1981

A user's manual for the generalized reactor profile steady state program (GRPSS)

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Appendix A: GRPSS-Steady State Program Manual

A USER'S MANUAL FOR THE GENERALIZED REACTOR PROFILE STEADY STATE PROGRAM (GRPSS)

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1. INTRODUCTION

Although there are several generalized steady state process simulation routines available, few are capable of describing what is taking place along the length of a chemical reactor. CHESS, for example, can simulate reactor units, however it is limited in that it can only qualitatively describe the reactions taking place over the entire reactor and there is no adjustment made for the heat of reaction. In some cases, quantitative information of temperature, concentration, and reaction rates are important in dynamic studies and reactor design. Thus, a generalized steady state simulaton, including calculations along a reactor length and other process units, would prove useful in these areas.

GRPSS is a generalized reactor-profile steady-state package for simulating an adiabatic, packed-bed reactor system, in this case, the methanation section for a high-BTU coal gasificaton plant. The system is modeled for the following reactions:

$$CO + 3H_2 = CH_4 + H_2O \qquad \text{methanation} \qquad [1]$$

$$CO + H_2O = CO_2 + H_2 \qquad \text{shift} \qquad [2]$$

GRPSS was developed from a steady state reactor program included in a report prepared by Lehigh University for the U.S. Department of Energy (1). As with these programs, GRPSS utilizes the DSS/2 (2) integration system to perform the calculations down the length of the reactor, while also performing calculations between reactors and in other processing units.

This manual is a brief guide for using GRPSS. Previous simulation experience, as well as knowledge of DSS/2, is useful but not necessary for using GRPSS. The present form of the program makes it very flexible for making changes and expanding the simulation itself, which are discussed later.

2. SYSTEM DESCRIPTION

The GRPSS simulation system consists of a collection of three major program sets:

- DSS/2 - A numerical integration package capable of solving initial value differential equations as defined in three user written subroutines, INITAL, DERV, and PRINT. DSS/2 is the main calling program for the entire simulation (2).

- PHYSICAL DATA BASE (PDATAB) - A data block containing the ideal gas physical properties of 41 chemical species (3).

- SSGEN - A collection of subroutines simulating the methanation reactor system; includes INITAL, DERV, and PRINT called by DSS/2.

Because GRPSS is a generalized simulation, the user must specify which of the five possible process units (reactor, heat exchanger, divider, mixer, and condenser) to use and in what order. This proceedure is described in a later section.

The following sets of information are required for GRPSS:

1. DSS/2 input information,
2. reactor grid specifications in dimensionless terms, in % length,
3. process topology,
4. feed and tear stream data (if required),
5. ordering of unit calculations,
6. specification of the number of calculation repetitions (for iterative calculations only).

Note that sets 1, 2, and 6 specify the performance of DSS/2 during the calculation.

In attempting to understand the GRPSS system, the user must keep in mind that the simulation's focus is on the state inside a reactor over a one dimensional grid. GRPSS involves the solution of three differential equations:

1. the conversion change by the methanation reaction [1] per unit length,

2. the conversion change by the shift reaction [2] per unit length,

3. the change in temperature per unit length.

The numerical solution of these three equations for each reactor by DSS/2 is what is sought, with the added convenience of modeling an entire reactor system through the unit subroutines contained in SSGEN.

As an initial step in the calculation, DSS/2 recognizes the differential equations being solved and their solutions through the /F/ and /Y/ COMMON blocks in SSGEN. The common block /T/ specifies the independent variable, in this case, dimensionless length.

Without proceeding into excessive detail on the workings of DSS/2 and the subroutines in SSGEN, the following five steps generally describe the calculations and calling sequence:

1. DSS/2 calls subroutines INITAL in SSGEN to:

    a. set the initial conditions for the CDEs,

    b. identify the compounds being used in the physical data program,

    c. identify the reactions taking place,

    d. read the process topology, stream and unit ordering information supplied by the user,

    e. calculate the heats of reaction;

2. DSS/2 calls subroutine PRINT, which prints DSS/2 and process topology information;

3. DSS/2 makes multiple calls to subroutine DERV, which calls any or all of the five unit subroutines in the specified order to perform the simulation calculations;

4. DSS/2 calls PRINT to print the calculated data for the reactor profile(s) and process streams;

5. if an iterative calculation is involved, PRINT checks the newly calculated tear stream data with the previous data to see if the program has converged to a solution:

   a. if the program has converged, stream and reactor profile information are punched onto cards and solution is printed,

   b. if the program has NOT converged, simulation is repeated from Step 3 until:

      i. convergence is obtained,

      ii. number of specified repetitions has been completed, (OR)

      iii. time limit for computation is reached.

Table 2-1 gives a listing of the subroutines found in SSGEN and a brief description of their function.

Table 2-1: SSGEN SUBROUTINE DESCRIPTIONS

- INITAL - Called by DSS/2; contains the initial conditions for the differential equations being solved, as well as obtains all information inputed to the system. Contains the subroutines IDENT, STOICH, FLOWST, and HPREP described below.

  * IDENT - States the number of compounds being used and identifies the compound with its corresponding number in the physical data block, PDATAB.

  * STOICH - Gives the stoichiometric coefficients for the reactions taking place involving the compound specified.

  * FLOWST - Reads the process flowsheet information for the process under study; feed and tear stream information and the ordering of unit calculations.

  * HPREP - Calculates heat capacity coefficients and heats of reaction from the data block, PDATAB.

- DERV - Called by DSS/2; calls the individual process unit subroutines in the sequence specified by the user in FLOWST. Units called include a reactor, heat exchanger, divider, mixer, and condenser. Only the reactor contains the differential equations to be solved by DSS/2.

  * RXR - Contains the ODEs being solved for each specified point along the length of the reactor; calculations involve YSFLOW, HRXYCP, and RATE listed below.

    - YSFLOW - Determines new component flows for each reactor point.

    - HRXYCP - Determines the heat of reaction for each reactor point.

    - RATE - Determines the rate of reaction(s) at the specified point given compound partial pressures and temperatures.

Table 2-1, continued

* HX - Simple routine calculating a new exit stream temperature given a constant heat duty, Q.

* DIV - Divides a stream into two specified fractions.

* MIXER - Mixes together two or three streams; determines composition and temperature of new stream. Calls subroutines HGAS, HILC, and TCALC to assist in calculation.

  - HGAS - Calculates the specific enthalpy of a gas using CPMEAN.

  - CPMEAN - Calculated average heat capacity using PDATAB.

  - HILC - Keeps track of high and low temperature values during mixer calculation.

  - TCALC - Calculates temperature of mixed stream.

* CCND(ENSER) - A combined heat excahanger-water condensate separation system. Given a required fraction of water removal, CCND calculates the temperture of condensation, and the amount of heat removal required for the system, in BTU per hour.

- <u>PRINT</u> - Called by DSS/2 to print inputed information and calculation results.

3. PROCESS TOPOLOGY

Because GRPSS is a "generalized" simulation system, the process topology must be entered into the program through the data deck. This section will describe the functions of the five process units available for simulation.

The topological data required in GRPSS falls under three catagories; process, unit and stream.

The process data give an overall view of the process being simulated. The total number of each type of process unit, the total number of streams, and the number of reactor grid points are all submitted together. The notation used in the program is:

- NRXR = number of reactors
- NHX = number of heat exchangers
- NDIV = number of stream dividers
- NMIX = number of stream mixers
- NCDR = number of condensers
- NSTMS = total number of process streams
- NTEAR = total number of torn streams
- NPTS = total number of grid points within each reactor

The unit data describe each process unit used in the model with the individual number of the unit, its type (i.e. reactor, etc.), the stream numbers entering and leaving the unit, and some other data depending on the unit's function. The program uses the notation below:

- IUNIT = individual unit number (note: some units will have their own unit number, i.e. IRXR, the individual reactor number),
- KT = unit type where: 1 = RXR, 2 = HX, 3 = MIX, 4 = DIV, 5 = CDR,
- IN(I) = stream number(s) entering unit (I = max of 3),

- NOUT(J) = stream number(s) exiting unit (J = max of 2),

- DUMDAT = data which are characteristic of the unit (i.e. reactor area, etc.),

- RLNTH = length of reactor (for reactors only).

Note the only required criteria for naming individual stream numbers is that the major product stream is given the highest stream number(i.e. NSTMS).

Finally, the stream data include the temperature, pressure, and composition of all feed and tear (if necessary) streams. The nomenclature in GRPSS is:

- IFD (ITR) = feed (tear) stream number,

- FFDSTM(I) (FTRSTM(I)) = molar flowrate per hour of compound I, where: 1 = CO, 2 = H2, 3 = CH4, 4 = H2O, 5 = CO2, 6 = N2,

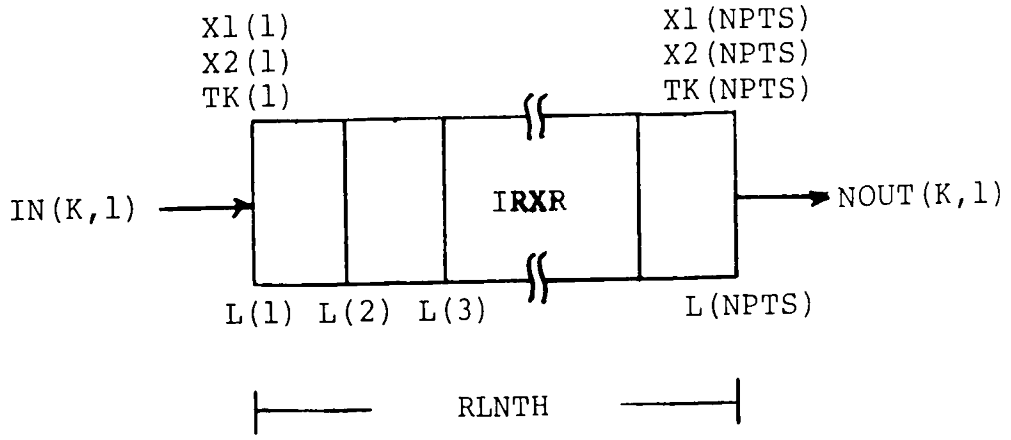
- PFDSTM (PTRSTM) = pressure of feed (tear) stream, psia,

- TFDSTM (TTRSTM) = temperature of feed (tear) stream, K,

The following is a discussion of the process unit subroutines available. Please note that K is defined as the individual unit number specified by the user.

3.1. Chemical Reactor - RXR(K)

This subroutine takes an input stream, IN(K,1), and calculates the fractional conversion of CO for each reaction along the length of the reactor at each point in the grid array, L. The grid may be of equal or unequal spacings, which are specified by the user. There are two reactions taking place, methanation [1] and shift [2], with the respective calculated conversions (X1,X2) and the temperature (TK) at a particular point determined by the solution of the three differential equations describing the reactor. The compositions and temperature at the last point along the reactor then describe the exit conditions, and the data are stored in the outlet stream array, NOUT(K,1). Additional data are required for the cross-sectional area, DUMDAT(K), in square feet, and the reactor length, RLNTH, in feet.



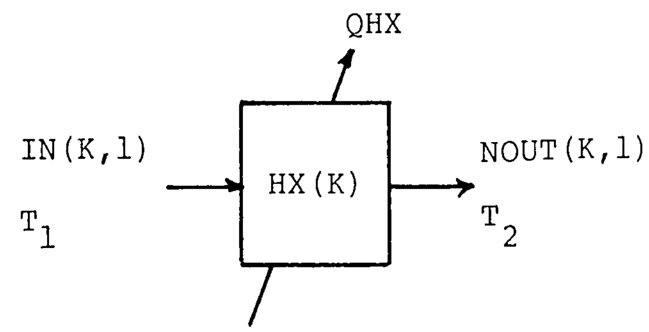
DUMDAT(K) = Cross-sectional Area, ft^2

RLNTH(IRXR) = Reactor Length, ft

Figure 3-1: Chemical Reactor Topology

3.2. Heat Exchanger - HX(K)

This subroutine describes a heat exchanger, very generally, by changing the temperature of an input stream to a specified value. It is assumed that the heating (or cooling) stream running counter to the flow is correctly adjusted to enable the outlet temperature to remain constant. A heat duty, QHX, is also calculated for each heat exchanger.



where:

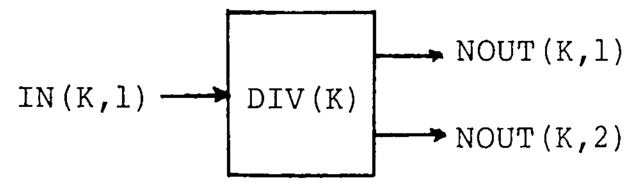
DUMDAT(K) = Desired Outlet Temperature, T_2, K

QHX = Heat Duty, BTU/lbmole

Figure 3-2: Heat Exchanger Topology

3.3. Stream Divider - DIV(K)

This subroutine separates a stream into two parts, by a fraction specified by DUMDAT. One must be careful in specifying the output streams for this unit, as shown by the diagram below:



where:

DUMDAT(K) = Fraction of input stream going to output stream 1, $0 \leq \text{DUMDAT} \leq 1$

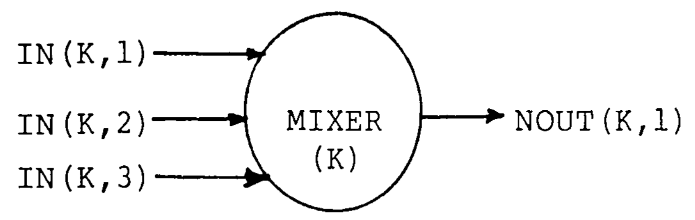
NOUT(K,1) = IN(K,1) * DUMDAT(K)

NOUT(K,2) = IN(K,1) * (1. - DUMDAT(K))

Figure 3-3: Stream Divider Topology

3.4. Stream Mixer - MIXER(K)

This subroutine simulates a mixer for up to three streams by summing the flows for each compound in all the streams. The exit temperature is also calculated by summing the enthalpies of each stream, and then performing an iteration to find the new temperature.



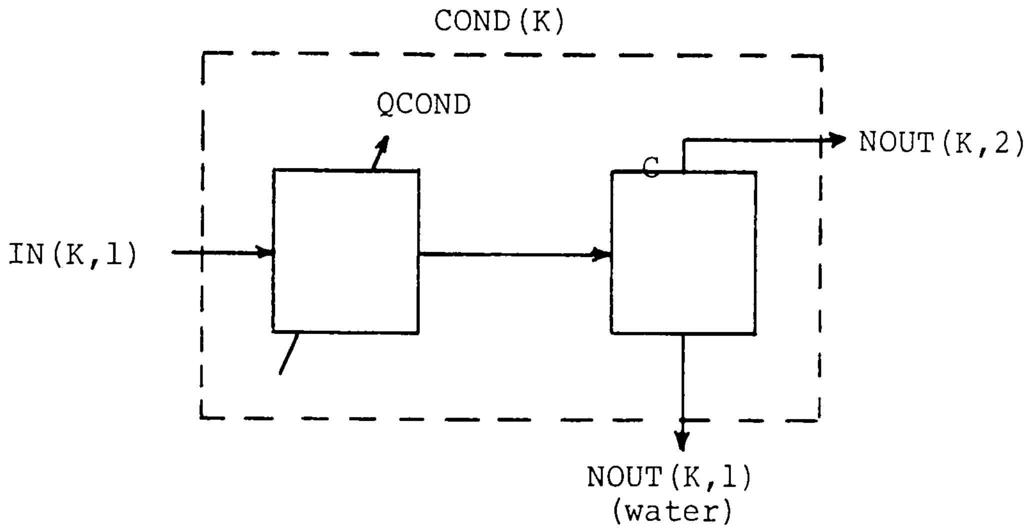
where:

DUMDAT(K) = 0.; No specific data required

Figure 3-4: Stream Mixer Topology

3.5. Condenser Unit - COND(K)

This subroutine simulates a condenser system consisting of a heat exchanger and a liquid separation unit. DUMDAT is specified as the desired fraction of water removal from the system. CCND then determines the exit temperature through an enthalpy balance (using HGAS and HWATER routines) and an iterative method called false position (FALPOS). Note that if the water removal fraction is set at zero, then the inlet stream is cooled to the saturation temperature. Of course, the second output stream being calculated is the flowrate of condensed water leaving the unit, and there is also a heat duty calculated, QCOND, in BTU per hour, for the exchanger.



where:

DUMDAT(K) = Fraction of water being removed from inlet stream

QCOND = Amount of heat removed from inlet stream, BTU/hr

for the water component only:

NOUT(K,2) = IN(K,1) * DUMDAT(K)

NOUT(K,1) = IN(K,1) * (1. - DUMDAT(K))

<u>NOTE</u>: Temperature of condenser is the temperature of the two outlet streams

Figure 3-5: Condenser Topology

3.6. Example 1

The reactor system shown in Figure 3-6, consisting of one each of the five possible process units, is to be simulated. Each unit has been numbered, as has each stream (prefixed S-) as shown in the figure. Table 3-1 contains a summary of the data required for the topology.

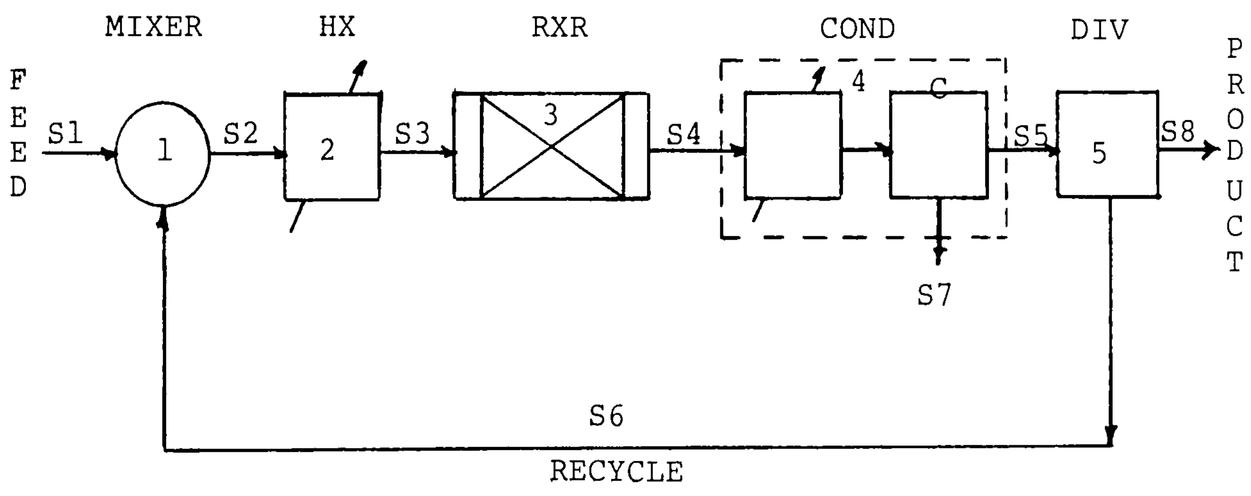


Figure 3-6: Topology Set-up For Example 1

Table 3-1: Summary of Topology Data, Example 1

UNIT NO.	UNIT TYPE	IN 1	IN 2	IN 3	OUT 1	OUT 2	DUMDAT	RLNTH	NOTES
1	4	1	6	0	2	0	0.	-	DUMDAT MUST BE SPECIFIED AS 0
2	2	2	0	0	3	0	559.	-	EXIT STREAM TEMP=559 K
3	1	3	0	0	4	0	3.142	5.	RXR DATA- AREA=3.142 SQ.FT. LENGTH=5FT
4	5	4	0	0	5	7	0.99	-	99% OF WATER TO BE
5	3	5	0	0	6	8	0.83	-	83% OF STREAM TO BE RECYCLED

3.7. Comments On Tearing Streams and Unit Ordering

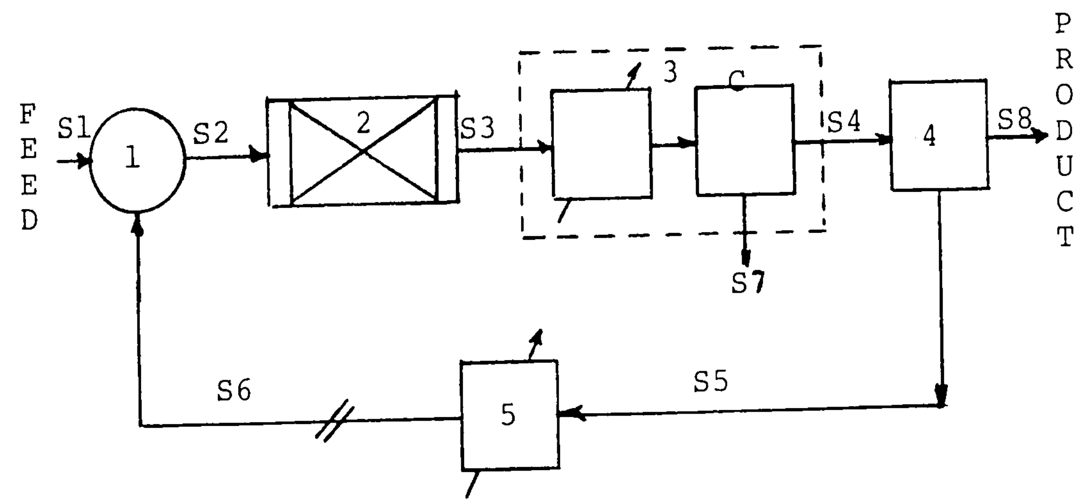
Whenever a stream is being recycled back to another unit, it creates a problem obtaining the solution for a process simulation. For example, take the process described in Example 1. If one were to try to calculate the process by solving Unit 1 first, then 2, and so forth, one has an immediate problem, because Stream 6 is unknown initially. This problem exists, not only for the mixer but for all the other units as well, because the only stream that is known is the feed stream, Stream 1.

