMON/TPROPI/ P,TBM(100),UBM(100),HBM(100),VBM(100),CPBM(100),
     1               AMWBM(100),RBM(100),PHE(100),AFR(100),XMFBM(100),
     2               XMPAM(100)
      COMMON/DPOPC/ HUTIM,DTPHY,XTLYO2,CPBAS,RHOD,TCRITF,XL298,
     1              XMBM(100),DVBDTH(100),DLDDTH(100),XMFLI(100),
     2              DI(100,3),DMFLI(100,3),DMLDT(100,3),XNDI(100,3),
     3              XKK(100,3)
      DO 1 I=1,II
      DNODT1(I)= 0.0
      IF (INO1.EQ.0 .OR. TBM(I).LT.1900. .OR. XO2(I).LE.1.E-15) GO TO 1
      T= TBM(I)
      RT= 1.987*T
C RATE CONSTANTS
      XKF1=       1.36E14*EXP(-75400./RT)
      XKB1=       3.12E13*EXP(-400./RT)
      XKF2= 1.33E10*T*EXP(-7080./RT)
      XKB2= 3.2E9*T      *EXP(-39100./RT)
      XKEQ3= 5.0*EXP(-58300./RT)
      XK1= CNOR*0.220782*(XKF1*XKEQ3)
      XK2 = (XKB1*XKB2/(XKF1*XKF2))
      XK3= XKB1/XKF2
      CORR1= 1.0- XK2*(XNONEQ(I)*XNONEQ(I))/(XN2(I)*XO2(I))
      CORR2= 1.0+ XK3*(XNONEQ(I)/XO2(I))
      CORR= CORR1/CORR2
      YNODT1= XK1*XN2(I)*SQRT(XO2(I)*P/T)*CORR
      YNODT1= (30./AMWBM(I))*XNODT1
      DNODT1(I)= (XMBM(I)-XMDF(I))*YNODT1
    1 CONTINUE
      RETURN
      END
```

```
*DECK RADHZ
      SUBROUTINE RADHZ(THP,    XMFB,VI,DQRDTH)
C RATE OF RADIATIVE H.T. FROM INDIVIDUAL HOT ZONE TO THE WALL
C BASED ON LOCAL ZONE TEMPERATURE
      COMMON/CONVF/ XJ,ATD,DTR,XK,SIG,R,RU,DTDTH,DTHDT,DTRDT,PI
      COMMON/ENGEO/ DE,RFW,RL,VC,SC,S,USI,CR,RPM,TW,DNOZZ,NNOZZ,DBOWL,
     1              VFJO
      ALFAH=0.9
      ALFAS=0.25
      XLI=S+SC
      AH= 1.570796327*DE*DE
      ASLVI= 3.14159*DE*XLI
      ALPH= (AH*ALFAH+ASLVI*ALFAS)/(AH+ASLVI)
      RHOFI=0.0
      IF (VI .GT. 1.0E-10) RHOFI= XMFB/VI
      RCP= 5.7E2*RHOFI
      VZE= VI/NNOZZ
      XXX= 6.0*VZE/PI
      PL=XXX**(0.3333333)
      AZE= 3.14159*PL*PL
      EPSA= ALPH*(1.0-EXP(-RCP*PL))
      XXX=(THP**4-TW **4)*SIG
      QRF= NNOZZ*EPSA*AZE*XXX
      DQRDTH=QRF*DTDTH
      RETURN
      END
```

```
*DECK RADHZZ
      SUBROUTINE RADHZZ
C RATE OF RADIATIVE H.T. FROM INDIVIDUAL HOT ZONE TO THE WALL
C BASED ON LOCAL ZONE TEMPERATURE
      COMMON/INTEGR/ IND1,INC2,ISOCT,IWETBT,NPRT,ICTAIL,NTER,NAXIL,
     1               NSHEL,NSZG,NITST,IBUG,II,III
      COMMON/CONVF/ XJ,ATD,DTR,XK,SIG,R,RU,CTDTH,DTHDT,DTRDT,PI
      COMMON/PRATEI/ DNODT1(100),DNODT2(100),DMSDT1(100),DMSDT2(100),
     1               DRMDTH(100),DLBDTH(100),XMDF(100)
      COMMON/TPROPI/ P,TBM(100),UBM(100),FBM(100),VBM(100),CPBM(100),
     1               AMWBM(100),RBM(100),PHE(100),AFR(100),XMFBM(100),
     2               XMPAM(100)
      COMMON/ENGEC/ DE,RFW,PL,VC,SC,S,USI,CR,RFM,TW,DNOZZ,NNOZZ,DBCWL,
     1              VFJO
      TW4= TW**4
      ALFAH=0.9
      ALFAS=0.25
      XLI=S+SC
      AH= 1.570796327*DE*DE
      ASLVI= 3.14159*DE*XLI
      ALPH= (AH*ALFAH+ASLVI*ALFAS)/(AH+ASLVI)
      DO 1 I= 1,II
      RHOFI=0.0
      IF (VBM(I) .GT. 1.0E-10) RHOFI= XMFBM(I)/VBM(I)
      RCP= 5.7E2*RHOFI
      VZE= VBM(I) /NNOZZ
      XXX= 6.0*VZE/PI
      PL=XXX**(0.3333333)
      AZE= 3.14159*PL*PL
      EPSA= ALPH*(1.0-EXP(-RCP*PL))
      XXX= (TBM(I)**4-TW4)*SIG
      QRF= NNOZZ*EPSA*AZE*XXX
      QRMDTH(I)= QRF*CTDTH
    1 CONTINUE
      RETURN
      END
```

```
*DECK SIZED
      SUBROUTINE SIZED(DELP,RHOA,FDEN,SURFT,XMUF,DNCZZ,SZBAR,GDSZ,NSZG)
C THIS ROUTINE CALCULATES THE INITIAL DROP-SIZE DISTRIBUTION OF A FUEL JET
      DIMENSION GDSZ( 5),SZBAR( 5)
      CM= 37.5
      DEL=0.85
      DPXX= DELP*1.01325E6
      DMAX= CM*(DNCZZ**.5)*(SURFT**.25)*(DPXX**(-0.375))*(FDEN**(-.125))
     1     *(XMUF**0.25)*(RHOA**(-0.2))
      DMIN= 0.01*DMAX
      DELD=(DMAX-DMIN)/NSZG
      DO 1 I=1,NSZG
      D1= DMIN+(I-1)*DELD
      D2= D1+DELD
      XX1= DEL*ALOG(D1/(DMAX-D1))
      IF(D2.LT.DMAX) XX2= DEL*ALOG(D2/(DMAX-D2))
      GDSZ(I)= 0.5*(1.0-ERF(XX1))
      IF(D2.LT.DMAX) GDSZ(I)= 0.5*(ERF(XX2)-ERF(XX1))
      SZBAR(I)= 0.5*(D1+D2)
      IF( D2.GE.DMAX) SZBAR(I)= 0.5*(DMAX+D1)
    1 CONTINUE
      SUM=0.0
      DO 2 I=1,NSZG
      SUM=SUM+GDSZ(I)
    2 CONTINUE
C  NORMALIZATION
      DO 3 I=1,NSZG
      GDSZ(I)= GDSZ(I)/SUM
    3 CONTINUE
      RETURN
      END
```