To get around this situation, one can "tear", or assume, the values for one stream, perform the necessary calculations, and then see how close the original assumptions were. Thus, if Stream 4 is torn, Unit 4 can be calculated, as can Unit 5 to determine the recycle stream (S6); then Unit 1 may now be calculated and so forth. After Unit 3 has been calculated, a new value for Stream 4 can be found. If the initial estimate was good, the difference between the old and new values will be small. If the error is beyond the set tolerances, the entire calculation must be repeated again, this time using the newly calculated stream values as the assumed stream values. This calculation sequence is repeated until the tolerences are met, thus, the solution has conveged.

In using GRPSS, provisions have been made for up to 10 tear streams. It is usually best to tear the minimun number of streams possible, but this is merely a guideline. Note that if more than one reactor is present, it is suggested that each stream exiting a reactor be torn to insure proper calculation during the first iteration. GRPSS checks <u>all</u> <u>torn</u> streams for convergence, so in some instances, it is better to tear some streams than others. Further information on tearing streams may be found in Steward (4).

Two further examples of tearing and ordering the unit calculatons are given below. [Note: In Example 2, Stream 6 was torn to show one possible ordering. In Example 3, Streams 5 and 9, both reactor outlet streams, were torn to insure proper calculation during the first iteration.]

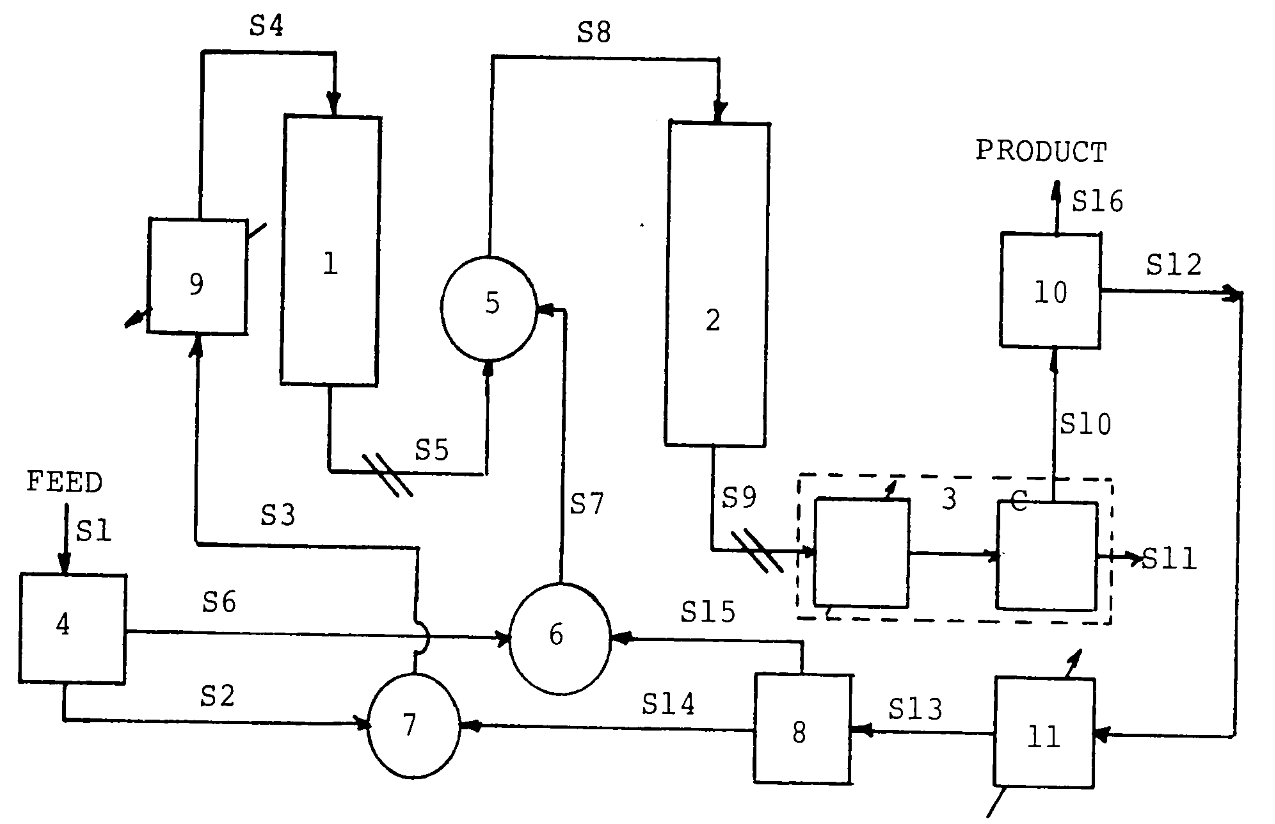
Example 2



Unit Calculation Order: 1 2 3 4 5
Tear Steam : S6

Figure 3-7: Topology For Example 2

Example 3



Unit Calculation Order: 4 3 10 11 8 7 9 6 1 5 2
Tear Streams : S5 S9

Figure 3-8: Topology For Example 3

4. Additional Information for using GRPSS

4.1. Present Simulation Capabilities

The following information gives an indication of the dimensional capacity of GRPSS. Use beyond these limits would require dimensional changes in most of the subroutines found in SSGEN. Listed is the varibale name and its nomenclature in the program.

- 8 Compounds - ID(8)
- 3 Reactions in reactor - A(3,10)
- Topology limits:
    * 5 reactors - IRXR(5)
    * 1 condenser - CDR
    * 15 units (total) - IUNIT(15)
    * 25 streams - FSTM(25,6)
    * 10 tear streams - ITEAR(10)
- 41 Reactor grid points - TK(41), X1(41), X2(41)
- Tolerance of flow stream conversion check: <0.5% of compound flow stream

In the present configuration, the entire package, DSS/2 (modified and shortened, listed in Appendix A), PDATAB, and SSGEN programs require slightly less than 110K memory on the CDC6400 computer.

4.2. Summary of Data Cards

CARD NO.	FORMAT	VARIABLE NAMES	USE
DSS Cards			
1	20A4	TITLE	Documentation
2	3E10.0	T0,TF,TP	Initial, final, and number of reactor grid points(include first and last pts.)
3	4I5,2X,A3, E10.0	N,NMAX, NTYPE,NPRINT IRRTYP,ERROR	Number of ODE's,ratio of print interval to minimum integration interval, integration algorithm,print option,type of error,max allowable integraton error
4	8E10	L(2)-L(TP-1)	All grid points along reactor between 0. and 100.
SSGEN Cards			
5	8A10	TEXT	Documentation for program run
6	8A10	TEXT	Documentation for program run
7	8I5	NRXR,NHX,NDIV, NMIX,NCDR,NSTMS, NTEAR,NPTS	No. of reactors,heat exchangers, dividers,mixers,condensers, streams,tear streams,no. rxr pts
ONE SET OF CARDS 8 & 9 FOR EACH UNIT			
8	7I5	IUNIT,KT, IN(3),NOUT(2)	Unit no.,unit type,stream numbers entering(3),stream numbers exiting(2)
9	F10.5	DUMDAT	Extra unit data
FOR REACTORS ONLY:			
9A	2F10.5	DUMDAT,RLNTH	Cross-sectional area, reactor length
ONE SET OF CARDS 10 & 11 FOR THE FEED STREAM			
10	I5,2F10.5	IFD,TFDSTM, PFDSTM	Feed stream no.,temp of stream (K),pressure of stream (psia),
11	6F10.5	FFDSTM(6)	Molar flow per hour of the six compounds in system in order of CO H2 CH4 H2O CO2 N2
12	20I5	IORD(I)	Unit order of calculation for I units

CARD NO.	FORMAT	VARIABLE NAMES	USE

SSGEN Cards, Cont'd

ONE SET OF CARDS 13 & 14 PER TEAR STREAM;
IGNORE IF THERE IS NO TEAR STREAM

13	I5,2F10.5	ITR,TTRSTM, PRSTM	Tear stream number, temp, and pressure
14	6F10.5	FTRSTM(6)	Molar flow per hour of the six compounds in system CO H2 CH4 H2O CO2 N2

DSS/2 CARDS

FOR MORE REPETITIONS INCLUDE CARDS 15 & 16
IGNORE IF NOT REQUIRED

15	A7	REPEATS	Tells DSS/2 to repeat calculation
16	I5	N	N is the number of repetitions
17	A11	END OF RUNS	Tells DSS/2 no further computations are necessary

4.3. Comments on Computation Time

GRPSS was developed on the CDC6400 computer at Lehigh University. Of course, computation time will vary with the number of reactor points, number of units, number of repeat runs for an iterative solution and amount of information printed. Table 4-1 provides several examples and the total length of time required by the computer system.

Table 4-1: Comparison of Computation Time

NO. RXRS	NO. UNITS	NO. RXR PTS.	ITERATIONS	SYS SEC.
1*	1	25	0	5.3
1*	1	41	0	5.7
1	3	25	8	11.5
1	3	41	8	18.0
1	5	25	16	26.5
2	12	25	16	34.8

* = no recycle used in reactor configuration

4.4. DSS/2 Modifiactions

While a grid of evenly spaced reactor points usually describes a reactor temperature profile well, it was found difficult to perform the calculation on a reactor with a very steep temperature gradient. Instead of using a very large number of grid points at a very small interval, which uses a great deal of computer time on points after the final equilibrium temperature has been reached, DSS/2 was modified to permit the user to pick the points for study. The changes are minor, and are all in the SYSTM2 deck of DSS/2. An output of the DSS/2 program so modified is included in Appendix B. All changes in the data cards for DSS/2 are included with that section.

5. Outline Of Possible Program Changes and Expansions

1. Change GRPSS for use with the FORTRAN 4 compiler: note that Lehigh will be changing to that system after June 81.

2. Re-dimension all unit and stream variables to provide for larger process simulations.

3. To change the reactions taking place, corrections will be needed in the following subroutines:

   - IDENT - re-identify compound for use with the physical property package,

   - STOICH - change stoichiometric ratios,

   - RATE - change rate kinetics.

4. More realistic simulation of heat exchanger and condenser units could be added.

5. Additional process units could be added to DERV by incrementing the unit number, type, etc.

6. Rewrite program for easy access via interactive terminals.

Appendix A: DSS/2 Program with Modificatons

HHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHH

```
      PROGRAM SYSTM(INPUT,OUTPUT,PUNCH,TAPE1,TAPE5=INPUT,TAPE6=OUTPUT,
     1 TAPE7=PUNCH)
C...
C...  COPYRIGHT - LEHIGH UNIVERSITY, 1976
C...
C...  DSS/2 - DIFFERENTIAL SYSTEMS SIMULATOR, VERSION 2
C...
C...  MACRODIAGRAM OF THE COMPLETE SYSTEM ORGANIZATION AND OPERATION
C...
C...                                    ........................
C...                                    .BEGIN EXECUTION OF MAIN.
C...                                    .    PROGRAM SYSTEM     .
C...                                    ........................
C...                                                .
C...                                                .
C...                                                .
C...                                                .
C...                                                + (+ DENOTES AN INPUT)
C...                                         ...............
C...                                         .  READ THREE  .
C...                      ...................+.DATA CARDS (1).
C...                      .                  ...............
C...                      .                             .
C...                      .                             .
C...                      .                             .
C...                      .                             .
C...                      .                             +
C...                      .                     ............       ......
C...                      .                     .END OF RUNS........+.STOP.
C...                      .                     . CARD READ .  YES   ......
C...                      .                     ............
C...                      .                             .
C...                      .                             .
C...                      .                             .NO
C...                      .                             .
C...                      .                             +
C...                      .                     ...........
C...                      .                     .PRINT DATA.
C...                      .                     . SUMMARY .
C...                      .                     ...........
C...                      .                             .
C...                      .                             .
C...                      .                             .
C...                      .                             .
C...                      .                             .
C...                      .                             +
C...              ................         ..........................
C...              . INCREMENT THE .        .   CALL SUBROUTINE INITAL .
C...              .RUN COUNTER (5).        .TO INITIALIZE THE MODEL (2).
C...              ................         ..........................
C...                      +                             .
C...                      .                             .
C...                      .                             .
C...                      .                             .
C...                      .                             +
C...                      .                ..............................
C...         ...................           .   CALL SUBROUTINE PRINT    .
C...         .PRINT ERROR SUMMARY.         .   TO PRINT THE NUMERICAL   .
C...         . IF REQUESTED (4)  .         .SOLUTION (INITIAL CONDITIONS.+....
C...         ...................           .  FOR FIRST CALL). STORE    .    .
C...                      +                .  SOLUTION FOR SUBSEQUENT   .    .
C...                      .                .         PLOTTING           .    .
C...                      .                ..............................    .
C...                      .                             .                    .
```

```
C...                   .                               .                         .
C...                   .                               .                         .
C...                   .                               .                         .
C...                   .                               +                         .
C...    .......................                 ..............                    .
C...    .CALL SUBROUTINE PLOTS.        YES      . END OF RUN .                    .
C...    .VIA SUBROUTINE PRINT .+...............(FINAL VALUE.                     .
C...    . TO PRINT THE ENTIRE .                .OF TIME) (3).                     .
C...    .  SOLUTION VS TIME   .                ..............                     .
C...    .......................                        .                          .
C...                                                   .                          .
C...                                                   .NO                        .
C...                                                   .                          .
C...                                                   +                          .
C...    ....................  COMMON/Y/  ........................                 .
C...    .  CALL SUBROUTINE .+............ CALL SUBROUTINE INTEG .                 .
C...    .  DERV TO COMPUTE .            . TO INTEGRATE THE MODEL.......
C...    .THE MODEL TEMPORAL.            . DIFFERENTIAL EQUATIONS.
C...    .  DERIVATIVES (6) ............+.OVER ONE PRINT INTERVAL.
C...    ....................  COMMON/F/  ........................
C...                 .      +
C...                 .      .
C...                 .      .
C...                 .      .
C...                 .      .
C...                 +      .
C...    ......................
C...    .CALL SYSTEM UTILITIES.
C...    .    TO ASSIST IN     .
C...    .   COMPUTATION OF    .
C...    .TEMPORAL DERIVATIVES .
C...    .         (7)         .
C...    ......................
C...
C...    EXPLANATORY NOTES FOR THE ABOVE MACRODIAGRAM
C...
C...    (1)   CARD 1 - TITLE(20) (READ VIA 900 FORMAT(20A4))
C...
C...          CARD 2 - TO,TF,TP (READ VIA 901 FORMAT(3E10.0))
C...
C...          CARD 3 - N,NMAX,NTYPE,NPRINT,IRRTYP,ERROR
C...                   (READ VIA 902 FORMAT(4I5,2X,3A1,E10.0))
C...
C...          IF **END OF RUNS** IS PUNCHED IN COLUMNS 1 TO 11 OF CARD 1 IN
C...          ANY SET OF THREE DATA CARDS, PROGRAM EXECUTION IS TERMINATED
C...          AND CARDS 2 AND 3 OF THAT SET ARE NOT REQUIRED.  MULTIPLE
C...          SETS OF DATA CARDS MAY BE USED, THREE CARDS PER SET.  THE
C...          MAIN PROGRAM WILL READ EACH SET AND EXECUTE A RUN UNTIL AN
C...          **END OF RUNS** CARD IS READ.
C...
C...    (2)   SUBROUTINE INITAL IS CALLED ONCE PER RUN.  THEREFORE DATA
C...          CARDS MAY BE READ FROM THIS SUBROUTINE TO DEFINE INITIAL
C...          PARAMETERS OF THE MODEL EQUATIONS FOR EACH RUN.  THE ADDI-
C...          TIONAL DATA CARDS WOULD BE STACKED BEHIND THE THREE BASIC
C...          DATA CARDS OF (1) ABOVE.
C...
C...    (3)   THE END OF RUN CONDITION IS T GE TF WHERE T IS THE FIRST ELE-
C...          MENT IN COMMON/T/ (GENERATED BY MAIN PROGRAM SYSTEM) AND TF
C...          IS READ FROM DATA CARD (2) OF (1) ABOVE.
C...
C...    (4)   NPRINT = 1 WILL PRINT A SUMMARY OF THE DEPENDENT VARIABLES IN
C...          COMMON/Y/ FOR WHICH THE ESTIMATED TEMPORAL INTEGRATION (TRUN-
C...          CATION) ERROR EXCEEDED THE MAXIMUM PERMISSIBLE VALUE, ERROR,
C...          (READ FROM DATA CARD (3) OF (1) ABOVE) AT ANY POINT DURING
C...          THE RUN.  IF NPRINT = 0, TEMPORAL INTEGRATION ERRORS WILL NOT
C...          BE REPORTED.
```

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C...                                                                    SYSTM2 131
C...  (5)  THE RUN COUNTER, SET BY MAIN PROGRAM SYSTEM, IS THE THIRD    SYSTM2 132
C...       ELEMENT IN COMMON/T/ E.G., COMMON/T/T,NFIN,NORUN             SYSTM2 133
C...                                                                    SYSTM2 134
C...  (6)  THE FUNDAMENTAL LINKAGE IN THIS SYSTEM IS THROUGH COMMON/Y/   SYSTM2 135
C...       WHICH CONTAINS THE MODEL DEPENDENT VARIABLE VECTOR AND COMMON SYSTM2 136
C...       /F/ WHICH CONTAINS THE VECTOR OF TEMPORAL DERIVATIVES OF THE  SYSTM2 137
C...       DEPENDENT VARIABLE VECTOR.  FOR EXAMPLE, THIS LINKAGE COULD  SYSTM2 138
C...       BE PROGRAMMED AS                                             SYSTM2 139
C...                                                                    SYSTM2 140
C...            COMMON/T/T,NFIN,NORUN/Y/U(11)/F/PUPT(11)                SYSTM2 141
C...                                                                    SYSTM2 142
C...       WHERE THE DEPENDENT VARIABLE VECTOR U(11) IS GENERATED BY THE SYSTM2 143
C...       TEMPORAL INTEGRATOR, SUBROUTINE INTEG, FROM THE DERIVATIVE   SYSTM2 144
C...       VECTOR, PUPT(11), GENERATED BY SUBROUTINE DERV.  IF THE USER SYSTM2 145
C...       PROVIDES ANOTHER TEMPORAL INTEGRATOR ROUTINE, PERHAPS FOR    SYSTM2 146
C...       IMPLICIT INTEGRATION, THE SAME LINKAGE MUST BE ESTABLISHED IN SYSTM2 147
C...       ORDER TO RUN ANY PART OF THE PROBLEM LIBRARY.                SYSTM2 148
C...                                                                    SYSTM2 149
C...  (7)  REPRESENTATIVE SYSTEM UTILITIES INCLUDE                      SYSTM2 150
C...                                                                    R012580 24
C...           LINT1 - SUBROUTINES FOR ONE, TWO AND THREE-DIMENSIONAL   SYSTM2 151
C...           LINT2   LINEAR INTERPOLATION (TABLE LOOKUP).             SYSTM2 152
C...           LINT3                                                    SYSTM2 153
C...                                                                    R012580 25
C...           DSS002 - DIFFERENTIATION ROUTINES FOR THE NUMERICAL      R012580 26
C...             TO     METHOD OF LINES INTEGRATION OF PARTIAL DIFFER-  R012580 27
C...           DSS030   ENTIAL EQUATIONS.                               R012580 28
C...                                                                    SYSTM2 154
C...  MAIN PROGRAM SYSTEM IS THE CALLING PROGRAM FOR A SERIES OF SUB-    SYSTM2 155
C...  ROUTINES WHICH DEFINE AND INTEGRATE THE TEMPORAL DIFFERENTIAL      SYSTM2 156
C...  EQUATIONS.  THE COMPLETE PROGRAM CONSISTS OF THE FOLLOWING         SYSTM2 157
C...  COMPONENTS                                                        SYSTM2 158
C...                                                                    SYSTM2 159
C...     (1)  MAIN PROGRAM SYSTEM - PERFORMS OVERALL CONTROL OF THE      SYSTM2 160
C...          THE TOTAL PROGRAM.                                        SYSTM2 161
C...                                                                    SYSTM2 162
C...     (2)  SUBROUTINE INITAL - SETS THE INITIAL CONDITIONS FOR THE    SYSTM2 163
C...          TEMPORAL INTEGRATION (PROVIDED BY THE USER).              SYSTM2 164
C...                                                                    SYSTM2 165
C...     (3)  SUBROUTINE DERV - DEFINES THE TEMPORAL DERIVATIVE VECTOR   SYSTM2 166
C...          (PROVIDED BY THE USER).                                   SYSTM2 167
C...                                                                    SYSTM2 168
C...     (4)  SUBROUTINE PRINT - PRINTS THE NUMERICAL SOLUTION (PROVIDED SYSTM2 169
C...          BY THE USER).                                             SYSTM2 170
C...                                                                    SYSTM2 171
C...     (5)  SUBROUTINE PLOTS - PLOTS THE NUMERICAL SOLUTION ON THE     SYSTM2 172
C...          LINE PRINTER.  PLOTS IS CALLED BY SUBROUTINE PRINT, AND IT SYSTM2 173
C...          IN TURN CALLS SUBROUTINES SKPT, TYPIT AND GZRO TO HANDLE   SYSTM2 174
C...          VARIOUS ASPECTS OF THE PLOTTING.  A SECOND PLOTTING ROU-   SYSTM2 175
C...          TINE, TPLOTS, IS ALSO AVAILABLE IN THE DSS SYSTEM TO       SYSTM2 176
C...          PRINT PLOTS WHICH FIT ON AN 8-1/2 X 11 INCH PAGE.  TPLOTS  SYSTM2 177
C...          IN TURN CALLS TSKPT, TTYPIT AND TGZRO TO HANDLE VARIOUS    SYSTM2 178
C...          ASPECTS OF THE PLOTTING.                                  SYSTM2 179
C...                                                                    SYSTM2 180
C...     (6)  SUBROUTINE INTEG - PERFORMS THE CENTRALIZED TEMPORAL       SYSTM2 181
C...          INTEGRATION.  SINCE THE PRECEDING DOCUMENTATION COMMENTS   SYSTM2 182
C...          WERE WRITTEN, THE GEAR/HINDMARSH INTEGRATOR HAS BEEN       SYSTM2 183
C...          ADDED TO THE DSS/2 SYSTEM.  THEREFORE THE INTEGRATION CAN  SYSTM2 184
C...          BE DONE BY EITHER SUBROUTINE INTEG (14 CLASSICAL RUNGE     SYSTM2 185
C...          KUTTA ALGORITHMS) OR BY SUBROUTINE GEARB (GEAR VARIABLE-   SYSTM2 186
C...          ORDER, VARIABLE-STEP ALGORITHM WITH EXTENDED STABILITY     SYSTM2 187
C...          DOMAIN FOR STIFFNESS).                                    SYSTM2 188
C...                                                                    SYSTM2 189
C...     (7)  OPTIONAL SYSTEM UTILITIES - CALLED BY SUBROUTINE DERV TO   SYSTM2 190
C...          ASSIST IN THE COMPUTATION OF THE TEMPORAL DERIVATIVE       SYSTM2 191
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C...         VECTOR.  FOR EXAMPLE, DSS CONTAINS SUBROUTINES LINT1,          SYSTM2 192
C...         LINT2 AND LINT3 FOR ONE, TWO AND THREE-DIMENSIONAL FUNC-       SYSTM2 193
C...         TION GENERATION (TABLE LOOKUP).                                SYSTM2 194
C...                                                                        SYSTM2 195
C...  DOCUMENTATION COMMENTS ARE GIVEN AT THE BEGINNING OF ALL OF THE       SYSTM2 196
C...  SYSTEM ROUTINES EXPLAINING THEIR OPERATION.                           SYSTM2 197
C...                                                                        SYSTM2 198
C...  ALL OF THE PROGRAMMING IS IN STANDARD FORTRAN IV AND THEREFORE        SYSTM2 199
C...  SHOULD BE ESSENTIALLY MACHINE INDEPENDENT.  THE PROGRAM WAS           SYSTM2 200
C...  DEVELOPED FOR CDC 6000 COMPUTERS.  STATEMENTS WHICH MIGHT REQUIRE     R012580 29
C...  MINOR MODIFICATION FOR ADAPTATION OF THE PROGRAM TO OTHER COMPU-      SYSTM2 202
C...  TERS ARE MARKED WITH LEADING AND TRAILING COMMENTS CONSISTING OF A    SYSTM2 203
C...  ROW OF ASTERISKS.  IN PARTICULAR, DATA STATEMENTS WHICH DEFINE        SYSTM2 204
C...  HOLLERITH STRINGS AND THE LOGICAL UNIT NUMBERS FOR THE FORTRAN        SYSTM2 205
C...  READ/WRITE STATEMENTS MAY REQUIRE MINOR MODIFICATION.  IF YOU         SYSTM2 206
C...  ENCOUNTER ANY PROBLEMS IN INSTALLING THIS PROGRAM ON YOUR COMPUTER    SYSTM2 207
C...  PLEASE CONTACT THE PROGRAM AUTHOR                                     SYSTM2 208
C...                                                                        SYSTM2 209
C...                 W. E. SCHIESSER                                        SYSTM2 210
C...                 WHITAKER NO. 5                                         R012580 30
C...                 LEHIGH UNIVERSITY                                      SYSTM2 213
C...                 BETHLEHEM, PENNSYLVANIA 18015                          SYSTM2 214
C...                                                                        SYSTM2 215
C...                 215-861-4264 (WHITAKER LABORATORY)                     SYSTM2 216
C...                 215-861-4137 (COMPUTING CENTER)                        SYSTM2 217
C...                                                                        SYSTM2 218
C...  THE TEMPORAL DIFFERENTIAL EQUATIONS AND ASSOCIATED INITIAL CONDI-     SYSTM2 219
C...  TIONS ARE PROGRAMMED IN SUBROUTINES DERV AND INITAL RESPECTIVELY.     SYSTM2 220
C...  SUBROUTINE INITAL IS CALLED ONCE AT THE BEGINNING OF EACH RUN TO      SYSTM2 221
C...  INITIALIZE THE PROBLEM SYSTEM.  THIS CALL THEREBY SETS THE INITIAL    SYSTM2 222
C...  VALUES OF THE DEPENDENT VARIABLES THAT ARE THEN PASSED TO SUBROU-     SYSTM2 223
C...  TINE DERV THROUGH COMMON/Y/.  THESE DEPENDENT VARIABLES CAN THERE-    SYSTM2 224
C...  FORE BE ASSUMED TO BE SET NUMERICALLY AT THE BEGINNING OF SUBROU-     SYSTM2 225
C...  TINE DERV AND THEY CAN BE USED IN SUBSEQUENT PROGRAMMING IN DERV.     SYSTM2 226
C...  THE FINAL PROGRAMMING IN DERV MUST NUMERICALLY SET ALL OF THE         SYSTM2 227
C...  DERIVATIVES DEFINED BY THE TEMPORAL DIFFERENTIAL EQUATIONS WHICH      SYSTM2 228
C...  APPEAR IN COMMON/F/.  IN SUMMARY, SUBROUTINE DERV RECEIVES A          SYSTM2 229
C...  VECTOR OF DEPENDENT VARIABLES THROUGH COMMON/Y/ AND RETURNS A         SYSTM2 230
C...  VECTOR OF DERIVATIVES THROUGH COMMON/F/.  THIS DERIVATIVE VECTOR      SYSTM2 231
C...  IS THEN USED BY SUBROUTINE INTEG TO MOVE THE SOLUTION AHEAD A STEP    SYSTM2 232
C...  IN TIME.  THE NEW SOLUTION VECTOR GENERATED BY INTEG AT THE AD-       SYSTM2 233
C...  VANCED POINT IN TIME IS THEN PASSED TO DERV THROUGH COMMON/Y/ AND     SYSTM2 234
C...  THE PROCESS IS REPEATED FOR THE NEXT STEP IN TIME.                    SYSTM2 235
C...                                                                        SYSTM2 236
C...  THE PROGRAM IS SET UP FOR MULTIPLE RUNS WITHIN A SINGLE SUBMISSION    SYSTM2 237
C...  TO THE COMPUTER.  EACH RUN REQUIRES THREE DATA CARDS, READ BY MAIN    SYSTM2 238
C...  PROGRAM SYSTEM, WHICH CONTAIN THE FOLLOWING INFORMATION               SYSTM2 239
C...                                                                        SYSTM2 240
C...    (1)  DATA CARD 1 - A DOCUMENTATION TITLE OF UP TO 80 CHARACTERS     SYSTM2 241
C...         (STORED IN ARRAY TITLE(20)), READ BY A 20A4 FORMAT (FORMAT     SYSTM2 242
C...         900).  THIS DOCUMENTATION TITLE IS MERELY PRINTED AT THE       SYSTM2 243
C...         BEGINNING OF EACH RUN.  A BLANK CARD CAN BE USED. HOWEVER,     SYSTM2 244
C...         A CARD MUST BE PROVIDED.                                       SYSTM2 245
C...                                                                        SYSTM2 246
C...    (2)  DATA CARD 2 - THE INITIAL (T0), FINAL (TF), AND PRINT          SYSTM2 247
C...         INTERVAL (TP) VALUES OF TIME, READ BY A 3E10.0 FORMAT          SYSTM2 248
C...         (FORMAT 901).  THE UNITS OF THE TIME VALUES READ FROM          SYSTM2 249
C...         THIS CARD MUST BE THE SAME AS FOR THE DERIVATIVES IN THE       SYSTM2 250
C...         TEMPORAL DIFFERENTIAL EQUATIONS (E.G., WEEKS, MONTHS,          SYSTM2 251
C...         YEARS).                                                        SYSTM2 252
C...                                                                        SYSTM2 253
C...    (3)  DATA CARD 3 - THE NUMBER OF DIFFERENTIAL EQUATIONS (N),        SYSTM2 254
C...         THE RATIO OF THE PRINT INTERVAL TO THE MINIMUM INTEGRATION     SYSTM2 255
C...         INTERVAL (NMAX, MAXIMUM VALUE OF 99999), THE INTEGRATION       SYSTM2 256
C...         ALGORITHM (NTYPE = 1 TO 16).  THE ERROR MESSAGE OPTION         R012580 31
C...         (NPRINT = 0 OR 1), THE TYPE OF ERROR CRITERION (IRRTYP =       SYSTM2 258
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C...         REL, CAN BE REL OR ABS), AND THE MAGNITUDE OF THE MAXI-
C...         MUM ALLOWABLE INTEGRATION ERROR (ERROR), READ BY A 4I5,
C...         2X,A3,E10.0 FORMAT (FORMAT 902).
C...
C...  AS THE PROGRAM GOES THROUGH SUCCESSIVE RUNS BY READING SETS OF
C...  THREE DATA CARDS, IT PROVIDES A RUN COUNTER, NORUN, IN COMMON/T/
C...  WHICH CAN BE USED TO BRANCH WITHIN SUBROUTINES INITAL, DERV AND
C...  PRINT.  FOR THE FIRST RUN, NORUN = 1, FOR THE SECOND, NORUN = 2,
C...  ETC.  NORUN CAN THEREFORE BE USED TO CHANGE THE PROBLEM SYSTEM
C...  PARAMETERS IN SUCCESSIVE RUNS THROUGH THE USE OF A COMPUTED GO TO
C...  OR OTHER BRANCHING STATEMENT.
C...
C...  THE USER MAY SELECT ONE OF 16 INTEGRATION ALGORITHMS BY PUNCHING
C...  A 1 TO 16 IN COLUMNS 14-15 OF THE THIRD DATA CARD (RIGHT JUSTI-
C...  FIED TO COLUMN 15).  ALSO, THE USER MAY SELECT A PRINT OPTION FOR
C...  ERRORS BY PUNCHING A 0 OR 1 IN COLUMN 20 OF THE THIRD DATA CARD OF
C...  EACH RUN (I.E., NPRINT = 0 OR 1).  IF 1 IS USED, THE PROGRAM WILL
C...  REPORT ANY TEMPORAL INTEGRATION ERRORS WHICH OCCURRED DURING THE
C...  RUN IN AN ERROR SUMMARY AT THE END OF THE RUN (I.E., THE DEPENDENT
C...  VARIABLES WHICH VIOLATED THE ERROR CRITERION DURING A RUN AS
C...  SPECIFIED ON THE THIRD DATA CARD OF THE RUN ARE REPORTED).
C...
C...  MAIN PROGRAM SYSTEM
C...
C...     (1)  READS THE DATA CARDS FOR MULTIPLE RUNS OF THE PROGRAM
C...
C...     (2)  TESTS FOR AN END OF RUNS CARD
C...
C...     (3)  PROVIDES OVERALL CONTROL FOR EACH RUN OF THE PROGRAM
C...
C...     (4)  CALLS SUBROUTINE INITAL FOR INITIALIZATION AND DATA INPUT
C...          AT THE BEGINNING OF EACH RUN.
C...
C...     (5)  TRANSFERS CONTROL TO SUBROUTINE INTEG OR SUBROUTINE GEARB
C...          TO INTEGRATE THE TEMPORAL DIFFERENTIAL EQUATIONS
C...
C...     (6)  CALLS SUBROUTINE PRINT TO PRINT AND PLOT THE NUMERICAL
C...          SOLUTION
C...
C...     (7)  PRINTS A SUMMARY OF ANY INTEGRATION ERRORS WHICH OCCURRED
C...          DURING A RUN.
C...
C...  *-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-
C...       THIS PROGRAM HAS BEEN MODIFIED TO PERMIT NUMERICAL
C...  INTEGRATION OVER AN UNEVEN PRINT INTERVAL.  ALL ADDITIONS TO
C...  THE ORIGINAL DSS PROGRAM ARE OFFSET FROM THE ORIGINAL
C...  IN A SIMILAR MANNER.
C...
C...  *-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-
C...  DEFINE THE COMMON AREA
C...
C...  COMMON/SYSTM1/ CONTAINS THE PROGRAM CONTROL DATA READ FROM THE
C...  SECOND AND THIRD DATA CARDS
      COMMON/SYSTM1/T0,TF,TP,N,NMAX,NTYPE,NPRINT,IRRTYP,ERROR
C...
C...  COMMON/T/ CONTAINS THE INDEPENDENT VARIABLE, RUN TERMINATION
C...  VARIABLE, CURRENT RUN NUMBER
      COMMON/T/T,NFIN,NORUN
C...
C...  COMMON/IO/ CONTAINS THE INPUT/OUTPUT UNIT (DEVICE) NUMBERS
      COMMON/IO/NI,NO
C...
C...  COMMON/GEARB/ CONTAINS THE COMPUTATIONAL STATISTICS FOR THE GEARB
C...  INTEGRATOR PRINTED BY FORMAT 911
      COMMON/GEARB/HUSED,NQUSED,NSTEP,NFE,NJE
C...
```

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C...  THE FOLLOWING COMMON BLOCKS CONTAIN THE ARRAYS WHICH MUST BE              SYSTM2 320
C...  EXPANDED IF DSS/2 IS TO ACCOMMODATE MORE THAN 250 ORDINARY                SYSTM2 321
C...  DIFFERENTIAL EQUATIONS.  ALSO, SOME OF THESE ARRAYS WILL REQUIRE          SYSTM2 322
C...  EXPANSION IF VARIOUS OPTIONS OF THE GEARB INTEGRATOR ARE TO BE            SYSTM2 323
C...  USED.  THIS EXPANSION CAN BE ACCOMPLISHED BY EITHER LOADING A             SYSTM2 324
C...  SUBROUTINE WITH THE EXPANDED ARRAYS BEFORE THIS MAIN PROGRAM OR           SYSTM2 325
C...  CHANGING THE COMMON STATEMENTS BELOW                                      SYSTM2 326
C...                                                                            SYSTM2 327
C...  COMMON/Y/ AND /F/ PROVIDE THE LINKAGE BETWEEN THE USER-SUPPLIED           SYSTM2 328
C...  SUBROUTINES DERV AND INITAL, AND THE INTEGRATION SUBROUTINE AS            SYSTM2 329
C...  EXPLAINED IN THE PRECEDING COMMENTS                                       SYSTM2 330
      COMMON/Y/Y(250)                                                    EXPAND SYSTM2 331
      COMMON/F/F(250)                                                    EXPAND SYSTM2 332
C...                                                                            SYSTM2 333
C...  COMMON/RK1/, /RK2/, /RK3/, /RK4/ AND /RK5/ CONTAIN THE RUNGE              SYSTM2 334
C...  KUTTA DERIVATIVES USED IN SUBROUTINE INTEG                                SYSTM2 335
      COMMON/RK1/K1(250)                                                 EXPAND SYSTM2 336
      COMMON/RK2/K2(250)                                                 EXPAND SYSTM2 337
      COMMON/RK3/K3(250)                                                 EXPAND SYSTM2 338
      COMMON/RK4/K4(250)                                                 EXPAND SYSTM2 339
      COMMON/RK5/K5(250)                                                 EXPAND SYSTM2 340
C...                                                                            SYSTM2 341
C...  COMMON/RK6/, /RK7/ AND /RK8/ CONTAIN THE ESTIMATED ERROR VECTOR,          SYSTM2 342
C...  DEPENDENT VARIABLE VECTOR AND DERIVATIVE VECTOR STORED AT THE             SYSTM2 343
C...  BEGINNING OF AN INTEGRATION STEP AND USED IN SUBROUTINE INTEG             SYSTM2 344
      COMMON/RK6/E(250)                                                  EXPAND SYSTM2 345
      COMMON/RK7/Y0(250)                                                 EXPAND SYSTM2 346
      COMMON/RK8/F0(250)                                                 EXPAND SYSTM2 347
C...                                                                            SYSTM2 348
C...  COMMON/SYSTM2/ AND /SYSTM3/ CONTAIN THE SUBSCRIPTS OF THE DE-             SYSTM2 349
C...  PENDENT VARIABLES VIOLATING THE USER-SPECIFIED ERROR CRITERION AT         SYSTM2 350
C...  EACH POINT ALONG THE SOLUTION AND ACCUMULATED FOR THE ENTIRE              SYSTM2 351
C...  SOLUTION, AND USED IN SUBROUTINE INTEG                                    SYSTM2 352
      COMMON/SYSTM2/NVAR,INTERR(250)                                     EXPAND SYSTM2 353
      COMMON/SYSTM3/NACC,INTACC(250)                                     EXPAND SYSTM2 354
C...                                                                            SYSTM2 355
C...  COMMON/GEAR2/ TO /GEAR10/ CONTAIN THE WORKING ARRAYS USED BY THE          SYSTM2 356
C...  GEAR/HINDMARSH INTEGRATOR IN SUBROUTINE DRIVEB AND THE SUBROUTINES        SYSTM2 357
C...  CALLED BY DRIVEB.  THEY ARE SIZED FOR THE DIAGONAL APPROXIMATION          SYSTM2 358
C...  OF THE JACOBIAN MATRIX (ALGORITHM NTYPE = 15, HINDMARSH METHOD            SYSTM2 359
C...  FLAG MF = 23).  FOR OTHER OPTIONS, THESE ARRAYS MUST GENERALLY BE         SYSTM2 360
C...  INCREASED ACCORDING TO THE INSTRUCTIONS IN THE GEARB MANUAL BY            R012580 35
C...  A. C. HINDMARSH CITED AS REFERENCE (2) AT THE BEGINNING OF SUBROU-        R012580 36
C...  TINE DRIVEB                                                               R012580 37
      COMMON/GEAR2/YMAX(250)                                             EXPAND SYSTM2 365
      COMMON/GEAR3/ERR(250)                                              EXPAND SYSTM2 366
      COMMON/GEAR4/SAVE1(250)                                            EXPAND SYSTM2 367
      COMMON/GEAR5/SAVE2(250)                                            EXPAND SYSTM2 368
      COMMON/GEAR6/PW(250)                                               EXPAND SYSTM2 369
      COMMON/GEAR7/IPIV(1)                                               EXPAND SYSTM2 370
      COMMON/GEAR10/Y1(250,6)                                            EXPAND SYSTM2 371
C...                                                                            SYSTM2 372
C...  COMMON/GEAR11/ CONTAINS INPUT/OUTPUT PARAMETERS FOR SUBROUTINE            SYSTM2 373
C...  DRIVEB, THE DRIVER FOR THE GEARB INTEGRATOR                               SYSTM2 374
      COMMON/GEAR11/H0,TOUT,EPS,MF,INDEX,ML,MU                                  SYSTM2 375
      REAL K1,K2,K3,K4,K5                                                       SYSTM2 376
C...                                                                            SYSTM2 377
C...  DIMENSION THE ARRAYS WHICH PROVIDE A DOCUMENTATION TITLE FOR EACH         SYSTM2 378
C...  RUN AND STORE THE CHARACTERS  END OF RUNS  AND  REPEATS                   SYSTM2 379
      DIMENSION TITLE(20),XTITLE(3),YTITLE(2)                                   SYSTM2 380
C...                                                                            SYSTM2 381
C...  ****************************************************************          SYSTM2 382
C...  THE FOLLOWING DATA STATEMENTS WHICH DEFINE THE CHARACTERS END OF          SYSTM2 383
C...  RUNS AND REPEATS MAY HAVE TO BE CHANGED FOR IMPLEMENTATION ON             SYSTM2 384
C...  COMPUTERS OTHER THAN THE CDC 6000 SERIES                                  SYSTM2 385
      DATA XTITLE(1),XTITLE(2),XTITLE(3)/4HEND ,4HOF R,4HUNS /                  SYSTM2 386
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```
      DATA YTITLE(1),YTITLE(2)/4HREPE,4HATS /
C...  DIMENSION FOR NUMBER OF PRINT INTERVALS BEING USED
C...
      DIMENSION TPT(50)
C...  *-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-
C...  *****************************************************************
C...  THE FOLLOWING DATA STATEMENT WHICH DEFINES THE CHARACTERS REL FOR
C...  A RELATIVE ERROR CRITERION MAY HAVE TO BE CHANGED FOR IMPLEMENTA-
C...  TION ON COMPUTERS OTHER THAN THE CDC 6000 SERIES
      DATA IHREL/3HREL/
C...  *****************************************************************
C...  THE FOLLOWING INITIALIZATION FOR THE INPUT/OUTPUT LOGICAL UNIT
C...  NUMBERS WHICH ARE USED IN THE FORTRAN READ/WRITE STATEMENTS MAY
C...  HAVE TO BE CHANGED FOR IMPLEMENTATION ON COMPUTERS OTHER THAN THE
C...  CDC 6000 SERIES
      NI=5
      NO=6
C...  *****************************************************************
C...
C...  THIS SECTION, CONCLUDING WITH THE CALL TO SUBROUTINE INITAL,
C...  INITIALIZES A DSS/2 RUN BY (GENERALLY) READING DATA CARDS AND
C...  PRINTING A DATA SUMMARY
C...
C...  INITIALIZE THE RUN NUMBER AND INCREMENT FOR EACH RUN, THE RUN
C...  TERMINATION VARIABLE, THE COUNTER FOR REPEAT RUNS
      NORUN=0
1     NORUN=NORUN+1
      NFIN=0
      NRPT=0
C...
C...  READ THE FIRST DATA CARD FOR THE NEXT RUN AND TEST FOR AN END OF
C...  RUNS CARD
      READ(NI,900)(TITLE(I),I=1,20)
      DO 2 I=1,3
      IF(TITLE(I).NE.XTITLE(I))GO TO 8
2     CONTINUE
C...
C...  AN END OF RUNS CARD HAS BEEN READ.  TERMINATE THE SERIES OF RUNS
      STOP
C...
C...  TEST FOR A REPEATS CARD
8     DO 9 I=1,2
      IF(TITLE(I).NE.YTITLE(I))GO TO 3
9     CONTINUE
C...
C...  A REPEATS CARD HAS BEEN READ.  READ THE NUMBER OF REPEAT RUNS
      READ(NI,902)NRPTS
C...
C...  STEP THROUGH NRPTS RUNS.  IN EACH RUN, RESET THE INITIAL VALUE OF
C...  THE INDEPENDENT VARIABLE
10    NRPT=NRPT+1
      T0=T0S
C...  *-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-
C...   SET COUNTER NN EQUAL TO ZERO.
C...
      NN = 0
C...  *-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-
C...
C...  FOR A REPEAT RUN, DATA CARDS ARE NOT READ
      GO TO 12
C...
C...  READ THE INITIAL, FINAL AND PRINT INCREMENT VALUES OF THE INDE-
C...  PENDENT VARIABLE
C...  *-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-
C...          ADDITIONS FOR VARYING PRINT INTERVALS
C...  ALL PRINT VALUES OF THE INDEPENDENT VARIABLE ARE BEING READ
```

```
C...  UNDER ARRAY TPT, NPTS IS THE TOTAL NUMBER OF POINTS BEING
C...  EVALUATED (INCLUDING ENDPOINTS),NN IS A COUNTER FOR TPT
C...
    3 READ(NI,914) T0,TF,NPTS
      IPT = NPTS - 2
      READ(NI,915) (TPT(I),I=1,IPT)
      NN = 0
C...  *-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-
C...
C...  STORE THE INITIAL INDEPENDENT VARIABLE IN CASE THE NEXT RUN(S) IS
C...  SPECIFIED VIA A REPEATS CARD IN WHICH CASE THIS VALUE IS NEEDED TO
C...  RESTART (INITIALIZE) THE REPEATS RUN(S)
      T0S=T0
C...
C...  READ THE NUMBER OF FIRST-ORDER ORDINARY DIFFERENTIAL EQUATIONS,
C...  RATIO OF PRINT INTERVAL TO MINIMUM INTEGRATION INTERVAL, NUMBER OF