```
*DECK SOOTP
      SUBROUTINE SOOTP(P,T8,AFV,YO28,V,T, IDIGI,XMSOT ,VBM, DMSDT,
     1 DMSDT1,DMSDT2)
C THIS ROUTINE ESTIMATE THE SOOT FORMATION AND DESTRUCTION RATE
      COMMON /AIRP/ XMAI,XMEJ,XMEGR,XMPD,XMAO,XMARC,XMAEGR,XMERD,XMEEGR,
     1              AMWA,AFRA,FARA,PHEA
      COMMON/FUELP/W,XX,YFL,ZFL,YSTOA,ZSTOA,API,FCEN,FAROS,AMWF,SURFT
     1            ,XMUF,CEN,CXST,HCOM
      COMMON/DROPC/ HUTIM,DTPHY,XTLYO2,CPBAR,RHOD,TCRITF,XL298,
     1              XMBM(100),DVBDTH(100),DLDDTH(100),XMFLI(100),
     2              DI(100,3),DMFLI(100,3),DMLDT(100,3),XNDI(100,3),
     3              XKK(100,3)
      COMMON /SOOTP/ SDEN,DSOOT, ASOTP,ASOTA,XMSOOT(100)
      IF(IDIGT.GT.2) GO TO 2
C VAPORIZING ZONE
    1 CONTINUE
      PFU= P/(1.0+AFV)
      PHEEV= PHEA*(1.0+(1.0+AFRA)/AFV)
      DMSDT= ASOTP*(VBM*VBM/V)*(T/T8) *(PHEEV**3)*PFU*EXP(-20000/T8)
      RETURN
C BURNING ZONE
    2 CONTINUE
C SOOT FORMATION RATE
      PHEB= 1.0/(AFV*FAROS)
      DMSDT1= ASOTA*(VBM*VBM/V)*(T/T8)*(PHEB**3)*P  *EXP(-20000./T8)
C SOOT OXIDIZATION RATE
      DMSDT2= 6.51E4*(XMSOT*YO28*P  )/(SDEN*DSOOT*SQRT(T8))*EXP(-19650./
     1 T8)
C NET PRODUCTION RATE
      DMSDT= DMSDT1- DMSDT2
      RETURN
      END
```

```
*DECK SOOTR7
      SUBROUTINE SOOTRZ(TAV,V)
C THIS ROUTINE ESTIMATE THE SOOT FORMATION AND DESTRUCTION RATE
      COMMON/INTEGR/ INO1,INO2,ISOOT,IWETBT,NPRT,IOTAIL,NTER,NAXIL,
     1               NSHEL,NSZG,NITST,IBUG,II,III
      COMMON/SPECYI/  XH2(100),XH2O(100),XCO(100),XCO2(100),XN2(100),
     1                XNO(100),XOH(100),XH(100),XO(100),XN(100),XO2(100)
     2                ,XCH4(100),XNONEQ(100)
      COMMON/PRATEI/ DNODT1(100),DNODT2(100),DMSDT1(100),DMSDT2(100),
     1               DRMDTH(100),DLBDTH(100),XMDF(100)
      COMMON/TPROPI/ P,TBM(100),UBM(100),HBM(100),VBM(100),CPBM(100),
     1               AMWBM(100),RBM(100),PHE(100),AFR(100),XMFBM(100),
     2               XMPAM(100)
      COMMON /AIRP/ XMAI,XMFJ,XMEGR,XMRD,XMAO,XMARD,XMAEGR,XMFRD,XMFEGR,
     1              AMWA,AFRA,FARA,PHEA
      COMMON/FUELP/W,XX,YFL,ZFL,YSTOA,ZSTOA,API,FDEN,FAROS,AMWF,SURFT
     1            ,XMUF,CEN,OXST,HCOM
      COMMON/DROPC/ HUTIM,DTPHY,XTLYO2,CPBAR,RHOD,TCRITF,XL298,
     1              XMBM(100),DVEDTH(100),CLODTH(100),XMFLI(100),
     2              DI(100,3),DMFLI(100,3),DMLDT(100,3),XNDT(100,3),
     3              XKK(100,3)
      COMMON /SOOTP/ SDEN,DSOOT, ASOTP,ASOTA,XMSOOT(100)
      DO 1 I=1,II
      DMSDT1(I)= 0.0
      DMSDT2(I)= 0.0
      IF (ISOOT.EQ.0) GO TO 1
      T8= TBM(I)
      YO28  = XO2(I)*32./AMWBM(I)
      AFOVAL= XMPAM(I)/(XMFBM(I)+XMFLI(I))
      PHEB= 1.0/(AFOVAL*FAROS)
C SOOT FORMATION RATE
      DMSDT1(I)= ASOTA*(VBM(I)*VBM(I)/V)*(TAV/T8)*(PHEB**3)*P*
     1           EXP(-20000./T8)
C SOOT OXIDIZATION RATE
      DMSDT2(I)= 6.51E4*(XMSOOT(I)*YO28*P  )/(SDEN*DSOOT*SQRT(T8))*
     1           EXP(-19650./T8)
    1 CONTINUE
      RETURN
      END
```

```
*DECK SPECY
      SUBROUTINE SPECY(PX,TX,PHEX,AMMC,XH2,XH2O,XCC,XCO2,XN2,XNO,XOH
     1  ,XH,XO,XN,XO2,XCH4)
C THIS ROUTINE CALCULATES THE EQUILIBRIUM SPECIES DISTRIBUTION OF A GIVEN
C STATE I.E. (P,T,PHE) FOR A SPECIFIC FUEL FROM TRIPLE TABLE INTERPOLATION
      COMMON/SPTAB/ NPTB,NTTB,NPHTB,PTB(7),TTB(13),PHETB(11),
     *              XH2TB(7,13,11),XH2OTB(7,13,11),XCOTB(7,13,11),
     1              XCO2TB(7,13,11),XN2TB(7,13,11),XNOTB(7,13,11),
     2              XOHTB(7,13,11),XHTB(7,13,11),XOTB(7,13,11),
     3              XNTB(7,13,11),XO2TB(7,13,11),XCH4TB(7,13,11)
      COMMON/XXCON/ IDP,IDT,IDPHE,
     1              IDP1,IDT1,IDPH1,DELP,DELT,DELPHE,DP1,DT1,DPHE1,
     2              DP2,DT2,DPHE2
      T=TX
      P=PX
      PHE= PHEX
      DO 1 IDP=2,NPTB
      IF (P.GE.PTB(IDP-1) .AND. P.LE.PTB(IDP)) GO TO 2
    1 CONTINUE
      WRITE(6,100) P
  100 FORMAT(* ERROR.... P OUT OF RANGE *, 1PE10.3)
      IF (P.LT.PTB(1)) GO TO 7
      P= PTB(NPTB)
      IDP= NPTB
      GO TO 2
    7 CONTINUE
      P= PTB(1)
      IDP= 2
    2 CONTINUE
      DO 3 IDT=2,NTTB
      IF (T.GE.TTB(IDT-1) .AND. T.LE.TTB(IDT)) GO TO 4
    3 CONTINUE
      WRITE(6,101) T
  101 FORMAT(* ERROR ..... T OUT OF RANGE * ,1PE10.3)
      IF (T.LT. TTB(1)) GO TO 8
      T= TTB(NTTB)
      IDT= NTTB
      GO TO 4
    8 CONTINUE
      T= TTB(1)
      IDT= 2
    4 CONTINUE
      DO 5 IDPHE= 2, NPHTB
      IF (PHE.GE.PHETB(IDPHE-1) .AND. PHE.LE.PHETB(IDPHE)) GO TO 6
    5 CONTINUE
      WRITE(6,102) PHE
  102 FORMAT(* ERROR ..... PHE OUT OF RANGE *,1PE10.3)
      IF (PHE.LT.PHETB(1)) GO TO 9
      PHE= PHETB(NPHTB)
      IDPHE= NPHTB
      GO TO 6
    9 CONTINUE
      PHE= PHETB(1)
      IDPHE= 2
    6 CONTINUE
      IDP1= IDP-1
      IDT1= IDT-1
      IDPH1= IDPHE-1
      DELP= PTB(IDP)- PTB(IDP1)
      DELT= TTB(IDT)- TTB(IDT1)
```