C...  THE INTEGRATION ALGORITHM, PRINT OPTION, TYPE OF INTEGRATION ERROR
C...  CRITERION, MAGNITUDE OF MAXIMUM ALLOWABLE INTEGRATION ERROR
      READ(NI,902)N,NMAX,NTYPE,NPRINT,IRRTYP,ERROR
C...
C...  PRINT THE DATA IN A SUMMARY FOR USER VERIFICATION
   12 WRITE(NO,903)NORUN,(TITLE(I),I=1,20)
C...  *-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-
      WRITE(NO,904)T0,TF
C...  *-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-
      WRITE(NO,905)N,NMAX,NTYPE
      WRITE(NO,908)
      IF(NTYPE.GT.14)WRITE(NO,910)
C...
C...  FOR NTYPE GT 14, ERROR MESSAGES ARE ALWAYS PRINTED AND A RELATIVE
C...  ERROR IS ALWAYS USED
      IF(NTYPE.GT.14)NPRINT=1
      IF(NTYPE.GT.14)IRRTYP=IHREL
      WRITE(NO,909)NPRINT,IRRTYP,ERROR
C...
C...  SET THE INITIAL CONDITIONS OF THE PROBLEM SYSTEM DEPENDENT VARI-
C...  ABLES (SET IN SUBROUTINE INITAL)
      T=T0
      CALL INITAL
C...
C...  ****************************************************************
C...
C...  THIS SECTION, CONCLUDING WITH STATEMENT 13, INTEGRATES THE
C...  TEMPORAL (INITIAL-VALUE) ORDINARY DIFFERENTIAL EQUATIONS BY ONE OF
C...  14 CLASSICAL RUNGE KUTTA ALGORITHMS (NTYPE = 1 TO 14)
      IF(NTYPE.GT.14)GO TO 13
C...
C...  INITIALIZE THE ARRAY CONTAINING THE SUBSCRIPTS OF THE DEPENDENT
C...  VARIABLES WHICH VIOLATE THE ERROR CRITERION DURING THE RUN
      NACC=0
      DO 6 I=1,N
    6 INTACC(I)=0
C...
C...  PRINT THE NUMERICAL SOLUTION
    4 CALL PRINT(NI,NO)
C...
C...  TEST FOR (1) A RUN TERMINATION IN SUBROUTINE DERV OR SUBROUTINE
C...  PRINT AND (2) THE END OF THE CURRENT RUN
      IF(NFIN.NE.0)GO TO 5
C...  *-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-
C...  BYPASS CHECK FOR END OF CURRENT RUN IF NN = 0
C...
      IF(NN.EQ.0) GO TO 50
      IF(T.GT.(TF-0.5*TP))GO TO 5
   50 CONTINUE
C...  *-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-
```

```
C...                                                                    SYSTM2 487
C...  TAKE THE NEXT STEP ALONG THE SOLUTION VIA INTEGRATION OF THE TEM- SYSTM2 488
C...  PORAL DIFFERENTIAL EQUATIONS                                      SYSTM2 489
      T0=T                                                              SYSTM2 490
C...  *-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*- FIX     37
C...  DETERMINE THE PRINT INTERVAL                                      FIX     38
C...                                                                    FIX     39
      NN = NN+1                                                         FIX     40
      IF(NN.GT.IPT) GO TO 52                                            FIX     41
      TP = TPT(NN) - T0                                                 FIX     42
      GO TO 54                                                          FIX     43
   52 TP = TF - T0                                                      FIX     44
   54 CONTINUE                                                          FIX     45
C...  *-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*- FIX     46
      CALL INTEG                                                        SYSTM2 491
C...                                                                    SYSTM2 492
C...  PRINT THE NUMERICAL SOLUTION AND CONTINUE THE INTEGRATION IF THE  SYSTM2 493
C...  RUN IS NOT FINISHED                                               SYSTM2 494
      GO TO 4                                                           SYSTM2 495
C...                                                                    SYSTM2 496
C...  PRINT A SUMMARY OF INTEGRATION ERRORS, IF REQUESTED, AND TERMINATE SYSTM2 497
C...  THE CURRENT RUN                                                   SYSTM2 498
5     IF((NPRINT.EQ.0).AND.(NRPT.EQ.0))GO TO 1                          SYSTM2 499
      IF((NPRINT.EQ.0).AND.(NRPT.NE.0))GO TO 11                         SYSTM2 500
C...                                                                    SYSTM2 501
C...  IF NO INTEGRATION ERRORS OCCURRED, AN ERROR SUMMARY IS NOT PRINTED SYSTM2 502
      IF((NACC.EQ.0).AND.(NRPT.EQ.0))GO TO 1                            SYSTM2 503
      IF((NACC.EQ.0).AND.(NRPT.NE.0))GO TO 11                           SYSTM2 504
C...                                                                    SYSTM2 505
C...  IF INTEGRATION ERRORS ARE REPORTED, NMAX, THE RATIO OF THE PRINT  SYSTM2 506
C...  INTERVAL TO THE MINIMUM ALLOWABLE INTEGRATION INTERVAL READ FROM  SYSTM2 507
C...  THE THIRD DATA CARD OF EACH RUN, SHOULD BE INCREASED.  ALSO, THE  SYSTM2 508
C...  ESTIMATED ERROR OF EACH DEPENDENT VARIABLE IS COMPARED WITH THE   SYSTM2 509
C...  MAXIMUM ERROR, ERROR, READ FROM THE THIRD DATA CARD.  THEREFORE,  SYSTM2 510
C...  THIS ERROR CRITERION CAN BE RELAXED (I.E. INCREASED) TO ELIMINATE SYSTM2 511
C...  REPORTED INTEGRATION ERRORS BUT THIS IN GENERAL WILL LEAD TO LESS SYSTM2 512
C...  ACCURATE SOLUTIONS.  ERROR = 0.001 (RELATIVE) IS RECOMMENDED AS A SYSTM2 513
C...  MAXIMUM ALLOWABLE ERROR (I.E. 0.1 PER CENT)                       SYSTM2 514
C...                                                                    SYSTM2 515
C...  PACK THE ARRAY CONTAINING THE SUBSCRIPTS OF THE VIOLATING DE-     SYSTM2 516
C...  PENDENT VARIABLES PRIOR TO PRINTING THE ERROR SUMMARY             SYSTM2 517
      J=0                                                               SYSTM2 518
      DO 7 I=1,N                                                        SYSTM2 519
      IF(INTACC(I).EQ.0)GO TO 7                                         SYSTM2 520
      J=J+1                                                             SYSTM2 521
      INTACC(J)=I                                                       SYSTM2 522
7     CONTINUE                                                          SYSTM2 523
C...                                                                    SYSTM2 524
C...  PRINT THE ERROR SUMMARY                                           SYSTM2 525
      WRITE(NO,906)(INTACC(I),I=1,NACC)                                 SYSTM2 526
      WRITE(NO,907)                                                     SYSTM2 527
C...                                                                    SYSTM2 528
C...  INITIATE THE NEXT RUN                                             SYSTM2 529
      IF(NRPT.EQ.0)GO TO 1                                              SYSTM2 530
C...                                                                    SYSTM2 531
C...  TEST IF THE TOTAL NUMBER OF REPEAT RUNS IS COMPLETE               SYSTM2 532
11    IF(NRPT.EQ.NRPTS)GO TO 1                                          SYSTM2 533
      NORUN=NORUN+1                                                     SYSTM2 534
      NFIN=0                                                            SYSTM2 535
      GO TO 10                                                          SYSTM2 536
C...                                                                    SYSTM2 537
C...  ************************************************************** SYSTM2 538
C...                                                                    SYSTM2 539
C...  THIS SECTION, CONCLUDING WITH STATEMENT 18, INTEGRATES THE        SYSTM2 540
C...  TEMPORAL (INITIAL-VALUE) ORDINARY DIFFERENTIAL EQUATIONS BY THE   SYSTM2 541
C...  GEAR/HINDMARSH ALGORITHM WITH DIAGONAL APPROXIMATION OF THE       SYSTM2 542
```

```
C...  JACOBIAN MATRIX (ALGORITHM NTYPE = 15, 16, HINDMARSH METHOD FLAG       SYSTM2 543
C...  = 23)                                                                  SYSTM2 544
13    IF(NTYPE.GT.16)GO TO 18                                                SYSTM2 545
C...                                                                         SYSTM2 546
C...  PRINT THE INITIAL CONDITIONS                                           SYSTM2 547
      CALL PRINT(NI,NO)                                                      SYSTM2 548
C...                                                                         SYSTM2 549
C...  CALL GEARB TO COVER ONE PRINT INTERVAL OF THE NUMERICAL SOLUTION       SYSTM2 550
16    CALL GEARB                                                             SYSTM2 551
C...                                                                         SYSTM2 552
C...  PRINT THE NUMERICAL SOLUTION                                           SYSTM2 553
      CALL PRINT(NI,NO)                                                      SYSTM2 554
C...                                                                         SYSTM2 555
C...  CHECK FOR A NORMAL RUN TERMINATION                                     SYSTM2 556
      IF(NFIN.NE.0)GO TO 14                                                  R012580 44
      IF(((INDEX-2)*INDEX.EQ.0).AND.(T.GT.(TF-0.5*TP)))GO TO 14              SYSTM2 557
C...                                                                         SYSTM2 558
C...  CHECK FOR AN ABNORMAL RUN TERMINATION (DUE TO AN ERROR CONDITION       SYSTM2 559
C...  REPORTED BY GEARB)                                                     SYSTM2 560
      IF((INDEX-2)*INDEX.NE.0)GO TO 15                                       SYSTM2 561
C...                                                                         SYSTM2 562
C...  TAKE THE NEXT STEP ALONG THE SOLUTION                                  SYSTM2 563
      GO TO 16                                                               SYSTM2 564
C...                                                                         SYSTM2 565
C...  REPORT THE COMPUTATIONAL STATISTICS OF THE GEARB INTEGRATOR            SYSTM2 566
14    WRITE(NO,911)NSTEP,NFE,NJE                                             SYSTM2 567
C...                                                                         SYSTM2 568
C...  TERMINATE THE CURRENT RUN                                              SYSTM2 569
17    IF(NRPT.EQ.0)GO TO 1                                                   SYSTM2 570
C...                                                                         SYSTM2 571
C...  TEST IF THE TOTAL NUMBER OF REPEAT RUNS IS COMPLETE                     SYSTM2 572
      IF(NRPT.EQ.NRPTS)GO TO 1                                               SYSTM2 573
      NORUN=NORUN+1                                                          SYSTM2 574
      GO TO 10                                                               SYSTM2 575
C...                                                                         SYSTM2 576
C...  PRINT AN ERROR MESSAGE FOR THE GEARB INTEGRATOR                        SYSTM2 577
15    WRITE(NO,912)INDEX                                                     SYSTM2 578
      GO TO 14                                                               SYSTM2 579
C...                                                                         SYSTM2 580
C...  ************************************************************          SYSTM2 581
C...                                                                         SYSTM2 582
C...  TEMPORAL (INITIAL-VALUE) INTEGRATORS CAN BE ADDED AT THIS POINT.       SYSTM2 583
C...  TEMPORARILY, AN ERROR MESSAGE MESSAGE IS PRINTED THAT THE INTE-        SYSTM2 584
C...  GRATOR NUMBER, NTYPE, READ FROM THE THIRD DATA CARD EXCEEDS 16         SYSTM2 585
C...  SINCE DSS/2 PRESENTLY CONTAINS 16 INTEGRATORS                          SYSTM2 586
18    WRITE(NO,913)                                                          SYSTM2 587
      GO TO 17                                                               SYSTM2 588
900   FORMAT(20A4)                                                           SYSTM2 589
901   FORMAT(3E10.0)                                                         SYSTM2 590
902   FORMAT(4I5,2X,A3,E10.0)                                                SYSTM2 591
903   FORMAT(1H1,10X,8HRUN NO. ,I2,3H - ,20A4,/)                             SYSTM2 592
904   FORMAT(11X,24HINITIAL VALUE OF TIME = ,E11.4,//,                       SYSTM2 593
     1       11X,22HFINAL VALUE OF TIME = ,E11.4,//,                         SYSTM2 594
C...  *-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-         FIX    47
     2       11X,68HPRINT INTERVAL OF TIME IS VARYING - SEE REACTOR PROF     FIX    48
     3ILE FOR SPACINGS,/)                                                    FIX    49
C...  *-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-         FIX    50
905   FORMAT(                                                                SYSTM2 596
     1 11X,47HNUMBER OF FIRST-ORDER DIFFERENTIAL EQUATIONS = ,I3,//,         SYSTM2 597
     2 11X,46HPRINT INTERVAL/MINIMUM INTEGRATION INTERVAL = ,I5,//,          SYSTM2 598
     3 11X,24HINTEGRATION ALGORITHM = ,I2,/,                                 SYSTM2 599
     4 16X,54H 1 - RUNGE KUTTA EULER                                 ,/,     SYSTM2 600
     5 16X,54H 2 - RUNGE KUTTA NIESSE                                ,/,     SYSTM2 601
     6 16X,54H 3 - RUNGE KUTTA MERSON                                ,/,     SYSTM2 602
     7 16X,54H 4 - RUNGE KUTTA TANAKA - 4                            ,/,     SYSTM2 603
     8 16X,54H 5 - RUNGE KUTTA TANAKA - 5                            ,/,     SYSTM2 604
```

```
     9 16X,54H 6 - RUNGE KUTTA CHAI                                 )         R012580 45
 908  FORMAT(                                                                 SYSTM2 606
     A 16X,54H 7 - RUNGE KUTTA ENGLAND                              , /,      SYSTM2 607
     B 16X,54H 8 - RUNGE KUTTA WES - 4/1                            , /,      SYSTM2 608
     C 16X,54H 9 - RUNGE KUTTA WES - 4/2                            , /,      SYSTM2 609
     D 16X,54H10 - RUNGE KUTTA WES - 4/3                            , /,      SYSTM2 610
     E 16X,54H11 - RUNGE KUTTA WES - 4/4                            , /,      SYSTM2 611
     F 16X,54H12 - RUNGE KUTTA WES - 4/5                            , /,      SYSTM2 612
     G 16X,54H13 - RUNGE KUTTA WES - 5/1                            , /,      SYSTM2 613
     H 16X,54H14 - RUNGE KUTTA WES - 5/2                            , /)      SYSTM2 614
 910  FORMAT(                                                                 SYSTM2 615
     1 16X,54H15 - GEAR/HINDMARSH INTEGRATOR FOR BANDED ODE SYSTEMS , /,      SYSTM2 616
     2 16X,54H      DIAGONAL APPROXIMATION OF THE JACOBIAN MATRIX   , /,      SYSTM2 617
     3 16X,54H      OUTPUT POINTS BY INTERPOLATION                  ,//,      SYSTM2 618
     4 16X,54H16 - GEAR/HINDMARSH INTEGRATOR FOR BANDED ODE SYSTEMS , /,      SYSTM2 619
     5 16X,54H      DIAGONAL APPROXIMATION OF THE JACOBIAN MATRIX   , /,      SYSTM2 620
     6 16X,54H      EXACT OUTPUT POINTS (NO INTERPOLATION)          , /)      SYSTM2 621
 909  FORMAT(                                                                 SYSTM2 622
     I 11X,15HPRINT OPTION = ,I1,/,                                           SYSTM2 623
     J 16X,36HNO INTEGRATION ERROR DIAGNOSTICS - 0,/,                         SYSTM2 624
     K 16X,36HSUMMARY OF INTEGRATION ERRORS    - 1,//,                        SYSTM2 625
     L 11X,28HTYPE OF INTEGRATION ERROR = ,A3,//,                             SYSTM2 626
     M 11X,28HMAXIMUM INTEGRATION ERROR = ,E10.3,/,                           SYSTM2 627
     N 1H1)                                                                   SYSTM2 628
 906  FORMAT(1H1,10X,55HINTEGRATION ERROR FOR THE FOLLOWING DEPENDENT VA      SYSTM2 629
     1RIABLES,/,(11X,10I5),/)                                                 SYSTM2 630
 907  FORMAT(11X,95HDEPENDENT VARIABLES REPORTED IN THE ERROR SUMMARY AR      SYSTM2 631
     1E NUMBERED IN THE SAME ORDER AS THEY APPEAR,/,11X,97HIN THE /Y/ SE      SYSTM2 632
     2CTION OF LABELLED COMMON (SEE THE COMMON AREA OF SUBROUTINES INITA      SYSTM2 633
     3L, DERV AND PRINT))                                                     SYSTM2 634
 911  FORMAT(1H1,//,                                                          SYSTM2 635
     1 16X,54HCOMPUTATIONAL STATISTICS FOR THE GEARB INTEGRATOR     , /,      SYSTM2 636
     2 16X,18H      RUN REQUIRED ,I5,29H STEPS                      , /,      SYSTM2 637
     3 16X,30H      DERIVATIVE EVALUATIONS = ,I5                    , /,      SYSTM2 638
     4 16X,30H      JACOBIAN EVALUATIONS   = ,I5,                   , /)      SYSTM2 639
 912  FORMAT(//,                                                              SYSTM2 640
     1 16X,54H ERROR CONDITION REPORTED BY THE GEARB INTEGRATOR     , /,      SYSTM2 641
     2 16X,13H      INDEX = ,I2,34H, CURRENT RUN TERMINATED         , /)      SYSTM2 642
 913  FORMAT(                                                                 SYSTM2 643
     1 16X,54HALGORITHM NUMBER READ FROM THIRD DATA CARD EXCEEDS 16 , /)      SYSTM2 644
C...  *-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-    FIX     51
C...  FORMATS ADDED FOR CHANGING PRINT INTERVAL                               FIX     52
C...                                                                          FIX     53
  914 FORMAT(2E10,I5)                                                         FIX     54
  915 FORMAT(8E10)                                                            FIX     55
C...  *-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-    FIX     56
      END                                                                     SYSTM2 645
      SUBROUTINE GEARB                                                        SYSTM2 646
C...                                                                          SYSTM2 647
C...  SUBROUTINE GEARB CALLS THE DRIVER ROUTINE FOR THE GEARB INTEGRA-        SYSTM2 648
C...  TOR, DRIVEB, TO MOVE THE SOLUTION THROUGH ONE INTERVAL BETWEEN          SYSTM2 649
C...  OUTPUT POINTS.  DRIVEB, WITH MINOR MODIFICATIONS, AND ASSOCIATED        SYSTM2 650
C...  ROUTINES WERE DEVELOPED BY DR. A. C. HINDMARSH OF THE LAWRENCE          SYSTM2 651
C...  LIVERMORE LABORATORY.  THE OPPORTUNITY TO USE THE GEARB INTEGRATOR      SYSTM2 652
C...  IN DSS/2 IS GRATEFULLY ACKNOWLEDGED.                                    SYSTM2 653
C...                                                                          SYSTM2 654
      COMMON/SYSTM1/T0,TF,TP,N,NMAX,NTYPE,NPRINT,IRRTYP,ERROR                 SYSTM2 655
      COMMON/T/T                                                              SYSTM2 656
      COMMON/Y/Y(1)                                                           SYSTM2 657
      COMMON/GEAR10/Y1(1,1)                                                   SYSTM2 658
      COMMON/GEAR11/H0,TOUT,EPS,MF,INDEX,ML,MU                                SYSTM2 659
C...                                                                          SYSTM2 660
C...  INITIALIZE THE GEAR/HINDMARSH INTEGRATOR.  NOTE THAT SOME RATHER        R012580 46
C...  ARBITRARY ASSUMPTIONS HAVE BEEN MADE HERE IN SETTING THE INITIAL        R012580 47
C...  INTEGRATION INTERVAL, H0, AND THE VALUE OF THE ALLOWABLE INTEGRA-       R012580 48
C...  TION ERROR, EPS (ERROR IS READ FROM THE THIRD DATA CARD OF A DSS/2      R012580 49
```

```
C...  RUN).  THESE VALUES OF H0 AND EPS MAY AFFECT THE PERFORMANCE OF
C...  THE GEAR/HINDMARSH INTEGRATOR AND THEREFORE SOME EXPERIMENTATION
C...  MAY BE REQUIRED IF THE PROBLEM SYSTEM ODES ARE NOT SUCCESSFULLY
C...  INTEGRATED.  OF COURSE, ONLY THE DIAGONAL APPROXIMATION OPTION
C...  (MF = 23) OF THE GEAR/HINDMARSH INTEGRATOR IS IMPLEMENTED.  OTHER
C...  OPTIONS WHICH USE MORE OF THE PROBLEM SYSTEM JACOBIAN MATRIX MAY
C...  BE REQUIRED, AND THEY CAN BE ADDED AFTER THE 3 CONTINUE STATEMENT
C...  BELOW, E.G., THE MF = 22 OPTION.  IN GENERAL, HOWEVER, MORE MEMORY
C...  WILL BE REQUIRED TO STORE THE ADDITIONAL ELEMENTS OF THE JACOBIAN
C...  MATRIX.  IN PARTICULAR, ARRAYS PW AND IPIV IN COMMON/GEAR6/ AND
C...  /GEAR7/ WILL HAVE TO BE EXPANDED IN ACCORDANCE WITH THE DIRECTIONS
C...  IN THE GEARB INTEGRATOR MANUAL (SEE REFERENCE (2) AT THE BEGINNING
C...  OF SUBROUTINE DRIVEB).  ARRAYS PW AND IPIV ARE DIMENSIONED AT THE
C...  BEGINNING OF THIS MAIN PROGRAM.  AN ALTERNATIVE IS TO CALL DRIVEB
C...  DIRECTLY (OUTSIDE DSS/2), AND PROVIDE THE REQUIRED DIMENSIONSING
C...  OF THE ARRAYS AS EXPLAINED IN THE GEARB MANUAL.  DETAILS FOR THIS
C...  SOMEWHAT MORE FLEXIBLE APPROACH ARE AVAILABLE FROM W. E. SCHIESSER
C...  (FOR THIS ALTERNATIVE, THE USER-SUPPLIED SUBROUTINES INITAL, DERV
C...  AND PRINT, AND THE SUBROUTINES CALLED BY THESE THREE SUBROUTINES,
C...  E.G., DSS002, REMAIN UNCHANGED).  EXTENDING THIS APPROACH FURTHER,
C...  ANY QUALITY INTEGRATOR FOR ODES CAN BE USED IN COMBINATION WITH
C...  SUBROUTINES INITAL, DERV AND PRINT.  ALL THAT IS REQUIRED IS THE
C...  USUAL INTERFACE THROUGH COMMON/T/, /Y/ AND /F/
      IF((T-T0-TP/2.).GT.0.)GO TO 10
      H0=TP/(FLOAT(NMAX)+1.0E+04)
      TOUT=T0
      EPS=ERROR
      INDEX=1
C...
C...  SELECT THE OPTION OF THE GEAR/HINDMARSH INTEGRATOR
10    NOPT=NTYPE-14
      GO TO(1,2,3),NOPT
C...
C...  NTYPE = 15, 16, GEARB INTEGRATOR WITH DIAGONAL APPROXIMATION OF
C...  THE JACOBIAN MATRIX, OUTPUT BY INTERPOLATION OR EXACT WITHOUT
C...  INTERPOLATION
1     CONTINUE
2     TOUT=TOUT+TP
      MF=23
      ML=1
      MU=1
C...
C...  CALL DRIVEB TO COVER ONE PRINT INTERVAL OF THE NUMERICAL SOLUTION
      CALL DRIVEB(N,T0,H0,Y,TOUT,EPS,MF,INDEX,ML,MU,Y1)
      T=TOUT
      IF(NTYPE.EQ.15)INDEX=2
      RETURN
C...
C...  OTHER OPTIONS OF THE GEARB INTEGRATOR CAN BE ADDED AT THIS POINT
3     CONTINUE
      RETURN
      END
      SUBROUTINE DIFFUN(N,TIME,Z,ZDOT)
C...
C...  SUBROUTINE DIFFUN IS AN INTERFACE BETWEEN THE GEAR/HINDMARSH INTE-
C...  GRATOR (CALLED BY DRIVEB AND ASSOCIATED SUBROUTINES) AND THE USER-
C...  SUPPLIED SUBROUTINE DERV WHICH DEFINES THE PROBLEM SYSTEM TEMPORAL
C...  DERIVATIVES
C...
      COMMON/T/T/Y/Y(1)/F/F(1)
      DIMENSION Z(N),ZDOT(N)
C...
C...  TRANSFER THE DEPENDENT VARIABLE VECTOR TO THE ARRAY USED BY SUB-
C...  ROUTINE DERV AND UPDATE THE INDEPENDENT VARIABLE
      DO 1 I=1,N
1     Y(I)=Z(I)
```

```
      T=TIME
C...
C...  COMPUTE THE PROBLEM SYSTEM TEMPORAL DERIVATIVES
      CALL DERV
C...
C...  TRANSFER THE TEMPORAL DERIVATIVE VECTOR TO THE ARRAY USED BY THE
C...  GEAR/HINDMARSH INTEGRATOR
      DO 2 I=1,N
2     ZDOT(I)=F(I)
      RETURN
      END
      SUBROUTINE COMPUR(UROUND)
C...
C...  SUBROUTINE COMPUR COMPUTES THE UNIT ROUNDOFF (MACHINE EPSILON)
C...  FOR USE IN THE GEARB INTEGRATOR.  UROUND IS THE SMALLEST POSITIVE
C...  U SUCH THAT (1+U).NE.1.  THIS ROUTINE WAS DEVELOPED AND TESTED BY
C...  D. M. LISTER AND D. G. BALL OF THE OAK RIDGE NATIONAL LABORATORY,
C...  OAK RIDGE, TENNESSEE  37830
C...
      U1=1.0E+0
      U2=1.0E+0
      TWO=2.0E+0
      HALF=0.5E+0
1     U2=U2*HALF
      U3=U1+U2
      IF(U3.NE.U1)GO TO 1
      UROUND=U2*TWO
      RETURN
      END
      SUBROUTINE PDB(N,T,Y,PW,NEBAND,ML,MU)
C...
C...  SUBROUTINE PDB IS CALLED BY THE GEARB INTEGRATOR FOR OPTIONS MF =
C...  11 AND 21, FOR WHICH THE USER SUPPLIES THE ODE SYSTEM ANALYTICAL
C...  JACOBIAN MATRIX IN PDB.  SINCE THESE OPTIONS ARE NOT IMPLEMENTED
C...  IN DSS/2, THIS DUMMY ROUTINE SHOULD NOT BE CALLED.  IF IT IS
C...  CALLED, AN ERROR MESSAGE IS PRINTED AND THE CURRENT DSS/2 RUN IS
C...  TERMINATED.
C...
      COMMON/IO/NI,NO
C...
C...  PRINT AN ERROR MESSAGE IF PDB IS CALLED
      WRITE(NO,1)
1     FORMAT(
     1 58H SUBROUTINE PDB WAS CALLED BY THE GEARB INTEGRATOR.  THIS , /,
     2 58H OCCURS FOR THE MF = 11, 21 GEARB OPTIONS WHICH ARE NOT    , /,
     3 58H IMPLEMENTED IN DSS/2, SO THE CURRENT RUN IS TERMINATED    )
      IF(N.GT.0)STOP
      RETURN
```

Appendix B: GRPSS Sample Program Output

TEST FOR NEW INPUTING OF INFO TO GEN
RC1 = 1000, R = 30, AREA=10, BRAUN DATA,INCREASE CO

PROCESS FLOWSHEET INFORMATION

KEY-UNIT TYPE(KT), 1=RXR, 2=HX, 3=DIV, 4=MIX, 5=DYR

		STM IN			STM OUT			
UNIT NO	TYPE	1	2	3	1	2	UNIT INFOR	RXR LENGTH
1	1	1	0	0	2	0	10.00000	30.00000

FEED STREAM INFORMATION

			FLOWRATES(LBMOLES/HR)					
STREAM	TK	PSIA	CO	H2	CH4	H2O	CO2	N2
1	551.0	1392.0	913.00	3650.00	14320.00	4473.00	365.00	0.00

STREAMS TORN NONE

UNIT ORDERING OF CALCULATION 1

FLOW STREAM INFORMATION

STREAM	TK	PSIA	CO	H2	CH4	H2O	CO2	N2	TOTAL
			FLOWRATES(LBMOLES/HR)						
1	551.0	1092.0	913.00	3650.00	14320.00	4473.00	365.00	0.00	23721.00
2	730.4	1092.0	10.15	941.45	15222.85	5375.85	365.00	0.00	21915.30

REACTOR NO. 1

LENGTH	XCO	TK	YCO	YH2	YCH4	YH2O	YCO2	DX1DL	DTKDL	RATE1	RATE2	CPAVG
0.000	.00000	551.0	.03849	.15387	.60368	.18857	.01539	6.4558E-02	1.2291E+01	1.9647E+01	0.	10.4265
2.50	.17404	583.8	.03222	.13559	.61867	.19792	.01560	7.4040E-02	1.3845E+01	2.2533E+01	0.	10.8168
5.00	.36458	613.1	.02516	.11500	.63555	.20845	.01583	7.6798E-02	1.4093E+01	2.3372E+01	0.	11.2365
7.50	.54883	652.6	.01813	.09449	.65237	.21894	.01607	6.8786E-02	1.2404E+01	2.0934E+01	0.	11.6539
10.00	.70168	680.0	.01214	.07701	.66671	.22788	.01627	5.2743E-02	9.3787E+00	1.6052E+01	0.	12.0047
12.50	.81195	693.5	.00772	.06412	.67727	.23448	.01641	3.5843E-02	6.3112E+00	1.0908E+01	0.	12.2606
15.00	.88406	712.2	.00479	.05557	.68428	.23885	.01651	2.2573E-02	3.9498E+00	6.8698E+00	0.	12.4293
17.50	.92842	719.9	.00297	.05026	.68864	.24157	.01657	1.3564E-02	2.3644E+00	4.1281E+00	0.	12.5336
20.00	.95467	724.5	.00188	.04710	.69123	.24318	.01661	7.8927E-03	1.3727E+00	2.4020E+00	0.	12.5955
22.50	.96978	727.1	.00126	.04527	.69272	.24412	.01663	4.4884E-03	7.7960E-01	1.3660E+00	0.	12.6312
25.00	.97831	728.6	.00090	.04424	.69357	.24465	.01664	2.5131E-03	4.3619E-01	7.6483E-01	0.	12.6513
27.50	.98306	729.4	.00071	.04367	.69404	.24494	.01665	1.3934E-03	2.4175E-01	4.2406E-01	0.	12.6626
30.00	.98568	729.9	.00060	.04335	.69430	.24510	.01665	7.6808E-04	1.3323E-01	2.3375E-01	0.	12.6688
32.50	.98713	730.1	.00054	.04317	.69445	.24519	.01665	4.2196E-04	7.3183E-02	1.2842E-01	0.	12.6722
35.00	.98792	730.3	.00050	.04308	.69453	.24524	.01665	2.3137E-04	4.0126E-02	7.0415E-02	0.	12.6741
37.50	.98836	730.4	.00049	.04302	.69457	.24527	.01665	1.2674E-04	2.1978E-02	3.8570E-02	0.	12.6751
40.00	.98859	730.4	.00048	.04299	.69459	.24528	.01665	6.9380E-05	1.2031E-02	2.1115E-02	0.	12.6757
42.50	.98872	730.4	.00047	.04298	.69461	.24529	.01665	3.7969E-05	6.5843E-03	1.1555E-02	0.	12.6760
45.00	.98880	730.4	.00047	.04297	.69461	.24530	.01665	2.0775E-05	3.6027E-03	6.3226E-03	0.	12.6762
47.50	.98883	730.4	.00047	.04296	.69462	.24530	.01665	1.1366E-05	1.9711E-03	3.4592E-03	0.	12.6762
50.00	.98886	730.4	.00046	.04296	.69462	.24530	.01665	6.2184E-06	1.0783E-03	1.8925E-03	0.	12.6763
52.50	.98887	730.4	.00046	.04296	.69462	.24530	.01665	3.4019E-06	5.8992E-04	1.0353E-03	0.	12.6763
55.00	.98887	730.4	.00046	.04296	.69462	.24530	.01666	1.8610E-06	3.2272E-04	5.6638E-04	0.	12.6763
57.50	.98888	730.4	.00046	.04296	.69462	.24530	.01666	1.0181E-06	1.7655E-04	3.0984E-04	0.	12.6763
60.00	.98888	730.4	.00046	.04296	.69462	.24530	.01666	5.5695E-07	9.6581E-05	1.6950E-04	0.	12.6763
62.50	.98888	730.4	.00046	.04296	.69462	.24530	.01666	3.0468E-07	5.2835E-05	9.2725E-05	0.	12.6764
65.00	.98888	730.4	.00046	.04296	.69462	.24530	.01666	1.6668E-07	2.8903E-05	5.0725E-05	0.	12.6764
67.50	.98888	730.4	.00046	.04296	.69462	.24530	.01666	9.1181E-08	1.5812E-05	2.7749E-05	0.	12.6764
70.00	.98888	730.4	.00046	.04296	.69462	.24530	.01666	4.9880E-08	8.6498E-06	1.5180E-05	0.	12.6764
72.50	.98888	730.4	.00046	.04296	.69462	.24530	.01666	2.7287E-08	4.7319E-06	8.3044E-06	0.	12.6764
75.00	.98888	730.4	.00046	.04296	.69462	.24530	.01665	1.4927E-08	2.5886E-06	4.5429E-06	0.	12.6764
77.50	.98888	730.4	.00046	.04296	.69462	.24530	.01666	8.1660E-09	1.4161E-06	2.4852E-06	0.	12.6764
80.00	.98888	730.4	.00046	.04296	.69462	.24530	.01666	4.4672E-09	7.7466E-07	1.3595E-06	0.	12.6764
82.50	.98888	730.4	.00046	.04296	.69462	.24530	.01666	2.4438E-09	4.2378E-07	7.4373E-07	0.	12.6764
85.00	.98888	730.4	.00046	.04296	.69462	.24530	.01666	1.3369E-09	2.3183E-07	4.0686E-07	0.	12.6764
87.50	.98888	730.4	.00046	.04296	.69462	.24530	.01666	7.3135E-10	1.2682E-07	2.2257E-07	0.	12.6764
90.00	.98888	730.4	.00046	.04296	.69462	.24530	.01666	4.0009E-10	6.9379E-08	1.2176E-07	0.	12.6764
92.50	.98888	730.4	.00046	.04296	.69462	.24530	.01666	2.1887E-10	3.7954E-08	6.6610E-08	0.	12.6764
95.00	.98888	730.4	.00046	.04296	.69462	.24530	.01665	1.1973E-10	2.0763E-08	3.6439E-08	0.	12.6764
97.50	.98888	730.4	.00046	.04296	.69462	.24530	.01666	6.5504E-11	1.1359E-08	1.9935E-08	0.	12.6764
100.00	.98888	730.4	.00046	.04296	.69462	.24530	.01666	3.5836E-11	6.2144E-09	1.0906E-08	0.	12.6764