```
      DELPHE= PHETB(IDPHE)- PHETB(IDPH1)
      DP1= (P-PTB(IDP1))/DELP
      DT1= (T-TTB(IDT1))/DELT
      DPHE1= (PHE-PHETB(IDPH1))/DELPHE
      DP2= (PTB(IDP)-P)/DELP
      DT2= (TTB(IDT)-T)/DELT
      DPHE2= (PHETB(IDPHE)- PHE)/DELPHE
      CALL TRIPIT(XH2TB,XH2)
      CALL TRIPIT(XH2OTB,XH2O)
      CALL TRIPIT(XCOTB,XCO)
      CALL TRIPIT(XCO2TB,XCO2)
      CALL TRIPIT(XN2TB,XN2)
      CALL TRIPIT(XNOTB,XNO)
      CALL TRIPIT(XOHTB,XOH)
      CALL TRIPIT(XHTB,XH)
      CALL TRIPIT(XOTB,XO)
      CALL TRIPIT(XNTB,XN)
      CALL TRIPIT(XO2TB,XO2)
      CALL TRIPIT(XCH4TB,XCH4)
      ANMC=2.*XH2+28.*XN2+18.*XH2O+17.*XOH+1.*XH+30.*XNO+14.*XN+32.*XO2
     1+16.*XO+44.*XCO2+28.*XCO+16.*XCH4
      RETURN
      END
```

```
*DECK SPECYZ
      SUBROUTINE SPECYZ
C THIS ROUTINE CALCULATES THE EQUILIBRIUM SPECIES DISTRIBUTION OF A GIVEN
C STATE I.E. (P,T,PHE) FOR A SPECIFIC FUEL FROM TRIPLE TABLE INTERPOLATION
      COMMON/INTEGR/ INO1,INO2,ISOCT,IWETBT,NPRT,IDTAIL,NTER,NAXIL,
     1               NSHEL,NSZG,NITST,IBUG,II,III
      COMMON/SPECYI/  XH2(100),XH2O(100),XCO(100),XCO2(100),XN2(100),
     1                XNO(100),XOH(100),XH(100),XO(100),XN(100),XO2(100)
     2                ,XCH4(100),XNONEG(100)
      COMMON/PRATEI/ DNOOT1(100),DNOOT2(100),DMSOT1(100),DMSOT2(100),
     1               DRMOTH(100),DLBOTH(100),XMDF(100)
      COMMON/TPROPI/ P,TBM(100),UBM(100),HBM(100),VBM(100),CPBM(100),
     1               AMWBM(100),RBM(100),PHE(100),AFR(100),XMFBM(100),
     2               XMPAM(100)
      COMMON/SPTAB/ NPTB,NTTB,NPHTB,PTB(7),TTB(13),PHETB(11),
     *              XH2TB(7,13,11),XH2OTB(7,13,11),XCOTB(7,13,11),
     1              XCO2TB(7,13,11),XN2TB(7,13,11),XNOTB(7,13,11),
     2              XOHTB(7,13,11),XHTB(7,13,11),XOTB(7,13,11),
     3              XNTB(7,13,11),XO2TB(7,13,11),XCH4TB(7,13,11)
      COMMON/XXCON/ IDP,IDT,IDPHE,
     1              IDP1,IDT1,IDPH1,DELP,DELT,DELPHE,DP1,DT1,DPHE1,
     2              DP2,DT2,DPHE2
      P1= P
      DO 1 IDP=2,NPTB
      IF(P1.GE.PTB(IDP-1) .AND. P1.LE.PTB(IDP)) GO TO 2
    1 CONTINUE
      WRITE(6,100) P1
  100 FORMAT(* ERROR.... P OUT OF RANGE *, 1PE10.3)
      IF(P1.LT.PTB(1)) GO TO 7
      P1= PTB(NPTB)
      IDP= NPTB
      GO TO 2
    7 CONTINUE
      P1= PTB(1)
      IDP= 2
    2 CONTINUE
      DO 10 I=1,II
      T1= TBM(I)
      PHE1= PHE(I)
      DO 3 IDT=2,NTTB
      IF (T1.GE.TTB(IDT-1) .AND. T1.LE.TTB(IDT)) GO TO 4
    3 CONTINUE
      WRITE(6,101) T1
  101 FORMAT(* ERROR ..... T OUT OF RANGE * ,1PE10.3)
      IF (T1.LT. TTB(1)) GO TO 8
      T1= TTB(NTTB)
      IDT= NTTB
      GO TO 4
    8 CONTINUE
      T1= TTB(1)
      IDT= 2
    4 CONTINUE
      DO 5 IDPHE= 2, NPHTB
      IF (PHE1.GE.PHETB(IDPHE-1) .AND. PHE1.LE.PHETB(IDPHE)) GO TO 6
    5 CONTINUE
      WRITE(6,102) PHE1
  102 FORMAT(* ERROR ..... PHE OUT OF RANGE *,1PE10.3)
      IF (PHE1.LT.PHETB(1)) GO TO 9
      PHE1= PHETB(NPHTB)
      IDPHE= NPHTB
```

```
      GO TO 6
    9 CONTINUE
      PHE1= PHETB(1)
      IDPHE= 2
    6 CONTINUE
      IDP1= IDP-1
      IDT1= IDT-1
      IDPH1= IDPHE-1
      DELP= PTB(IDP)- PTB(IDP1)
      DELT= TTB(IDT)- TTB(IDT1)
      DELPHE= PHETB(IDPHE)- PHETB(IDPH1)
      DP1= (P1-PTB(IDP1))/DELP
      DT1= (T1-TTB(IDT1))/DELT
      DPHE1= (PHE1-PHETB(IDPH1))/DELPHE
      DP2= (PTB(IDP)-P1)/DELP
      DT2= (TTB(IDT)-T1)/DELT
      DPHE2= (PHETB(IDPHE)- PHE1)/DELPHE
      CALL TRIPIT(XH2TB,XH2(I))
      CALL TRIPIT(XH2OTB,XH2O(I))
      CALL TRIPIT(XCOTB,XCO(I))
      CALL TRIPIT(XCO2TB,XCO2(I))
      CALL TRIPIT(XN2TB,XN2(I))
      CALL TRIPIT(XNOTB,XNO(I))
      CALL TRIPIT(XOHTB,XOH(I))
      CALL TRIPIT(XHTB,XH(I))
      CALL TRIPIT(XOTB,XO(I))
      CALL TRIPIT(XNTB,XN(I))
      CALL TRIPIT(XO2TB,XO2(I))
      CALL TRIPIT(XCH4TB,XCH4(I))
      AMWBM(I)= 2.*XH2(I)+ 28.*XN2(I)+ 18.*XH2O(I)+ 17.*XOH(I)+ 1.*XH(I)
     1          + 30.*XNO(I)+ 14.*XN(I)+ 32.*XO2(I)+ 16.*XO(I)+ 44.*
     2            XCO2(I)+ 28.*XCO(I)+ 16.*XCH4(I)
   10 CONTINUE
      RETURN
      END
```

```
*DECK SPRAY
      SUBROUTINE SPRAY(RHOR,OMEGA,DELP,SEFJ,CDCHG)
C THIS ROUTINE SIMULATES THE STEADY STATE FUEL JET SPRAY AND DEFINES THE
C TRAJECTORIES OF FUEL ELEMENTS AND A/F  VIA SIMILARITY ASSUMPTION
      DIMENSION BRB(20)
      COMMON/INTEGR/ INO1,INC2,ISOOT,IWETBT,NPRT,IDTAIL,NTER,NAXIL,
     1               NSHEL,NSZG,NITST,IBUG,II,III
      COMMON/SCA/ THEMAX,THEIJ,THEIG,DINJ,THENE,THEVO,THEVC,DTINJ,
     1            DTHMIN,DTHMED,DTHMAX,DTHETA,DT
      COMMON/ENGEO/ DE,RFW,RL,VC,SC,S,USI,CR,RPM,TW,DNOZZ,NNOZZ,DBOWL,
     1              VFJO
      COMMON/FUELP/W,XX,YFL,ZFL,YSTOA,ZSTOA,API,FDEN,FAROS,AMWF,SURFT
     1             ,XMUF,CEN,OXST,HCOM
      COMMON/JETP/ DJF,XS(20),YS(20,4),VS(20,4),RHOF(20,4),AFT(20,4),
     1             PTIM(20,4),ETAI(20,5),DYS(20,4), GDSZ(3),SZBAR(3),
     2             D(25,4,3),XSS(25,4),YSS(25,4),DYSS(25,4),TAFV(25,4),
     3             AFV(25,4),XMFVS(25,4),XMSOT(25,4),TO(25,4),PO(25,4),
     4             IDIG(25,4)
      COMMON/CONVF/ XJ,ATO,DTR,XK,SIG,P,RU,CTDTH,CTHDT,DTRDT,PI
      NAMELIST/GIVEN/ FDEN,SURFT,XMUF,DELP,RHOR,DNOZZ,DBOWL,VFJO,CIF
     1            ,CWF,CJF,XI,BI,NSHEL,NAXIL,NSZG ,DJF,DX,XWALL,BO,XMAX
      XIF1= 1.3446
      XIF2= 0.8105
      XIF3=0.559272539
      XIF4= 0.4209
      XIF5= 0.33115
      XIF6= 0.2709
      XIF7= 0.2276
      XI2= 2.8274
      XI3= 2.3122
      XI4= 1.9854
      XI5= 1.74872
      XI6= 1.57383
      XI7= 1.437
      CIF=0.135*(1.0+RHOR/FDEN)
      CJF=0.175
      CWF=0.204
      RBOWL= 0.5*DBOWL
      RNOZZ=0.5*DNOZZ
      ANOZZ= PI*RNOZZ*RNOZZ
      XJF= FDEN*VFJO*ANOZZ*CDCHG
      XJM= XJF*VFJO
      DJF= XJF/NSHEL
C  DEFINING THE DIMENSION OF INITIAL REGION
      PIF= PI/XIF3
      XI= (SQRT(PIF)-1.0)*RNOZZ/CIF
      BI= CIF*XI+RNOZZ
C     XWALL= (RBOWL+CJF*XI-BI)/(1.0+CJF)
      XWALL= RBOWL
      BO= BI+(XWALL-XI)*CJF
      XMAX= XWALL+(PI*DBOWL/NNOZZ)-RO
      DX= XMAX/(NAXIL-1)
C CALCULATE DROPSIZE DISTRIBUTION
      CALL SIZED(DELP,RHOR,FDEN,SURFT,XMUF,DNOZZ,SZBAR,GDSZ,NSZG)
      IF (IDTAIL.NE.0) WRITE(6,GIVEN)
      DO 3 J= 1, NSHEL
      PTIM(1,J)= 0.0
    3 CONTINUE
      XS(1)  = XI
      DO 1 I=1,NAXIL
```

```
      X= XI+(I-1)*DX
      IF(X.GT.XWALL)  GO TO 8
C FREE JET REGION
      B= BI+CJF*(X-XI)
      BB= XJF/(RHOR*B*B*XIF3)
      CC= -BB*VFJO
      XXX= BB*BB-4.0*CC
      VCL= 0.5*(-BB+SQRT(XXX))
      IF (VCL.GT. VFJO) VCL= VFJO
      RHOFCL= XJF/(VCL* B*B*XIF3)
      AFCL= RHOR/RHOFCL
      GO TO 4
    8 CONTINUE
      IF ((X-DX).GT.XWALL) GO TO 12
C WALL TRANSIENT ZONE
      BW= B
      XO= X-DX
      RHOCLP= XI2*XJF/(BW*BW*VCL*XIF2*XI3)
      XXX= XI2*(RHOR*XIF6+RHOFCL*XIF7)/(XIF2*(RHOR*XI6+RHOCLP*XI7))
      VCLP= VCL*SQRT(XXX)
      BOP= XIF2*BW*VCL/(XI2*VCLP)
      XJMP= VCLP*VCLP*BW*BOP*(RHOR*XI4+RHOCLP*XI5)
      IF (IBUG.EQ.0) GO TO 14
      WRITE(6,118)
      WRITE(6,112) B,RHOFCL,VCL,XJM
      WRITE(6,113) BOP,RHOCLP,VCLP,XJMP
   14 CONTINUE
      VCL= VCLP
       B= BOP
      RHOFCL= RHOCLP
C WALL REGION
   12 CONTINUE
      RX= X-XO
      B= B + CWF*RX
      AA= (RX+BW)*B*RHOR*XI4
      BB= XI5/XI3*XJF
      CC=-XJMP
      XXX= BB*BB- 4.0*AA*CC
      VCL= -BB+SQRT(XXX)/(2.0*AA)
      RHOFCL= XJF/(VCL*(RX+BW)*B*XI3)
      AFCL= RHOR/RHOFCL
C     WRITE(6,104) I,B,XP2,XN1U,XN2U,XMM,USI,VCL,RHOFCL,AFCL
    4 CONTINUE
      ETAI(I,1)= 0.0
      ETAI(I,NSHEL+1)= 1.0
      ETA=0.1
      DO 2 J=1,NSHEL
      IF (X.GT. XWALL) GO TO 7
C FREE JET REGION
      IF (J.EQ.NSHEL) GO TO 16
      GO=(FLOAT(J)    )*DJF/(2.0*PI*RHOFCL*VCL*B*B)
      DO 5 ITER=1,20
      ETA1= 0.5*(ETA*ETA)
      ETA2= 0.85714*(ETA**3.5)
      ETA3= 0.6*(ETA**5)
      ETA4= 0.15384*(ETA**6.5)
      G= ETA1-ETA2+ETA3-ETA4 -GO
      CHK= ABS(G/GO)
      IF (CHK.LT.1.0E-5 ) GO TO 6
      ETA32= ETA**1.5
```