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Appendix B: Listing of Steady State Program Portion (SSGEN) of GRPSS

```
      SUBROUTINE INITAL
C
C
C        SUBROUTINE INITAL SETS THE INITIAL CONDITIONS FOR THE
C        DIFFERENTIAL EQUATIONS BEING SOLVED AND ACCESSES ALL
C        OTHER REQUIRED INFORMATION VIA CALLS TO OTHER SUBROUTINES.
C
C
C
      REAL L,KCHEM
      COMMON/T/L,NFIN,NRUN/Y/X1(5),X2(5),TK(5)/F/DX1DL(5),DX2DL(5),
     1  DTKDL(5)
      COMMON/STOIC/ A(3,10), DELA(3)
      COMMON/PRTPLT/ IPLOT,NLINE,NPTS,Q(16),IPT
      COMMON/POINT/ ID(8)
      COMMON/INDAT/ NUNITS,NSTMS,NTEAR,IORD(15)
      COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
      COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
      COMMON/PARM/ N,M,TFDSTM,PFDSTM,P(5),IFD,ITR(10),Y(5,8)
      COMMON/UNIT/ NRXR,NHX,NDIV,NMIX,IRXR(5),NCDR,RLNTH(5),IHX(5),
     1              ICDR(5),QCOND(5),QHX(5)
      COMMON/FLAG/ FLAG1,FLAG2,NFLAG,FLAG3
C
C
C     NOTATION
C
C        DTKDL(I)=FIRST DERIVATIVE OF TK(I) W/R TO DIMENSIONLESS LENGTH
C        FLAG3=FLAG TO STOP PROGRAM WHEN IT HAS CONVERGED TO A SOLUTION
C        IPT=NUMBER OF AN INDIVIDUAL POINT ALONG REACTOR GRID
C        IRXR(I)=UNIT NUMBER OF AN INDIVIDUAL REACTOR I
C        IN(IR,1)=NUMBER OF STREAM ENTERING REACOT IR
C        L = DIMENSIONLESS LENGTH
C        NFLAG=FLAG CONTROLLING THE PRINTING OF SIMULATION INFOR. BY PRI
C        NLINE=LINE ON PRINT OUT PAGE
C        NPTS=TOTAL NUMBER OF POINTS ALONG REACTOR GRID
C        NRUN=RUN NUMBER
C        NRXR=TOTAL NUMBER OF REACTORS IN SIMULATION,READ FROM FLOWST
C        P(I)=PRESSURE IN REACTOR I, ASSUMED CONSTANT, PSIA
C        PRSTM(NSS)=PRESSURE OF STREAM NSS, PSIA
C        TK(I)=TEMPERATURE AT SPECIFIED PT. IN REACTOR I, DEG K
C        TKSTM(NSS)=TEMPERATURE OF STREAM NSS,DEG K
C        X1(I)=CONVERSION AT SPECIFIED PT. OF METHANATION REACTION
C              IN REACTOR I, PERCENT
C        X2(I)=CONVERSION AT SPECIFIED PT. OF SHIFT REACTION
C              IN REACTOR I, PERCENT
C
C
C        IF CALCULATION HAS CONVERGED ON PREVIOUS RUN,
C        STOP THE CALCULATION ( FLAG3 = 1 )
C
C
      IF (NRUN.EQ.1) GO TO 5
      IF (FLAG3.NE.0.) STOP
    5 CONTINUE
C
C        CALL SUBROUTINES  FOR ALL OTHER REQUIRED INFORMATION
C
      CALL IDENT
      CALL STOICH
      CALL FLOWST
      CALL HPREP
C
C
      IPLOT = 0
      NLINE = 0
      IPT = 0
      FLAG1 = 0.
      FLAG2 = 0.
      FLAG3 = 0.
      NFLAG = 0
C
C
C           INITIALIZE REACTION CONVERSIONS FOR ALL RXRS
C
C       INCLUDES FOR ALL REACTOR SPACES AS DIMENSIONED FOR (5)
C
      DO 10 I = 1, 5
```

```
      X1(I) = 0.
      X2(I) = 0.
   10 CONTINUE
      IF (NRUN.GT.1) GO TO 50
C
C          INITIALIZE THE TEMPERATURE PROFILES IN ALL RXRS
C
C      THIS IS DONE FOR ALL REACTOR SPACES ACCOUNTED FOR IN THE
C       PROGRAMING (IN THIS CASE 5)
C
      DO 20 I = 1, 5
      TK(I) = TFDSTM
      P(I) = PFDSTM
   20 CONTINUE
C
C          IF NRXR IS LESS THAN FIVE,SET THE REMAINING
C          REACTOR SPACES IN /F/ TO ZERO
C
      IF (NRXR.EQ.5) GO TO 40
      NS = NRXR + 1
      DO 30 I = NS,5
      DX1DL(I) = 0.
      DX2DL(I) = 0.
      DTKDL(I) = 0.
   30 CONTINUE
   40 CONTINUE
C
C      AFTER INITIAL RUN, SET FIRST GRID TEMP EQUAL TO
C           THE INLET STREAM TEMP TO THE REACTOR
C
      IF (NRUN.EQ.1) GO TO 60
   50 CONTINUE
      DO 15 I = 1, NRXR
      IR = IRXR(I)
      NSS = IN(IR,1)
      TK(I) = TKSTM(NSS)
      P(I) = PRSTM(NSS)
   15 CONTINUE
   60 CONTINUE
      CALL DERV
      RETURN
      END


      SUBROUTINE IDENT
C...
C...
C...  SUBROUTINE IDENT IDENTIFIES WHICH CHEM SPECIES FROM BLOCK DATA IS
C...  THE FIRST COMPONENT, WHICH IS THE SECOND, ETC FOR USE IN
C...  SUBSEQUENT CALCULATIONS.
C...
C             CALLED FROM INITAL
C...
      COMMON/POINT/ ID(8)
      COMMON/PARM/  N,M,TFDSTM,PFDSTM,P(5),IFD,ITR(10)
C
C        N = NUMBER OF COMPOUNDS
C
      N = 6
C
C       ID = CODE NUMBER OF COMPOUND FROM THERMO DATA BOOK
C
C             IN THIS CASE:
C               1=CO  2=H2  3=CH4  4=H2O  5=CO2  6=N2
C
      ID(1) = 4
      ID(2) = 3
      ID(3) = 13
      ID(4) = 12
      ID(5) = 5
      ID(6) = 1
      RETURN
      END
```

```
                   SUBROUTINE STOICH
            C...
            C...
            C...   SUBROUTINE STOICH SETS THE STOICHIOMETRIC COEFFICIENTS FOR THE
            C...   CHEM REACTIONS ENCOUNTERED.
            C...
            C              CALLED FROM INITAL
            C...
      2            COMMON/STOIC/ A(3,10), DELA(3)
      2            COMMON/PARM/ N,M,TFDSTM,PFDSTM,P(5),IFD,ITR(10)
            C
            C          M = NUMBER OF CHEMICAL REACTIONS
            C
      2            M = 2
            C
            C          A(J,I) = STOICHIOMETRIC COEFFICIENTS FOR
            C                   JTH REACTION, ITH COMPOUND
            C
      4            A(1,1) = -1.
     11            A(1,2) = -3.
     15            A(1,3) =  1.
     22            A(1,4) =  1.
     26            A(1,5) =  0.
     33            A(1,6) =  0.
     37            A(2,1) = -1.
     44            A(2,2) =  1.
     50            A(2,3) =  0.
     54            A(2,4) = -1.
     61            A(2,5) =  1.
     66            A(2,6) =  0.
     73            RETURN
     73            END


                   SUBROUTINE FLOWST
            C
            C
            C         SUBROUTINE FLOWST READS THE PROCESS FLOWSHEET
            C         INFORMATION FOR THE PROCESS UNDER STUDY
            C
            C              CALLED FROM INITAL
            C
            C
      2            COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
      2            COMMON/INDAT/ NUNITS,NSTMS,NTEAR,IORD(15)
      2            COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
      2            COMMON/T/L,NFIN,NRUN/Y/X1(5),X2(5),TK(5)/F/DX1DL(5),DX2DL(5)
      2            COMMON/UNIT/ NRXR,NHX,NDIV,NMIX,IRXR(5),NCDR,RLNTH(5),IHX(5),
                 1             ICDR(5),QCOND(5),QHX(5)
      2            COMMON/PARM/ N,M,TFDSTM,PFDSTM,P(5),IFD,ITR(10),Y(5,8)
      2            COMMON/PRTPLT/ IPLOT,NLINE,NPTS,Q(16),IPT
      2            DIMENSION FFDSTM(8), FTRSTM(8)
            C
            C
            C      NOTATION
            C
            C         DUMDAT(JJ) = DUMMY ARRAY CONTAINING REQUIRED DATA
            C                      FOR UNIT JJ
            C         FFDSTM(I)(FTRSTM) = MOLAR FLOWRATE OF COMPOUND I,
            C                             IN FEED (TEAR) STREAM, LBMOL/HR
            C         IFD = FEED STREAM NUMBER
            C         IN(J,I) = STREAM NUMBER ENTERING UNIT J FROM INLET POSITION I
            C         IORD(I) = ORDER IN WHICH UNIT I IS CALCULATED
            C         IRXR(I) = INDIVIDUAL REACTOR NUMBER OF J-TH UNIT(IF IT IS A RXR
            C         ITR(J) = J-TH TEAR STREAM NUMBER
            C         IUNIT(J) = INDIVIDUAL UNIT NUMBER FOR J-TH UNIT
            C         KT(J) = TYPE OF INDIVIDUAL UNIT FOR J-TH UNIT, WHERE-
            C                   1 = REACTOR
            C                   2 = HEAT EXCHANGER
            C                   3 = STREAM DIVIDER
            C                   4 = STREAM MIXER
            C                   5 = DRYER/CONDENSER
            C         JR = REACTOR COUNTER
            C         NDIV = TOTAL NUMBER OF DIVIDERS
            C         NDRY = TOTAL NUMBER OF DRYERS
```

```
              C         NHX = TOTAL NUMBER OF HEAT EXCHANGERS
              C         NMIX = TOTAL NUMBER OF DIVIDERS
              C         NRXR = TOTAL NUMBER OF REACTORS
              C         NOUT(J,I) = STREAM NUMBER EXITING UNIT J FROM OUTLET POSITION I
              C         NTEAR = NUMBER OF TEAR STREAMS
              C         NUNITS = TOTAL NUMBER OF UNITS
              C         PFDSTM(PTRSTM) = PRESSURE OF FEED (TEAR) STREAM, PSIA
              C         PRSTM(I) = PRESSURE OF STREAM I, PSIA
              C         Q(I) = ARRAY FOR TEXT CARDS
              C         RLNTH(I) = LENGTH OF REACTOR I, FT
              C         TFDSTM(TTRSTM) = TEMPERATURE OF FEED (TEAR) STREAM, DEG K
              C         TKSTM(I) = TEMPERATURE OF STREAM I, DEG K
              C
              C
              C
              C
     2              IF (NRUN.GT.1) RETURN
              C
              C              READ TEXT CARDS
              C
     5              READ 105,(Q(I),I=1,16)
    20          105 FORMAT (8A10)
    20              READ 100,   NRXR,NHX,NDIV,NMIX,NCDR,NSTMS,NTEAR,NPTS
    44          100 FORMAT(8I5)
              C
    44              NUNITS = NRXR + NHX + NDIV + NMIX + NCDR
              C
              C            READ PROCESS FLOWSHEET
              C
    51              JR = 0
    52              JHX = 0
    53              JCDR = 0
    54              DO 10 J = 1, NUNITS
    55              READ 110,      (IUNIT(J),KT(J),(IN(J,I),I = 1,3),(NOUT(J,I),I=1,2))
   110          110 FORMAT (7I5)
              C
              C           DETERMINE THE REACTOR NUMBER FOR FUTURE USE
              C
   110              IF(JR.EQ.NRXR) GO TO 50
   113              IF (KT(J).EQ.1) GO TO 55
   117              GO TO 50
   120           55 CONTINUE
   120              JR = JR + 1
   122              IRXR(JR) = IUNIT(J)
   127           50 CONTINUE
              C
              C            DETERMINE HX NUMBER FOR FUTURE USE
              C
   127              IF(JHX.EQ.NHX) GO TO 70
   132              IF(KT(J).EQ.2) GO TO 75
   136              GO TO 70
   137           75 CONTINUE
   137              JHX = JHX + 1
   141              IHX(JHX) = IUNIT(J)
   146           70 CONTINUE
              C
              C            DETERMINE COND NUMBER FOR FUTURE USE
              C
   146              IF(JCDR.EQ.NCDR) GO TO 80
   151              IF(KT(J).EQ.5) GO TO 85
   155              GO TO 80
   156           85 CONTINUE
   156              JCDR = JCDR + 1
   160              ICDR(JCDR) = IUNIT(J)
   165           80 CONTINUE
              C
              C           READ OTHER REQUIRED DATA FOR UNIT TYPE, FOR A REACTOR,
              C           ALSO READ THE LENGTH OF REACTOR
              C
   165              JJ = IUNIT(J)
   170              IF (KT(J).EQ.1) GO TO 60
   174              READ 112,      DUMDAT(JJ)
   203          112 FORMAT (F10.5)
   203              GO TO 65
   204           60 CONTINUE
   204              READ 111, DUMDAT(JJ), RLNTH(JR)
   216          111 FORMAT(2F10.5)
```

```
216      65 CONTINUE
216      10 CONTINUE
      C
      C           READ FEED STREAM INFORMATION
      C
221         READ 120,     IFD,TFDSTM,PFDSTM,(FFDSTM(I),I=1,N)
242     120 FORMAT (I5,2F10.3,/,6F10.5)
242         SUMF = 0.
243         DO 30 J = 1, N
245         FSTM(IFD,J) = FFDSTM(J)
253         SUMF = SUMF + FFDSTM(J)
257      30 CONTINUE
261         TTFSTM(IFD) = SUMF
264         TKSTM(IFD) = TFDSTM
267         PRSTM(IFD) = PFDSTM
      C
      C           READ ORDER OF UNIT CALCULATION
      C
272         READ 130,    (IORD(I), I=1,NUNITS)
306     130 FORMAT (20I5)
      C
      C           READ TEAR STREAM INFORMATION
      C
306         IF (NTEAR.EQ.0) GO TO 44
310         DO 40 J = 1, NTEAR
312         READ 120, ITR(J),TTRSTM,PTRSTM,(FTRSTM(I),I=1,N)
334         IS = ITR(J)
337         SUMF = 0.
340         DO 42 I = 1, N
342         FSTM(IS,I) = FTRSTM(I)
350         SUMF = SUMF + FTRSTM(I)
354      42 CONTINUE
356         TTFSTM(IS) = SUMF
361         TKSTM(IS) = TTRSTM
364         PRSTM(IS) = PTRSTM
367      40 CONTINUE
372      44 CONTINUE
372         RETURN
373         END


            SUBROUTINE HPREP
      C...
      C...
      C...  SUBROUTINE HPREP CALCULATES TEMPERATURE INDEPENDENT THERMODYNAMIC
      C...  CONSTANTS THAT ONLY NEED BE CALCULATED ONCE, BUT ARE USED
      C...  FREQUENTLY BY SUBSEQUENT TEMPERATURE DEPENDENT THERMODYNAMIC
      C...  CALCULATIONS.
      C...
      C              CALLED FROM INITAL
      C
      C...
  2         COMMON/HPASS/ HRX537(3),DELALF(3),DELBET(3),DELGT2(3),DEGOV2(3),
           1  HI537(3),HO(3),HRXT(3),CPAVG(5),GRX537(3),GI537(3),
           2  GO(3),GOVT(3),KCHEM(3),LL,RATE1(5),RATE2(5),IER,ILR
  2         COMMON/PARM/ N,M,TFDSTM,PFDSTM,P(5)
  2         COMMON/POINT/ IC(8)
  2         COMMON/STOIC/ A(3,10), DELA(3)
  2         COMMON/PDATA/ DUM22(990),GF537(45),HF537(45),HCOMB(45),
           1  ALPHA(45),BETA(45),GAMT2(45),GAMOV2(45)
      C
      C         NOTATION:
      C              DELA = DIFF IN STOICHIOMETRIC COEFFICIENTS
      C              DELALF = DIFF IN ALPHAS IN CP GAS
      C              DELBET = DIFF IN BETAS IN CP GAS
      C              DELGT2 = DIFF IN GAMT2 IN CP GAS
      C              GAMT2 = COEFF OF FORM  GAMMA*T*T
      C              DEGOV2 = DIFF IN GAMOV2 IN CP GAS
      C              GAMOV2 = COEFF OF FORM GAMMA/T
      C              HRX537 = HEAT OF REACTION AT 537 R
      C              GRX537 = FREE ENERGY OF RX AT 537 R
      C
  2         DO 12 J = 1, M
  4         DELA(J) = 0.0
  6         DELALF(J) = 0.0
 11         DELBET(J) = 0.0
```

```
  14          DELGT2(J) = 0.0
  17          DEGOV2(J) = 0.0
  22          HRX537(J) = 0.0
  25          GRX537(J) = 0.0
  30       12 CONTINUE
  33          DO 20 J = 1, M
  34          DO 10 I = 1, N
  35          ACOEFF = A(J,I)
  42          IF (ABS(ACOEFF).LT.0.001 ) GO TO 10
  50          NC = ID(I)
  53          DELA(J) = DELA(J) + ACOEFF
  61          DELALF(J) = DELALF(J) + ACOEFF*ALPHA(NC)
  71          DELBET(J) = DELBET(J) + ACOEFF*BETA(NC)
 102          DELGT2(J) = DELGT2(J) + ACOEFF*GAMT2(NC)
 112          DEGOV2(J) = DEGOV2(J) + ACOEFF*GAMOV2(NC)
 123          HRX537(J) = HRX537(J) + ACOEFF*HF537(NC)
 133          GRX537(J) = GRX537(J) + ACOEFF*GF537(NC)
 144       10 CONTINUE
 147       20 CONTINUE
        C
        C                 HI537 = CONST USED IN CALC OF HEAT OF
        C                         REACTION AT TEMP TK
        C                 GI537 = FREE ENERGY SIMILAR TC HI537
        C                 HO = CONST DEFINED BY FOLLOWING EQN
        C                      IS USED IN CALCULATING HEAT OF
        C                      REACTION AT TEMPERATURE TK
        C                 GO = FREE ENERGY SIMILAR TO HO
 151          CO 14 J = 1, M
 153          HI537(J) = DELALF(J)*537. + DELBET(J)/2.*537.*537. + DELGT2(J)/3.
             1  *537.*537.*537. - DEGOV2(J)/537.
 175          HO(J) = HRX537(J) - HI537(J)
 204          GI537(J) = HO(J)/537. - DELALF(J)*ALOG(537.) - DELBET(J)/2.*537.-
             1  DELGT2(J)/6.*537.*537. - DEGOV2(J)/2./537./537.
 233          GO(J) = GRX537(J)/537. - GI537(J)
 243       14 CONTINUE
 245          RETURN
 246          END


              SUBROUTINE DERV
        C
        C
        C          SUBROUTINE DERV CALLS THE INDIVIDUAL PROCESS SUBROUTINES
        C          IN THE SEQUENCE SPECIFIED BY THE ORDER OF UNIT CALCULATIONS.
        C
        C
   2          COMMON/T/L,NFIN,NRUN/Y/X1(5),X2(5),TK(5)/F/DX1DL(5),DX2DL(5),
             1  DTKDL(5)
   2          COMMON/PRTPLT/ IPLOT,NLINE,NPTS,Q(16),IPT
   2          COMMON/PARM/ N,M,TFDSTM,PFDSTM,P(5),IFD,ITR(10),Y(5,8)
   2          COMMON/INDAT/ NUNITS,NSTMS,NTEAR,IORD(15)
   2          COMMON/OUT/ TKOUT,PSIAOT,FOUT(8),FTOTOT
   2          COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
   2          COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
   2          COMMON/UNIT/ NRXR,NHX,NDIV,NMIX,IRXR(5),NCDR,RLNTH(5)
        C
        C           USE ORDERING OF UNIT CALCULATIONS (IORD) TO
        C           PERFORM STREAM OPERATIONS BETWEEN REACTORS AND
        C           THEN DETERMINE THE REACTOR*S ODE*S
        C
   2          DO 100 I = 1, NUNITS
   4          J = 0
   5       90 CONTINUE
   5          J = J + 1
   7          IF (IORD(I).EQ.IUNIT(J)) GO TO 95
  15          GO TO 90
  16       95 CONTINUE
  16          K = IUNIT(J)
  21          JKT = KT(J)
        C
        C           BYPASS ALL NONREACTOR CALCULATIONS DURING
        C           CALCULATION OF REACTOR PROFILE (I.E. AFTER
        C           FIRST CALL TO DERV)
        C
  24          IF ((IPT.GT.0).AND.(JKT.NE.1))GO TO 100
  35          GO TO (110,120,130,140,150),JKT
```

```
110 CONTINUE
    CALL RXR(K)
    GO TO 100
120 CONTINUE
    CALL HX(K)
    GO TO 100
130 CONTINUE
    CALL DIV(K)
    GO TO 100
140 CONTINUE
    CALL MIXER(K)
    GO TO 100
150 CONTINUE
    CALL COND(K)
100 CONTINUE
    RETURN
    END


    SUBROUTINE RXR(KK)
C...
C...
C         SUBROUTINE RXR CONTAINS THE DIFFERENTIAL EQUATIONS TO
C         BE SOLVED FOR EACH POINT ALONG THE REACTOR BEING CALCULATED
C
C              CALLED FROM DERV
C
C
C
      COMMON/T/L,NFIN,NRUN/Y/X1(5),X2(5),TK(5)/F/DX1DL(5),DX2DL(5),
     1  DTKDL(5)
      COMMON/HPASS/ HRX537(3),DELALF(3),DELBET(3),DELGT2(3),DEGOV2(3),
     1  HI537(3),HO(3),HRXT(3),CPAVG(5),GRX537(3),GI537(3),
     2  GO(3),GOVT(3),KCHEM(3),LL,RATE1(5),RATE2(5),IER,ILR
      COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
      COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
      COMMON/PARM/ N,M,TFDSTM,PFDSTM,P(5),IFD,ITR(10),Y(5,8)
      COMMON/UNIT/ NRXR,NHX,NDIV,NMIX,IRXR(5),NCDR,RLNTH(5)
      COMMON/OUT/ TKOUT,PSIAOT,FTOTOT
      COMMON/PRTPLT/ IPLOT,NLINE,NPTS,Q(16),IPT
C
C
C     NOTATION
C
C
C         AREA=CROSSECTIONAL AREA OF REACTOR, SQ.FT.
C         CPAVG(LL)=AVERAGE HEAT CAPACITY OF REACTOR LL AT THE GIVEN PT.
C         FSTM(I,1)=MOLAR FLOWRATE OF STREAM I, MOLES/HR.
C         FTOTOT=TOTAL MOLAR FLOWRATE LEAVING THE REACTOR
C         HRXT(1)=HEAT OF REACTION OF METHANATION REACTION
C         HRXT(2)=HEAT OF REACTION OF SHIFT REACTION
C         IER=STREAM NUMBER ENTERING REATOR
C         ILR=STREAM NUMBER LEAVING REACTOR
C         KK = UNIT NUMBER
C         LL = INDIVIDUAL REACTOR NUMBER
C         RLNTH(LL)=LENGTH OF REACTOR LL, FT.
C         TKOUT=TEMPERATURE OF STREAM LEAVING THE REACTOR, DEG K
C         P(LL)=PREASSURE OF REACTOR LL, TAKEN FROM INLET STREAM
C         PSIAOT=PRESSURE OF STREAM LEAVING THE REACTOR, PSIA
C
C
C
C
C      DETERMINE THE STREAM NUMBERS BEING USED
C
      IER = IN(KK,1)
      ILR = NOUT(KK,1)
      DO 10 J = 1, NRXR
   10 IF (IRXR(J).EQ.IUNIT(KK)) LL = J
      P(LL) = PRSTM(IER)
      AREA = DUMDAT(KK)
      IF(IPT.EQ.0) TK(LL) = TKSTM(IER)
      CALL YSFLOW
      CALL HRXYCP
      CALL RATE
C
      TERM3 = FSTM(IER,1)*100./AREA/RLNTH(LL)
      DX1DL(LL) = RATE1(LL)/TERM3
      DX2DL(LL) = RATE2(LL)/TERM3
```