```
      FC= 1.0-ETA32
      DGDE= (FC**3)*ETA
      ETA= ETA- G/DGDE
      IF(ETA.LT.0.0) ETA=0.0001
      IF(ETA.GT.1.0) ETA=0.9999
    5 CONTINUE
      WRITE(6,103) J,I,G,QQ,ETA
      STOP
C A/F, VELOCITY DISTRIBUTIONS--- FREE JET REGION
    6 CONTINUE
      ETAI(I,J+1)= ETA
   16 FC= 1.0-(0.5*(ETAI(I,J+1)+ETAI(I,J)))**1.5
      RHOF(I,J)= RHOFCL*FC
      R1= ETAI(I,J)*B
      R2= ETAI(I,J+1)*B
      DAREA= PI*(R2*R2-R1*R1)
      VBAR2= DJF/RHOF(I,J)/DAREA
      VS(I,J)= VBAR2/VFJO
      AFT(I,J)= (1.0/VS(I,J))-1.0
      AFT(I,J)= RHOR/RHOF(I,J)
      GO TO 9
    7 CONTINUE
C WALL JET REGION
      IF (J.EQ.NSHEL) GO TO 17
      QQ= FLOAT(J)*DJF/(2.0*PI*(RX+BW)*B*VCL*RHOFCL)
      DO 10 ITER=1,20
      ETA1= ETA
      ETA2=(3.0/2.5)*(ETA**2.5)
      ETA3= (3.0/4.0)*(ETA**4)
      ETA4=(1.0/5.5)*(ETA**5.5)
      G= ETA1-ETA2+ETA3-ETA4- QQ
      CHK= ABS(G/QQ)
      IF (CHK.LT.1.0E-5 ) GO TO 11
      ETA32= ETA**1.5
      FC= 1.0-ETA32
      DGDE= FC**3
      ETA= ETA- G/DGDE
      IF(ETA.LT.0.0) ETA=0.0001
      IF(ETA.GT.1.0) ETA=0.9999
   10 CONTINUE
      WRITE(6,103) J,I,G,QQ,ETA
      STOP
   11 CONTINUE
C A/F, VELOCITY DISTRIBUTIONS--- WALL JET REGION
      ETAI(I,J+1)= ETA
   17 FC= 1.0-(0.5*(ETAI(I,J+1)+ETAI(I,J)))**1.5
      RHOF(I,J)= RHOFCL*FC
      R1= ETAI(I,J)*B
      R2= ETAI(I,J+1)*B
      DAREA= 2.0*PI*(RX+BW)*(R2-R1)
      VBAR2= DJF/RHOF(I,J)/DAREA
      VS(I,J)= VBAR2/VFJO
      AFT(I,J)= RHOR/RHOF(I,J)
    9 CONTINUE
      YS(I,J)= 0.5*(R1+R2)
      DYS(I,J)= R2-R1
      IF (I.LE.1) GO TO 2
C INTEGRATING FOR PENETRATION TIME
      VBAR= 0.5*(VS(I-1,J)+VS(I,J))*VFJO
      PTIM(I,J)= PTIM(I-1,J)+ (DX/VBAR)
```

```
    2 CONTINUE
      XS(I)  = X
      BBB(I)= B
    1 CONTINUE
C EFFECT OF SWIRL CN ENTRINNMENT
      USBAR= 0.25*CBOWL*OMEGA
      ER=  1.0+ SEFJ*(USBAR/VFJO)
      DO 21 J=1,NSHEL
      DO 21 I=1,NAXIL
      AFT(I,J)= ER*AFT(I,J)
   21 CONTINUE
C DETAIL OUTPUT
      IF (IDTAIL.EG.0) GO TO 22
      WRITE(6,116) (I,I=1,NSZG)
      WRITE(6,117)     (SZBAR(I),I=1,NSZG)
      WRITE(6,115)     ( GDSZ(I),I=1,NSZG)
      WRITE(6,98)
      WRITE(6,107)    (XS(I  ),I=1,20)
      WRITE(6,106)    ( BBB(I)  ,I=1,20)
      DO 20 J=1,NSHEL
      WRITE(6,98)
      WRITE(6,108)    (  YS(I,J),I=1,20)
      WRITE(6,114)    ( DYS(I,J),I=1,20)
      WRITE(6,109) (RHOF(I,J),I=1,20)
      WRITE(6,119) (AFT(I,J),I=1,20)
      WRITE(6,110)    (VS(I,J),I=1,20)
      WRITE(6,111)      (PTIM(I,J),I=1,20)
   20 CONTINUE
   22 CONTINUE
   98 FORMAT(/)
  103 FORMAT(/1X,* JET SPRAY LOCUS ITERATICN GOES NCT CONVERGE *,2I5,
     1 1P5E10.3)
  106 FORMAT(1X,* B *,20F6.2)
  107 FORMAT(1X,* X *,20F6.3)
  108 FORMAT(1X,* Y *,20F6.4)
  109 FORMAT(1X,*ROF*,20F6.4)
  110 FORMAT(1X,* V *,20F6.4)
  111 FORMAT(1X,*TIM*,20F6.4)
  112 FORMAT(1X,*BEFORE TRANSITION*,2X,1P9E12.3)
  113 FORMAT(1X,*AFTER  TRANSITICN*,2X,1P9E12.3)
  114 FORMAT(1X,*DY *,20F6.4)
  115 FORMAT(1X,*GROUP MASS FRACTICN*,5E12.3)
  116 FORMAT(/1X,*DROPLET SIZE GROUP *,5(7X,I5))
  117 FORMAT(1X,*MEAN GROUP SIZE    *,5E12.3)
  118 FORMAT(/27X,1HB,9X,6HRHOFCL,6X,3HVCL,9X,3HXJM)
  119 FORMAT(1X,*AFT*,20F6.2)
      RETURN
      END
```

```
*DECK TAPEIN
      SUBROUTINE TAPEIN
C  SPECIES TABLE INPUT FROM A TAPE
      COMMON/SPTAB/ NPTB,NTTB,NPHTB,PTB(7),TTB(13),PHETB(11),
     *              XH2TB(7,13,11),XH2OTB(7,13,11),XCOTB(7,13,11),
     1              XCO2TB(7,13,11),XN2TB(7,13,11),XNOTB(7,13,11),
     2              XOHTB(7,13,11),XHTB(7,13,11),XOTB(7,13,11),
     3              XNTB(7,13,11),XO2TB(7,13,11),XCH4TB(7,13,11)
      NPTB= 7
      NTTB= 13
      NPHTB= 11
C SET ZERO
      DO 84 I=1,12043
      PTB(I)= 0.0
   84 CONTINUE
      DO 81 IPHTB=1, NPHTB
      DO 81 IPTB=1,NPTB
      READ (8,121) PTB(IPTB),PHETB(IPHTB)
      READ (8,122) (TTB(I),I=1,NTTB)
      IF(PHETB(IPHTB).LE.0.05) GO TO 82
      READ (8,122) (XH2TB(IPTB,I,IPHTB),I=1,NTTB)
      READ (8,122) (XH2OTB(IPTB,I,IPHTB),I=1,NTTB)
      READ (8,122) ( XCOTB(IPTB,I,IPHTB),I=1,NTTB)
      READ (8,122) (XCO2TB(IPTB,I,IPHTB),I=1,NTTB)
   82 CONTINUE
      READ (8,122) ( XN2TB(IPTB,I,IPHTB),I=1,NTTB)
      READ (8,122) ( XNOTB(IPTB,I,IPHTB),I=1,NTTB)
      IF(PHETB(IPHTB).LE.0.05) GO TO 83
      READ (8,122) ( XOHTB(IPTB,I,IPHTB),I=1,NTTB)
      READ (8,122) (  XHTB(IPTB,I,IPHTB),I=1,NTTB)
   83 CONTINUE
      READ (8,122) (  XOTB(IPTB,I,IPHTB),I=1,NTTB)
      READ (8,122) (  XNTB(IPTB,I,IPHTB),I=1,NTTB)
      READ (8,122) ( XO2TB(IPTB,I,IPHTB),I=1,NTTB)
      IF(PHETB(IPHTB).LE.0.05) GO TO 81
      READ (8,122) (XCH4TB(IPTB,I,IPHTB),I=1,NTTB)
   81 CONTINUE
  121 FORMAT(1X,1P3E10.3)
  122 FORMAT(6X,1P13E10.3)
      RETURN
      END
```

```
*DECK TPROP
      SUBROUTINE TPROP(TX,PX,V,CV,CP,U,H  ,AMW,GAM  ,R,PHEX)
C*********** THIS ROUTINE CALCULATES --------
C********** EQUILIBRIUM THERMODYNAMICS OF COMBUSTION PRODUCTS
C********** U(P,T,PHE) AND R(P,T,PHE) AND THEIR DERIVATIVES
      COMMON/FUELP/W,XX,YFL,ZFL,YSTOA,ZSTOA,API,FDEN,FAROS,AMWF,SURFT
     1             ,XMUF,CEN,OXST,HCOM
      COMMON/RANGS/ TRANG1,TRANG2,PRANG1,PRANG2,PHERG1,PHERG2
      COMMON /PDRVT/ PUPP,PUPT,PRPF,PUPF,PRFT,PRPP
      COMMON /HPCOE/ AA1(6),BB1(6),DD1(11),RR1(8), AA2(6),BB2(6),DD2(11)
     1               ,RR2(8)
      P1= PX
      T1= TX
      PHE= PHEX
      IF (PX.GT.PRANG2) P1= PRANG2
      IF (TX.GT.TRANG2) T1= TRANG2
      IF (PHEX.GT.PHERG2) PHE= PHERG2
      TI=1000./T1
      T2= T1*T1
      T3= T2*T1
      T4= T3*T1
      T5= T4*T1
      PHE2 = PHE*PHE
      PHE3= PHE*PHE2
      ALOGP= ALOG(P1)
      IF (PHE.GT.1.0) GO TO 2
    1 CONTINUE
C FUEL LEAN
      A= AA1(1)+AA1(2)*T1+AA1(3)*T2 +AA1(4)*T3 +AA1(5)*T4 +AA1(6)*T5
      B= BB1(1)+BB1(2)*T1+BB1(3)*T2 +BB1(4)*T3 +BB1(5)*T4 +BB1(6)*T5
      D1=  DD1(1)+DD1(2)*PHE+ DD1(3)*PHE3
      D2= (DD1(4)+DD1(5)*PHE+ DD1(6)*PHE3)*TI
      D30=((DD1(7)+DD1(8)*PHE+ DD1(9)*PHE3)+ (DD1(10)+DD1(11)*PHE)*TI)
      D3= D30*ALOGP
      XXX=D1+D2+D3
      IF (XXX.LT.-200.) XXX=-200.
      D= EXP(XXX)
      UX= A- B*PHE+ D
      XXX= (RR1(3)+ RR1(4)*TI+ RR1(5)*ALOGP)*PHE+ RR1(6)+ RR1(7)*TI+
     1RR1(8)*ALOGP
      IF (XXX.LT.-200.) XXX=-200.
      C= EXP(XXX)
      RX= RR1(1)+ RR1(2)*PHE + C
      HX=UX+RX*T1
      AP= AA1(2)+2.0*AA1(3)*T1+ 3.0*AA1(4)*T2+ 4.0*AA1(5)*T3+ 5.0*AA1(6)
     1     *T4
      BP= BB1(2)+2.0*BB1(3)*T1+ 3.0*BB1(4)*T2+ 4.0*BB1(5)*T3 +5.0*BB1(6)
     1     *T4
      D2P= -(DD1(4)+ DD1(5)*PHE+ DD1(6)*PHE3)*1000./T2
      D3P= -(DD1(10)+ DD1(11)*PHE)*1000./T2* ALOGP
      DP = C*(D2P+D3P)
      CVX= AP-BP*PHE+DP
      CPX=CVX+RX
CONVERT UNIT TO  PER  MASS OF MIXTURE
      XBASE= 1.0+FAROS*PHE
      F1= 1.0/XBASE
      U= UX*F1
      H= HX*F1
      R=RX*F1
      AMW= 1.987/R
```

```
      V= 41.6*P*T1/P1
      CV=CVX*F1
      CP=CPX*F1
      GAM= CP/CV
C  PARTIAL DERIVATIVES OF U AND R W.R.T. P,T, AND PHE
      D1PF = DD1(2)+3.0*DD1(3)*PHE2
      D2PF = (DD1(5)+3.0*DD1(6)*PHE2)*TI
      D3PF =((DD1(9)+3.0*DD1(9)*PHE2)+ DD1(11)*TI)*ALOGP
      DPF= D*(D1PF+D2PF+D3PF)
      PF1PF= -F1*F1*FAROS
      PUPP=     F1*D*(D30/P1)
      PUPT = CV
      PUPF= F1*(-B+DPF)+ PF1PF*UX
      PRPP= F1*C*(RR1(5)*PHE+RR1(8))/P1
      PRPT= -F1*C*(RR1(4)*PHE+RR1(7))*1000./T2
      PRXPF= RR1(2)+ C*(RR1(3)+ RR1(4)*TI+ RR1(5)*ALOGP)
      PRPF= F1*PRXPF+ PF1PF*RX
      RETURN
    2 CONTINUE
C FUEL RICH
      A= AA2(1)+AA2(2)*T1+AA2(3)*T2 +AA2(4)*T3 +AA2(5)*T4 +AA2(6)*T5
      B= BB2(1)+BB2(2)*T1+BB2(3)*T2 +BB2(4)*T3 +BB2(5)*T4 +BB2(6)*T5
      D1=  DD2(1)+DD2(2)*PHE+ DD2(3)*PHE3
      D2= (DD2(4)+DD2(5)*PHE+ DD2(6)*PHE3)*TI
      D30=((DD2(7)+DD2(8)*PHE+ DD2(9)*PHE3)+ (DD2(10)+DD2(11)*PHE)*TI)
      D3= D30*ALOGP
      XXX=D1+D2+D3
      IF (XXX.LT.-200.) XXX=-200.
      D= EXP(XXX)
      UX= A- B*PHE+ D
      XXX= (RR2(3)+ RR2(4)*TI+ RR2(5)*ALOGP)*PHE+ RR2(6)+ RR2(7)*TI+
     1RR2(8)*ALOGP
      IF (XXX.LT.-200.) XXX=-200.
      C= EXP(XXX)
      RX= RR2(1)+ RR2(2)*PHE + C
      HX=UX+RX*T1
      AP= AA2(2)+2.0*AA2(3)*T1+ 3.0*AA2(4)*T2+ 4.0*AA2(5)*T3+ 5.0*AA2(6)
     1     *T4
      BP= BB2(2)+2.0*BB2(3)*T1+ 3.0*BB2(4)*T2+ 4.0*BB2(5)*T3 +5.0*BB2(6)
     1     *T4
      D2P= -(DD2(4)+ DD2(5)*PHE+ DD2(6)*PHE3)*1000./T2
      D3P= -(DD2(10)+ DD2(11)*PHE)*1000./T2* ALOGP
      DP = D*(D2P+D3P)
      CVX= AP-BP*PHE+DP
      CPX=CVX+RX
CONVERT UNIT TO  PER  MASS OF MIXTURE
      XBASE= 1.0+FAROS*PHE
      F1= 1.0/XBASE
      U= UX*F1
      H= HX*F1
      R=RX*F1
      AMW= 1.987/R
      V= 41.6*R*T1/P1
      CV=CVX*F1
      CP=CPX*F1
      GAM= CP/CV
C  PARTIAL DERIVATIVES OF U AND R W.R.T. P,T, AND PHE
      D1PF = DD2(2)+3.0*DD2(3)*PHE2
      D2PF = (DD2(5)+3.0*DD2(6)*PHE2)*TI
      D3PF =((DD2(8)+3.0*DD2(9)*PHE2)+ DD2(11)*TI)*ALOGP
```