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      C
            DTKDL(LL) = (-HRXT(1)*DX1DL(LL) - HRXT(2)*DX2DL(LL))/
         1    (FTOTOT/FSTM(IER,1)*CPAVG(LL))
            TKSTM(ILR) = TKOUT
            PRSTM(ILR) = PSIAOT
            TTFSTM(ILR) = FTOTOT
            RETURN
            END


            SUBROUTINE HX(KK)
      C
      C
      C        SUBROUTINE HX CHANGES THE TEMPERATURE OF A PROCESS
      C        STREAM TO A SPECIFIED VALUE, WITHOUT INVOLVING
      C        DETAILED HEAT EXCHANGER CALCULATIONS.
      C
      C              CALLED FROM DERV
      C
      C
            COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
            COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
            COMMON/PARM/ N,M,TFDSTM,PFDSTM,P(5),IFD,ITR(10),Y(5,8)
            COMMON/UNIT/ NRXR,NHX,NDIV,NMIX,IRXR(5),NCDR,RLNTH(5),IHX(5),
         1               ICDR(5),QCOND(5),QHX(5)
            COMMON/POINT/ ID(8)
            DIMENSION YY(8)
      C
      C
      C     NOTATION
      C
      C        IEH = STREAM NUMBER ENTERING HX
      C        ILH = STREAM NUMBER LEAVING HX
      C        DUMDAT = NEW TEMPERATURE OF STREAM, DEG K
      C
      C
            IEH = IN(KK,1)
            ILH = NOUT(KK,1)
            TKSTM(ILH) = DUMDAT(KK)
            PRSTM(ILH) = PRSTM(IEH)
            DO 10 K = 1, NHX
         10 IF(IHX(K).EQ.IUNIT(KK)) LL=K
            DO 2 J = 1, N
            YY(J) = FSTM(IEH,J)/TTFSTM(IEH)
          2 FSTM(ILH,J) = FSTM(IEH,J)
            TTFSTM(ILH) = TTFSTM(IEH)
      C
      C          CALCULATE THE HEAT DUTY FOR THE EXCHANGER
      C
            TIEH = TKSTM(IEH) * 1.8
            TILH = TKSTM(ILH) * 1.8
      C
      C          CALCULATE CPAVG IN BTU/(LBMOLE)(DEG R)
      C
            CALL HGAS (ID,N,TIEH,YY,CPAVG,HIEH)
            CALL HGAS (ID,N,TILH,YY,CPAVG,HILH)
      C
      C          CALCULATE QHX IN BTU/(HR)
      C
            QHX(LL) = CPAVG * (TILH  - TIEH) * TTFSTM(IEH)
            RETURN
            END


            SUBROUTINE DIV(I)
      C
      C
      C        SUBROUTINE DIV ACTS AS A STREAM DIVIDER
      C
      C              CALLED FROM DERV
      C
            COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
            COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
            COMMON/PARM/ N,M,TFDSTM,PFDSTM,P(5),IFD,ITR(10),Y(5,8)
      C
```

```
         C      NOTATION
         C
         C         DUMDAT = FRACTION OF INLET STREAM BEING
         C                DIVERTED TO OUTLET STREAM NO. 1 (DIVFRC)
         C         FSUM1 (FSUM2) = TOTAL FLOWRATE OF STREAM LEAVING
         C                   FROM POSITION 1 (2)
         C         IED = STREAM NUMBER ENTERING DIVIDER
         C         IOD1 = STREAM NUMBER LEAVING DIVIDER FROM POSITION 1
         C         IOD2 = STREAM NUMBER LEAVING DIVIDER FROM POSITION 2
         C
         C
     6          DIVFRC = DUMDAT(I)
    11          IED = IN(I,1)
    16          IOD1 = NOUT(I,1)
    22          IOD2 = NOUT(I,2)
    27          FSUM1 = 0.
    30          FSUM2 = 0.
    31          DO 2 J = 1, N
    33          FSTM(IOD1,J) = FSTM(IED,J) * DIVFRC
    44          FSTM(IOD2,J) = FSTM(IED,J) * (1. - DIVFRC)
    57          FSUM1 = FSUM1 + FSTM(IOD1,J)
    64          FSUM2 = FSUM2 + FSTM(IOD2,J)
    71        2 CONTINUE
    73          TTFSTM(IOD1) = FSUM1
    76          TTFSTM(IOD2) = FSUM2
   101          TKSTM(IOD1) = TKSTM(IED)
   106          PRSTM(IOD1) = PRSTM(IED)
   113          TKSTM(IOD2) = TKSTM(IED)
   120          PRSTM(IOD2) = PRSTM(IED)
   125          RETURN
   126          END


                SUBROUTINE MIXER(I)
         C
         C
         C         SUBROUTINE MIXER COMBINES THE CONTENTS OF TWO OR THREE
         C         STREAMS, AND THEN DETERMINES THE NEW STREAM TEMPERATURE
         C
         C               CALLED FROM DERV
     6          COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
     6          COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
     6          COMMON/UNIT/ NRXR,NHX,NDIV,NMIX
     6          COMMON/PARM/ N,M,TFDSTM,PFDSTM,P(5),IFD,ITR(10),Y(5,8)
     6          COMMON/FLAG/ FLAG1,FLAG2
     6          COMMON/POINT/ ID(8)
     6          DIMENSION DMCOMP(8),IEM(4),SUMF(8)
         C
         C
         C      NOTATION
         C
         C         DMCOMP(J) = DUMMY VARIABLE FOR THE MOL FRACTION OF
         C                   COMPOUND J IN STREAM ILM
         C         HOUT = ENTHALPY OF OUTLET STREAM, CAL
         C         HSUM = SUM OF INLET STREAM ENTHALPIES, CAL
         C         IEM(K) = STREAM NUMBER ENTERING MIXER FROM POSITION K
         C         ILM = STREAM NUMBER LEAVING MIXER
         C         K = COUNTER FOR THE INLET STREAM POSITIONS, NUMBERED 1, 2, OF 3
         C         SUMF(J) = SUM OF EACH COMPOUND J IN NEW STREAM, LBMOL/HR
         C         TKDUM = DUMMY VARIABLE FOR THE TEMP OF ONE OF THE ENTERING
         C                STREAMS, DEG R
         C         TNEW = TEMPERATURE OF OUTLET STREAM, DEG R
         C         TSUMF = TOTAL FLOW OF NEW STREAM, LBMOL/HR
         C
         C
         C
         C            DETERMINE STREAM NUMBERS ENTERING AND LEAVING MIXER
         C
     6          DO 1 K = 1, 3
     7          IEM(K) = IN(I,K)
    15        1 CONTINUE
    17          ILM = NOUT(I,1)
         C
         C            SUM COMPONENT FLOWS OF ALL STREAMS AND GET NEW TOTAL FLOW
         C
    24          TSUMF = 0.
```

```
      DO 3 J = 1, N
      SUMF(J) = 0.
      DO 5 K = 1, 3
      IED = IEM(K)
      IF(IED.EQ.0) GO TO 5
      SUMF(J) = SUMF(J) + FSTM(IED,J)
    5 CONTINUE
      TSUMF = TSUMF + SUMF(J)
      FSTM(ILM,J) = SUMF(J)
    3 CONTINUE
      TTFSTM(ILM) = TSUMF
C
C          CALCULATE INDIVIDUAL STREAM ENTHALPIES
C          CALCULATE NEW OUTLET STREAM TEMPERATURE
C
      THI = 0.
      TLO = 0.
      HSUM = 0.
      DO 7 K = 1, 4
      IF (K.EQ.4) GO TO 6
      IED = IEM(K)
      IF(IED.EQ.0) GO TO 7
      TKDUM = TKSTM(IED)*1.8
      GO TO 8
    6 CONTINUE
      IED = ILM
    8 CONTINUE
      DO 9 J = 1, N
C
C          CALCULATE STREAM COMPOSITION
C
      DMCOMP(J) = FSTM(IED,J)/TTFSTM(IED)
    9 CONTINUE
C
C          CALCULATE INDIVIDUAL STREAM ENTHALPIES
C
      IF (K.EQ.4) GO TO 7
C
C        KEEP TRACK OF THE HI AND LO TEMPERATURES
C
      CALL HGAS(ID,N,TKDUM,DMCOMP,CPIGM,HDUM)
      CALL HILO (K,TKDUM,THI,TLO,HDUM,HHI,HLO)
      HSUM = HSUM + HDUM*TTFSTM(IED)
    7 CONTINUE
      HOUT = HSUM/TSUMF
C
C        CALCULATE TEMPERATURE OF STREAM LEAVING MIXER
C
      CALL TCALC (ID,N,DMCOMP,THI,TLO,HHI,HLO,TNEW,HOUT)
      TKSTM(ILM) = TNEW/1.8
      IEDD = IN(I,1)
      PRSTM (ILM) = PRSTM(IEDD)
      RETURN
      END


      SUBROUTINE HILO(K,XDUM,XHI,XLO,YDUM,YHI,YLO)
C
C          THIS SUBROUTINE KEEPS TRACK OF PRESENT HI AND LO TEMP VALUES
C          AND THEIR CORRESPONDING ENTHALPIES
C
C        CALLED FROM MIXER
C
C     NOTATION
C
C        HHI = HI ENTHALPY VALUE
C        HLO = LO ENTHALPY VALUE
C        K = POSITION NUMBER FOR INLET STREAM
C        XDUM = PRESENT TEMP VALUE BEING CONSIDERED
C        XHI = HI TEMP VALUE
C        XLO = LO TEMP VALUE
C        YDUM = PRESENT ENTHALPY VALUE BEING CONSIDERED
C
C
C
      IF(K.GT.1) GO TO 12
```

```
    15          XLO = XDUM
    16          YLO = YDUM
    17          GO TO 18
    20       12 CONTINUE
    20          IF (K.GT.2) GO TO 16
    23          IF (XDUM.GE.XLO) GO TO 13
    26          GO TO 15
    27       13 CONTINUE
    27          XHI = XDUM
    30          YHI = YDUM
    31       15 CONTINUE
    31          IF (XDUM.LT.XLO) GO TO 14
    34          GO TO 18
    35       14 CONTINUE
    35          XHI = XLO
    36          YHI = YLO
    40          XLO = XDUM
    40          YLO = YDUM
    42          GO TO 18
    42       16 CONTINUE
    42          IF (XDUM.GE.XHI) GO TO 17
    45          GO TO 19
    46       17 CONTINUE
    46          XHI = XDUM
    47          YHI = YDUM
    50       19 CONTINUE
    50          IF (XDUM.LE.XLO) GO TO 21
    53          GO TO 18
    54       21 CONTINUE
    54          XLO = XDUM
    55          YLO = YDUM
    56       18 CONTINUE
    56          RETURN
    57          END


                SUBROUTINE COND(KK)
     6          COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
     6          COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
     6          COMMON/PARM/ N,M,TFDSTM,PFDSTM,P(5),IFD,ITR(10),Y(5,8)
        C
     6          COMMON/UNIT/ NRXR,NHX,NDIV,NMIX,IRXR(5),NCDR,RLNTH(5),IHX(5),
               1            ICDR(5),QCOND(5),QHX(5)
     6          COMMON/POINT/ ID(8)
        C            SUBROUTINE COND SIMULATES A CONDENSOR UNIT.  GIVEN A
        C            PARTICULAR STREAM AND THE DESIRED PERCENTAGE OF WATER
        C            REMOVAL, COND WILL CALCULATE THE TEMPERATURE AND THE
        C            WATER CONTENT OF BOTH STREAMS LEAVING THE UNIT.
        C            ** NO RATING OF THE CONDENSOR IS PROVIDED **
        C            THE WATER VAPOR PRESSURE IS DETERMINED FROM THE
        C            ANTOINE EQUATION.
        C
     6          DIMENSION T(25),YIEC(8),YILC1(8)
        C
        C
        C       NOTATION
        C
        C          IED = STREAM NUMBER ENTERING DRYER
        C          ILD1 = STREAM NUMBER LEAVING DRYER FROM POSITION 1
        C          ILD2 = STREAM NUMBER LEAVING DRYER FROM POSITION 2
        C                 ( CONTAINS WATER ONLY )
        C
     6          LOOP = 1
     7          TOL = 0.5
    11          IEC = IN(KK,1)
    15          ILC1 = NOUT(KK,1)
    22          ILC2 = NOUT(KK,2)
    26          DO 5 K = 1, NCDR
    30        5 IF(ICDR(K).EQ.IUNIT(KK)) LL=K
    41          CFRAC = DUMDAT(KK)
    44          PCOND = PRSTM(IEC)
    47          FTOL = FSTM(IEC,4) * CFRAC
        C            INITIALLY SET THE FLOW RATES OUT OF THE CONDENSOR*S TWO STMS
        C
    54          DO 10 I = 1, N
    56          FSTM(ILC1,I) = FSTM(IEC,I)
```

```
   10 FSTM(ILC2,I) = 0.
C
C           CALCULATE THE FLOWRATE OF THE INERTS
      FINRT = TTFSTM(IEC) - FSTM(IEC,4)
C           ASSUME AN INITIAL TEMPERATURE
C
      T(LOOP) = 500.
   20 CONTINUE
C           CALCULATE WATER VAPOR PRESSURE AT THE ASSUMED TEMPERATURE
C           USING THE ANTOINE EQUATION (CONSTANTS TAKEN FROM PRS),IN PSIA
C
      VPH2O = (EXP(18.3036 - 3816.44/(T(LOOP) - 46.13))) * 14.7/760.
C           CALCULATE INERTS PRESSURE, IN PSIA
C
      PINRT = PCOND - VPH2O
      IF (PINRT.LE.0.) GO TO 25
C           CALCULATE LBMOLES OF STEAM CONDENSING
C
      FVAP = FINRT * VPH2O / PINRT
      FCOND = FSTM(IEC,4) - FVAP
C           CHECK FOR CONVERGENCE
C
      DEL = FCOND - FTOL
      ADEL = ABS(DEL)
      IF (ADEL.LE.TOL) GO TO 30
C           CALL FALSE POSITION ROUTINE TO CONVERGE TO A SOLUTION
C
      CALL FALPOS (T(LOOP),DEL,LOOP,TNEW)
      LOOP = LOOP + 1
      T(LOOP) = TNEW
      IF (LOOP.EQ.26) GO TO 40
      GO TO 20
   25 CONTINUE
C           USE THIS ROUTE IF THE VPH2O IS .GT. THE CONDENSOR PRESS.
C
      T(LOOP) = T(LOOP) - 100.
      GO TO 20
   30 CONTINUE
      TKSTM(ILC1) = T(LOOP)
      TKSTM(ILC2) = T(LOOP)
      PRSTM(ILC1) = PCOND
      PRSTM(ILC2) = PCOND
      FSTM(ILC1,4) = FVAP
      FSTM(ILC2,4) = FCOND
      TTFSTM(ILC1) = 0.
      TTFSTM(ILC2) = 0.
      DO 35 I = 1, N
      TTFSTM(ILC1) = TTFSTM(ILC1) + FSTM(ILC1,I)
      TTFSTM(ILC2) = TTFSTM(ILC2) + FSTM(ILC2,I)
   35 CONTINUE
C
C       CALCULATE THE MOLE FRACTION FOR THE STREAMS
      DO 45 I = 1, N
      YIEC(I) = FSTM(IEC,I) / TTFSTM(IEC)
      YILC1(I) = FSTM(ILC1,I) / TTFSTM(ILC1)
   45 CONTINUE
C
C           CALCULATE HEAT DUTY OF CONDENSOR, QCOND, IN BTU/HR
      TRIEC = TKSTM(IEC) * 1.8
      CALL HGAS(ID,N,TRIEC,YIEC,CPIEC,HIEC)
      TRILC1 = TKSTM(ILC1) * 1.8
      CALL HGAS(ID,N,TRILC1,YILC1,CPILC1,HILC1)
      CALL HWATER(TKSTM(ILC2),HW)
      QCOND(LL) = (HIEC*TTFSTM(IEC)) - (HILC1*TTFSTM(ILC1))
     1      - (HW*TTFSTM(ILC2))
      RETURN
   40 WRITE (NO,100)
  100 FORMAT (/,10X,*COND IN TROUBLE*)
      LM1 = LOOP - 1
      RETURN
      END
```