```
DPF= D*(D1PF+D2PF+D3PF)
PF1PF= -F1*F1*FAROS
PUPP=     F1*D*(D30/P1)
PUPT = CV
PUPF= F1*(-D+DPF)+ PF1PF*UX
PRPP= F1*C*(RR2(5)*PHE+RR2(8))/P1
PRPT= -F1*C*(RR2(4)*PHE+RR2(7))*1000./T2
PRXPF= RR2(2)+ C*(RR2(3)+ RR2(4)*TI+ RR2(5)*ALOGP)
PRPF= F1*PRXPF+ PF1PF*RX
RETURN
END
```

```
*DECK TPROPZ
      SUBROUTINE TPROPZ
C**********  THIS ROUTINE CALCULATES --------
C********** EQUILIBRIUM THERMODYNAMICS OF COMBUSTION PRODUCTS
C********** U(P,T,PHE) AND R(P,T,PHE) AND THEIR DERIVATIVES
      COMMON/INTEGR/ INO1,INO2,ISOOT,IWETBT,NPRT,ICTAIL,NTER,NAXIL,
     1               NSHEL,NSZG,NITST,IBUG,II,III
      COMMON/TPROPI/ P,TBM(100),UBM(100),HBM(100),VBM(100),CPBM(100),
     1               AMWBM(100),RBM(100),PHE(100),AFR(100),XMFBM(100),
     2               XMPAM(100)
      COMMON/FUELP/W,XX,YFL,ZFL,YSTOA,ZSTOA,API,FDEN,FAROS,AMWF,SURFT
     1            ,XMUF,CEN,OXST,HCOM
      COMMON/RANGS/ TRANG1,TRANG2,PRANG1,PRANG2,PHERG1,PHERG2
      COMMON/PDPVIZ/ PUPPBM(100),PUPTBM(100),PRPFBM(100),PUPFBM(100),
     1               PRPTBM(100),PRFPBM(100)
      COMMON /HPCOE/ AA1(6),BB1(6),DD1(11),RR1(8), AA2(6),BB2(6),DD2(11)
     1              ,RR2(8)
      P1= P
      IF (P1.GT.PRANG2) P1= PRANG2
      DO 10 I=1,II
      T1= TBM(I)
      PHE1= PHE(I)
      IF (T1.GT.TRANG2) T1= TRANG2
      IF (PHE1.GT.PHERG2) PHE1= PHERG2
      TI=1000./T1
      T2= T1*T1
      T3= T2*T1
      T4= T3*T1
      T5= T4*T1
      PHE2 = PHE1*PHE1
      PHE3= PHE1*PHE2
      ALOGP= ALOG(P1)
      IF (PHE1.GT.1.0) GO TO 2
    1 CONTINUE
C FUEL LEAN
      A= AA1(1)+AA1(2)*T1+AA1(3)*T2 +AA1(4)*T3 +AA1(5)*T4 +AA1(6)*T5
      B= BB1(1)+BB1(2)*T1+BB1(3)*T2 +BB1(4)*T3 +BB1(5)*T4 +BB1(6)*T5
      D1=  DD1(1)+DD1(2)*PHE1+ DD1(3)*PHE3
      D2= (DD1(4)+DD1(5)*PHE1+ DD1(6)*PHE3)*TI
      D30=((DD1(7)+DD1(8)*PHE1+ DD1(9)*PHE3)+ (DD1(10)+DD1(11)*PHE1)*TI)
      D3= D30*ALOGP
      XXX=D1+D2+D3
      IF (XXX.LT.-200.) XXX=-200.
      D= EXP(XXX)
      UX= A- B*PHE1+ D
      XXX= (RR1(3)+ RR1(4)*TI+ RR1(5)*ALOGP)*PHE1+ RR1(6)+ RR1(7)*TI+
     1RR1(8)*ALOGP
      IF (XXX.LT.-200.) XXX=-200.
      C= EXP(XXX)
      RX= RR1(1)+ RR1(2)*PHE1+ C
      HX=UX+RX*T1
      AP= AA1(2)+2.0*AA1(3)*T1+ 3.0*AA1(4)*T2+ 4.0*AA1(5)*T3+ 5.0*AA1(6)
     1     *T4
      BP= BB1(2)+2.0*BB1(3)*T1+ 3.0*BB1(4)*T2+ 4.0*BB1(5)*T3 +5.0*BB1(6)
     1     *T4
      D2P= -(DD1(4)+ DD1(5)*PHE1+ DD1(6)*PHE3)*1000./T2
      D3P= -(DD1(10)+ DD1(11)*PHE1)*1000./T2* ALOGP
      DP = D*(D2P+D3P)
      CVX= AP-BP*PHE1+DP
      CPX=CVX+RX
```

```
CONVERT UNIT TO  PER  MASS OF MIXTURE
      XBASE= 1.0+FAROS*PHE1
      F1= 1.0/XBASE
      UBM(I)= UX*F1
      HBM(I)= HX*F1
      RBM(I)= RX*F1
      AMWBM(I)= 1.987/RBM(I)
      VX= 41.6*RBM(I)*T1/P1
      CV=CVX*F1
      CPBM(I)= CPX*F1
      GAM= CPBM(I)/CV
C  PARTIAL DERIVATIVES OF U AND R W.R.T. P,T, AND PHE
      D1PF  = DD1(2)+3.0*DD1(3)*PHE2
      D2PF  = (DD1(5)+3.0*DD1(6)*PHE2)*TI
      D3PF =((DD1(8)+3.0*DD1(9)*PHE2)+ DD1(11)*TI)*ALOGP
      DPF= D*(D1PF+D2PF+D3PF)
      PF1PF= -F1*F1*FAROS
      PUPPBM(I)= F1*D*(D30/P1)
      PUPTBM(I) = CV
      PUPFBM(I)= F1*(-B+DPF)+ PF1PF*UX
      PRPPBM(I)= F1*C*(RR1(5)*PHE1+RR1(8))/P1
      PRPTBM(I)= -F1*C*(RR1(4)*PHE1+RR1(7))*1000./T2
      PRXPF= PR1(2)+ C*(RR1(3)+ RR1(4)*TI+ RR1(5)*ALOGP)
      PRPFBM(I)= F1*PRXPF+ PF1PF*RX
      GO TO 10
    2 CONTINUE
C FUEL RICH
      A= AA2(1)+AA2(2)*T1+AA2(3)*T2 +AA2(4)*T3 +AA2(5)*T4 +AA2(6)*T5
      B= BB2(1)+BB2(2)*T1+BB2(3)*T2 +BB2(4)*T3 +BB2(5)*T4 +BB2(6)*T5
      D1=  DD2(1)+DD2(2)*PHE1+ DD2(3)*PHE3
      D2= (DD2(4)+DD2(5)*PHE1+ DD2(6)*PHE3)*TI
      D30=((DD2(7)+DD2(8)*PHE1+ DD2(9)*PHE3)+ (DD2(10)+DD2(11)*PHE1)*TI)
      D3= D30*ALOGP
      XXX=D1+D2+D3
      IF (XXX.LT.-200.) XXX=-200.
      D= EXP(XXX)
      UX= A- B*PHE1+ D
      XXX= (RR2(3)+ RR2(4)*TI+ RR2(5)*ALOGP)*PHE1+ RR2(6)+ RR2(7)*TI+
     1RR2(8)*ALOGP
      IF (XXX.LT.-200.) XXX=-200.
      C= EXP(XXX)
      RX= RR2(1)+ RR2(2)*PHE1+ C
      HX=UX+RX*T1
      AP= AA2(2)+2.0*AA2(3)*T1+ 3.0*AA2(4)*T2+ 4.0*AA2(5)*T3+ 5.0*AA2(6)
     1     *T4
      BP= BB2(2)+2.0*BB2(3)*T1+ 3.0*BB2(4)*T2+ 4.0*BB2(5)*T3 +5.0*BB2(6)
     1     *T4
      D2P= -(DD2(4)+ DD2(5)*PHE1+ DD2(6)*PHE3)*1000./T2
      D3P= -(DD2(10)+ DD2(11)*PHE1)*1000./T2* ALOGP
      DP = D*(D2P+D3P)
      CVX= AP-BP*PHE1+DP
      CPX=CVX+RX
CONVERT UNIT TO  PER  MASS OF MIXTURE
      XBASE= 1.0+FAROS*PHE1
      F1= 1.0/XBASE
      UBM(I)= UX*F1
      HBM(I)= HX*F1
      RBM(I)= RX*F1
      AMWBM(I)= 1.987/RBM(I)
      VX= 41.6*RBM(I)*T1/P1
```

```
      CV=CVX*F1
      CPBM(I)= CPX*F1
      GAM= CPBM(I)/CV
C  PARTIAL DERIVATIVES OF U AND R W.R.T. P,T, AND PHE
      D1PF = DD2(2)+3.0*DD2(3)*PHE2
      D2PF = (DD2(5)+3.0*DD2(6)*PHE2)*TI
      D3PF =((DD2(8)+3.0*DD2(9)*PHE2)+ DD2(11)*TI)*ALOGP
      DPF= C*(D1PF+D2PF+D3PF)
      PF1PF= -F1*F1*FAROS
      PUPPBM(I)= F1*D*(D30/P1)
      PUPTBM(I) = CV
      PUPFBM(I)= F1*(-R+DPF)+ PF1PF*UX
      PRPPBM(I)= F1*C*(RR2(5)*PHE1+RR2(8))/F1
      PRPTBM(I)= -F1*C*(RR2(4)*PHE1+RR2(7))*1000./T2
      PRXPF= RR2(2)+ C*(RR2(3)+ RR2(4)*TI+ RR2(5)*ALOGP)
      PRPFBM(I)= F1*PRXPF+ PF1PF*RX
   10 CONTINUE
      RETURN
      END
```

```
*DECK TRIPIT
      SUBROUTINE TRIPIT(Q,QI)
C  TRIPLE INTERPOLATION OF A TABLE FUNCTION Q(P,T,PHE)
      DIMENSION Q(7,13,11)
      COMMON/XXCON/ IDP,IDT,IDPHE,
     1              IDP1,IDT1,IDPH1,DELP,DELT,DELPHE,DP1,DT1,DPHE1,
     2              DP2,DT2,DPHE2
      QJ1K1= Q(  IDP,IDT,IDPHE)*DP1+ Q(  IDP1,IDT,IDPHE)*DP2
      QJ1K = Q(  IDP,IDT,IDPH1)*DP1+ Q(  IDP1,IDT,IDPH1)*DP2
      QJK1 = Q(  IDP,IDT1,IDPHE)*DP1+ Q(  IDP1,IDT1,IDPHE)*DP2
      QJK  = Q(  IDP,IDT1,IDPH1)*DP1+ Q(  IDP1,IDT1,IDPH1)*DP2
      Q2= QJ1K1*DT1+ QJK1*DT2
      Q1= QJ1K*DT1+ QJK*DT2
      QI    = Q2*DPHE1+ Q1*DPHE2
      RETURN
      END
```

```
*DECK VOLM
      SUBROUTINE VOLM(THETAI,DSDTH,DVDTH,V)
C*****  THIS ROUTINE CALCULATES THE TOTAL VOLUME AT CURRENT CA
      COMMON/ENGEO/ DE,RFW,RL,VC,SC,S,USI,CR,RPM,TW,DNOZZ,NNOZZ,DBOWL,
     1              VFJO
      COMMON/CONVF/ XJ,ATD,DTR,XK,SIG,R,RU,DTDTH,DTHDT,DTRDT,PI
      XX2= THETAI*DTR
      SINT=SIN(XX2)
      COST= COS(XX2)
      RLR= RFW/RL
      XXX= 1.0-(RLR*SINT)**2
      XXX= SQRT(XXX)
      S= RFW*(1.0-COST +(1.0-XXX)/RLR)
      DSDTH= RFW *SINT *(1.0+COST*RLR/XXX)  *DTR
      DVDTH= 0.7853981635*DE*DE*DSDTH
      V= VC+ 0.7853981635*DE*DE*S
      RETURN
      END
```

```
*DECK WETBT
      SUBROUTINE WETBT(P,T8,AMWA,AMWF,A,B,C,TW,XL)
C     ESTIMATE STABLE WET-BULB TEMPERATURE (N-HEPTANE)
      COMMON/DROPC/ HUTIM,DTPHY,XTLYC2,CPBAR,RHOD,TCRITF,XL298,
     1              XMBM(100),DVEDTH(100),DLDDTH(100),XMFLI(100),
     2              DI(100,3),DMFLI(100,3),DMLDT(100,3),XNDI(100,3),
     3              XKK(100,3)
      DTW= 0.05*(TCRITF-298.)
      TW= 298.- DTW
      DO 1 ITER=1,50
      TW= TW+ DTW
      IF (TW.GE.TCRITF) GO TO 3
      XL= XL298*((TCRITF-TW)/(TCRITF-298.))**0.38
      XRHS= CPBAR*(T8-TW)/XL
      XXX= A- B/(TW-C)
      PFL= 10.**XXX
      XXX= PFL*AMWF
      YFL= XXX/(XXX+(P-PFL)*AMWA)
      XLHS= YFL/(1.0-YFL)
      CHK= (XRHS-XLHS)/XRHS
      IF (ABS(CHK).LT.0.01) GO TO 2
      IF (ITER.EQ.1) CHK1= CHK
      IF (CHK*CHK1 .LT. 0.0) GO TO 3
      GO TO 1
    3 CONTINUE
      TW= TW- DTW
      DTW= 0.5*DTW
    1 CONTINUE
      WRITE(6,100) ITER,P,T8,TW,XRHS,XLHS,DTW
  100 FORMAT(1X,*..... ERROR IN WETBT ITERATION...*,I3,1P7E10.3)
      STOP
    2 CONTINUE
      RETURN
      END
```

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16. ABSTRACT

A mathematical model describing heat release and pollutant formation in direct injection diesel engines has been developed and tested. The model includes several empirical constants which can be tuned to fit the requirements of a particular engine. Sensitivity studies indicate that the model is most responsive to those constants which control fuel/air mixing. Numerical experiments strongly suggest that diffusion flames modelled by spherical droplet flames are unsuitable for this type of system. The model has been tested against results obtained with a single cylinder diesel engine. Reasonable predictions of the influence of engine design and operation parameters on NO_x emissions were obtained. However, predictions of smoke emissions were not satisfactory.

17. KEY WORDS AND DOCUMENT ANALYSIS

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