```
      SUBROUTINE HWATER(TEMPK,HW)
C
C
C          SUBROUTINE HWATER CALCULATES THE SPECIFIC ENTHALPY OF
C          LIQUID WATER IN UNITS OF BTU/LBMOLE.  THE BASIS IS H = 0 AT
C          TBASE = 255.6 K(460. R).  NOTE THAT THE TEMPERATURE T
C          IS IN DEGREES K.
C
      TBASE = 460./1.8
      CPAVE = (CP2(TEMPK) + CP2(TBASE))/2.
      HW = CPAVE*(TEMPK - TBASE) * 18.
      RETURN
      END


      FUNCTION CP2(TEMPK)
C
C
C          FUNCTION CP2 CALCULATES THE HEAT CAPACITY OF LIQUID
C          WATER IN BTU/LBLK AS A FUNCTION OF TEMPERATURE.
C          NOTE THAT THE TEMPERATURE IS IN DEGREES K.
C
      CP2 = 1.8 + 0.13 * (TEMPK - 293.)/(508. - 293.)
      RETURN
      END


      SUBROUTINE FALPOS (T,DELTA,LOOP,TNEW)
C
C...  THIS ROUTINE USES A BRACKETTING METHOD TO
C...  CONVERGE UPON THE DEPENDENT VALUE OF A FUNCTION
C...  WHEN IT CROSSES THE X-AXIS AT POINT A.
C...  LETTING     F = F(P)   ,
C...  AN INITIAL ESTIMATE OF THE ROOT (P1) IS
C...  USED TO ARRIVE AT ANOTHER ESTIMATE (P2)
C...  SUCH THAT F1 AND F2 ARE OF OPPOSITE SIGN.
C...  ADDITIONAL TRIAL VALUES (P(1)) ARE CALCULATED
C...  FROM THE EQUATION
C...        P(1) = P1 - ((P2-P1)/F2-F1)*F1
C...  AS THE PROCEDURE CONVERGES, THE VALUES
C...  FOR (P1,F1) OR (P2,F2) WILL BE REPLACED
C...  BY THE NEWLY GENERATED COORDINATES FOR
C...  A MORE ACCURATE ESTIMATE.
C
C
C...  INITIALIZE VALUES FOR 1ST RUN THROUGH THE ROUTINE
C
      IF(LOOP.NE.1) GO TO 5
      TPOS = 0.
      TNEG = 0.
      DELTAP = 0.
      DELTAN = 0.
    5 CONTINUE
C
C...  DETERMINE THE PLACEMENT OF THE PRESENT DEPENDENT VALUE,
C...  ON THE POSITIVE OR NEGATIVE SIDE OF X-AXIS
C
      IF(DELTA.LT. 0.) GO TO 10
      TPOS = T
      DELTAP = DELTA
      GO TO 12
   10 CONTINUE
      TNEG = T
      DELTAN = DELTA
   12 CONTINUE
C
C...  Q-- HAS THE DEPENDENT VARIABLE BRACKETTED ZERO
C...          Y--CALCULATE PNEW VIA THE GIVEN EQ.
C...                 N--INCREMENT P FOR A NEW PNEW
C...
C
      IF((DELTAN.NE.0.).AND.(DELTAP.NE.0.)) GO TO 20
      IF(DELTAN.EQ.0.) GO TO 22
      TNEW = T - 100.
      RETURN
```

```
   42        22 CONTINUE
   42           TNEW = T + 100.
   44           RETURN
   44        20 CONTINUE
   44           TNEW = TNEG - ((TPOS-TNEG)/(DELTAP-DELTAN))*DELTAN
   54           RETURN
   55           END


                SUBROUTINE YSFLOW
          C...
          C...
          C...  SUBROUTINE YSFLOW CALCULATES MOLE FRACTION AND THE OUTLET VECTOR
          C...  OF TEMP., PRESS, AND FLOW OF EACH SPECIES IN MOLES PER HR.  VECTOR
          C...  IS CALCULATED AT EACH PT. IN REACTOR AND OVERWRITTEN SUCH THAT
          C...  ONLY OUTLET IS AVAILABLE FOR SUBSEQUENT USE.
          C...
          C              CALLED FROM RXR
          C...
    2           COMMON/T/L,NFIN,NRUN/Y/X1(5),X2(5),TK(5)/F/DX1DL(5),DX2DL(5),
               1  DTKDL(5)
    2           COMMON/STOIC/ A(3,10), DELA(3)
    2           COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
    2           COMMON/OUT/ TKOUT,PSIAOT,FTOTOT
    2           COMMON/PARM/ N,M,TFDSTM,PFDSTM,P(5),IFD,ITR(10),Y(5,8)
    2           COMMON/HPASS/ HRX537(3),DELALF(3),DELBET(3),DELGT2(3),DEGOV2(3),
               1  HI537(3),HO(3),HRXT(3),CPAVG(5),GRX537(3),GI537(3),
               2  GO(3),GOVT(3),KCHEM(3),LL,RATE1(5),RATE2(5),IER,ILR
    2           DIMENSION TOTMIN(5)
          C
          C
    2           JE = IER
    4           JL = ILR
    5           TKOUT = TK(LL)
   10           PSIAOT = PRSTM(JE)
   13           TOTMIN(LL) = TTFSTM(JE)/FSTM(JE,1)
   24           TOTMOL = TOTMIN(LL) + DELA(1)*X1(LL) + DELA(2)*X2(LL)
   41           FTOTOT = TOTMOL * FSTM(JE,1)
   47           DO 10 I = 1, N
   50           FSTM(JL,I) = FSTM(JE,I) + FSTM(JE,1)*(A(1,I)*X1(LL)+A(2,I)*X2(LL))
  103           Y(LL,I) = FSTM(JL,I)/FTOTOT
  115        10 CONTINUE
  117           RETURN
  120           END


                  SUBROUTINE HRXYCP

          C
          C           SUBROUTINE HRXYCP CALCULATES HEAT OF REACTION, FREE ENERGY
          C           OF REACTION, AND THE AVERAGE HEAT CAPACITY AT THE POINT OF
          C           CALCULATION UTILIZING DATA CALCULATED IN HPREP
          C
          C                 CALLED FROM RXR
    2             REAL KCHEM
    2           COMMON/T/L,NFIN,NRUN/Y/X1(5),X2(5),TK(5)/F/DX1DL(5),DX2DL(5),
               1  DTKDL(5)
    2             COMMON/HPASS/HRX537(3),DELALF(3),DELBET(3),DELGT2(3),DEGOV2(3),
               1  HI537(3),HO(3),HRXT(3),CPAVG(5),GRX537(3),GI537(3),
               2  GO(3),GOVT(3),KCHEM(3),LL,RATE1(5),RATE2(5),IER,ILR
    2           COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
    2           COMMON/PARM/ N,M,TFDSTM,PFDSTM,P(5),IFD,ITR(10),Y(5,8)
    2             COMMON /PDATA/ DUM22(990), GF537(45), HF537(45), HCOMB(45),
               1                 ALPHA(45), BETA(45), GAMT2(45), GAMOV2(45)
    2           COMMON/POINT/ ID(8)
          C
          CC...                              HRXT = HEAT OF REACTION AT TK IN
          CC...                                     CAL / G MOLE
          CC...                              GOVT = FREE ENERGY OF RX AT TK OVER T
    2           JE = IER
    4           JL = ILR
    5           TT = TK(LL) * 1.8
   11            DO 10 J=1,M
   12            HRXT(J) = HO(J) + DELALF(J)*TT + DELBET(J)/2.*TT*TT + DELGT2(J)
               *  /3.*TT*TT*TT - DEGOV2(J)/TT
```

```
          HRXT(J) = HRXT(J)/1.8
          GOVT(J) = GO(J) + HO(J)/TT - DELALF(J)*ALOG(TT) - DELBET(J)/2.*TT
     *     - DELGT2(J)/6.*TT*TT - DEGOV2(J)/2./TT/TT
          KCHEM(J) = EXP ( - GOVT(J)/1.987 )
   10 CONTINUE
CC...                                   CPAVG = HEAT CAPACITY OF ALL COMPOUND
CC...                                         IN THE REACTOR AT THE POINT OF
CC...                                         CALCULATION AT TEMP TT
CC...                                         IN CAL / G MOLE / DEG C
      CPAVG(LL) = 0.
        DO 11 I=1,N
        NC = ID(I)
      CPAVG(LL) = CPAVG(LL) + Y(LL,I)*(ALPHA(NC) + BETA(NC)*TT +
     1      GAMT2(NC)*TT*TT + GAMOV2(NC)/TT/TT)
   11 CONTINUE
        RETURN
        END


        SUBROUTINE RATE
C
C
C          SUBROUTINE RATE DETERMINES THE RATE OF REACTION TAKING
C          PLACE AT THE POINT OF CALCULATION.  THE METHANATION RATE
C          EQUATION IS OF THE FORM OF LEE*S EQUATION, WITH THE
C          RATE CONSTANT DETERMINED FROM EXAMINATION OF PILOT PLANT
C          DATA AS PRESENTED BY LEPPIN.  A NEGLIGIBLE SHIFT REACTION
C          IS ASSUMED FOR LOW CO CONCENTRATIONS.  LEE*S EQUATION WAS
C          DETERMINED FROM EXPERIMENTAL DATA BETWEEN THE TEMPERATURES
C          OF 547 AND 755 DEG K, USING 1/4IN HARSHAW NI-0104T
C          NICKEL CATALYST.  THEREFORE ANY GRID POINT TEMPERATURE
C          OUTSIDE THESE BOUNDS SHOULD BE EXAMINED FOR POSSIBLE ERROR.
C
C                 CALLED FROM RXR
C
       COMMON/T/L,NFIN,NRUN/Y/X1(5),X2(5),TK(5)/F/DX1DL(5),DX2DL(5),
     1   DTKDL(5)
       COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
       COMMON/HPASS/ HRX537(3),DELALF(3),DELBET(3),DELGT2(3),DEGOV2(3),
     1   HI537(3),HO(3),HRXT(3),CPAVG(5),GRX537(3),GI537(3),
     2   GO(3),GOVT(3),KCHEM(3),LL,RATE1(5),RATE2(5),IER,ILR
       COMMON/PARM/ N,M,TFDSTM,PFDSTM,P(5),IFD,ITR(10),Y(5,8)
        REAL KCHEM,KP
C
C
C      NOTATION
C
C          JE = STREAM NUMBER ENTERING REACTOR
C          JL = STREAM NUMBER LEAVING REACTOR
C          PCO,PH2... = PARTIAL PRESSURE OF CO,H2,..., PSIA
C          RATE1 = RATE OF METHANATION REACTION, CO + 3H2 = CH4 + H2O
C                  IN LBMOL/HR/CU FT CAT
C                  IN LBMOL/HR/CU FT CAT
C          RATE2 = RATE OF SHIFT REACTION, CO + H2O = CO2 + H2
       JE = IER
       JL = ILR
       TT = TK(LL)
       PCO  = Y(LL,1)*P(LL)
       PH2  = Y(LL,2)*P(LL)
       PCH4 = Y(LL,3)*P(LL)
       PH2O = Y(LL,4)*P(LL)
       PCO2 = Y(LL,5)*P(LL)
       IF (PH2.LE.0.) GO TO 8
       GO TO 10
    8  CONTINUE
       PH2 = 0.001*P(LL)
   10  CONTINUE
        KP=KCHEM(1)/14.69/14.69
       A = PCH4*PH2O/PCO/PH2/PH2/PH2/KP
       RC1 = 79.4 * EXP(-3473./TT)
       RTE1= RC1*PCO*SQRT(PH2)*(1-A)/(1+0.1*PH2+0.05*PCH4)
       RTE2 = 0.
        IF (RTE1 .LT.0.0) RTE1 =0.0
        IF (RTE2 .LT.0.0) RTE2 =0.0
       RATE1(LL) = RTE1
       RATE2(LL) = RTE2
```

```
 135          RETURN
 136          END


              SUBROUTINE CPMEAN(ID,NC,THI,TLO,Y,CPIGM)
       C...
       C...   THIS SUBROUTINE CALCULATES THE INTEGRATED MEAN IDEAL GAS HEAT
       C...   CAPACITY BETWEEN TWO TEMPERATURES THI AND TLO.
       C
       C               CALLED FROM HGAS
       C
       C...
       C...      INPUT
       C...         ID     ARRAY WHICH HOLDS THE IDENTIFICATION NUMBERS OF THE
       C...                SPECIES OF INTEREST.  FOR EXAMPLE, FOR THE ORDER
       C...                CARBON MONOXIDE, HYDROGEN, METHANE, WATER, CARBON
       C...                DIOXIDE
       C...                        ID (1) = 4
       C...                        ID (2) = 3
       C...                        ID (3) = 13
       C...                        ID (4) = 12
       C...                        ID (5) = 5
       C...         NC     NUMBER OF COMPONENTS IN GAS
       C...         THI    HIGH TEMPERATURE OF INTEREST IN R.
       C...         TLO    LOW TEMPERATURE OF INTEREST IN R.
       C...         Y      MOLE FRACTION ARRAY IN THE SAME ORDER AS THE SPECIES
       C...                HAVE BEEN SET UP IN THE ID ARRAY.
       C...      OUTPUT
       C...         CPMEAN INTEGRATED MEAN IDEAL GAS HEAT CAPACITY IN
       C...                BTU/LB MOLE R  OR CAL/G MOLE K
       C...
  11            COMMON /PDATA/ DUM22(990), GF537(45), HF537(45), HCOMB(45),
               1              ALPHA(45), BETA(45), GAMT2(45), GAMOV2(45)
  11          DIMENSION ID(8), Y(8)
  11          AMIX = 0.0
  12          BMIX = 0.0
  13          GT2MIX = 0.0
  14          GOVMIX = 0.0
  15          DO 1 I = 1, NC
  16          J = ID(I)
  21          AMIX = AMIX + Y(I)*ALPHA(J)
  27          BMIX = BMIX + Y(I)*BETA(J)
  35          GT2MIX = GT2MIX + Y(I)*GAMT2(J)
  42          GOVMIX = GOVMIX + Y(I)*GAMOV2(J)
  50        1 CONTINUE
  52          CPIGM = AMIX + 0.5*BMIX*(THI+TLO) + GT2MIX/3.*
             1 (THI*THI + THI*TLO + TLO*TLO) + GOVMIX/THI/TLO
  70          RETURN
  70          END


              SUBROUTINE TCALC(ID,NC,Y,T1,T2,H1,H2,T,H)
       C...
       C...
       C...
       C...   SUBROUTINE TCALC CALCULATES THE TEMPERATURE OF A GAS STREAM
       C...   GIVEN ITS SPECIFIC ENTHALPY.  IT IS USED WHEN TWO GAS STREAMS
       C...   ARE COMBINED TO GIVE A NEW GAS STREAM.  AN INTERVAL HALVING
       C...   ITERATION METHOD IS USED TO CONVERGE TO THE CORRECT TEMPERATURE.
       C...
       C               CALLED FROM MIXER
       C
       C...
       C...   INPUT
       C...      ID        ARRAY WHICH HOLDS THE IDENTIFICATION NUMBERS
       C...                FOR THE COMPONENTS OF INTEREST.  FOR EXAMPLE,
       C...                FOR THE ORDER CO, H2, CH4, H2O, AND CO2
       C...                        ID(1) =  4
       C...                        ID(2) =  3
       C...                        ID(3) = 13
       C...                        ID(4) = 12
       C...                        ID(5) =  5
       C...      NC        NUMBER OF COMPONENTS IN GAS
       C...      Y         MOLE FRACTION ARRAY IN THE SAME ORDER AS THE
       C...                COMPONENTS HAVE BEEN SET UP IN THE ID ARRAY
       C...      T1,T2     INITIAL GUESSES OF TEMPERATURE IN R
       C...      H1,H2     SPECIFIC ENTHALPIES OF GAS AT GUESSED TEMPERATURES
```

```
          C...                T1 AND T2 IN UNITS OF BTU/LB-MOLE
          C...      H         SPECIFIC ENTHALPY OF COMBINED GAS STREAM IN BTU/LB-MOLE
          C...    OUTPUT
          C...      T         CALCULATED TEMPERATURE OF COMBINED GAS STREAM IN R.
          C...
  14              DIMENSION ID(8), Y(8)
  14              IF (H2.NE.H1) GO TO 1
  16              TEST = T1
  17              GO TO 2
  20            1 TEST = (H-H1)*(T2-T1)/(H2-H1) + T1
  31            2 LOOP = 0
  32              FLAGM = -1.
  34              FLAGP = -1.
  35              DT = 10.
  37           50 LOOP = LOOP + 1
  41              IF (LOOP.GT.200) GO TO 101
  44              CALL HGAS (ID,NC,TEST,Y,CPIGM,HCALC)
  50              PCERR = ABS((HCALC-H)/H*100.)
  61              IF (PCERR.LT.0.1) GO TO 100
  67              IF (HCALC-H) 10,10,20
  73           10 IF (FLAGP.LT.0.) GO TO 11
  76              DT = DT/2.
 100           11 TEST = TEST + DT
 102              FLAGM = 1.
 104              GO TO 50
 104           20 IF (FLAGM.LT.0.) GO TO 21
 107              DT = DT/2.
 111           21 TEST = TEST - DT
 113              FLAGP = 1.
 115              GO TO 50
 115          100 T = TEST
 117              RETURN
 120          101 PRINT 150
 124          150 FORMAT (10X,21HENDLESS LOOP IN TCALC)
 124              STOP
 126              END


                  SUBROUTINE HGAS (ID,NC,T,Y,CPIGM,H)
  11              DIMENSIOK ID(8), Y(8)
  11              TBASE = 460.
          C...
          C...
          C...    SUBROUTINE HGAS CALCULATES THE SPECIFIC ENTHALPY OF A GAS
          C...    STREAM IN UNITS OF BTU/LB-MOLE.  THE BASIS FOR ALL CALCULATIONS
          C...    IS THAT ALL COMPONENTS HAVE H = 0 AT TBASE = 460 R.  IT SHOULD BE
          C...    NOTED THAT HGAS IS ONLY VALID IF NO REACTIONS OCCUR AND IF THE
          C...    HEAT OF MIXING OF THE GAS COMPONENTS IS ZERO.  NOTE ALSO THAT THE
          C...    TEMPERATURE T IS IN DEGREES R.
          C...
          C               CALLED FROM TCALC AND MIXER
          C
  12              CALL CPMEAN (ID,NC,T,TBASE,Y,CPIGM)
  15              H = CPIGM*(T-TBASE)
  24              RETURN
  24              END


                  SUBROUTINE PRINT(NI,NO)
   6              REAL IL
   6              REAL L,KCHEM
   6              COMMON/T/L,NFIN,NRUN/Y/X1(5),X2(5),TK(5)/F/DX1DL(5),DX2DL(5),
                 1  DTKDL(5)
   6              COMMON/STOIC/ A(3,10), DELA(3)
   6              COMMON/PRTPLT/ IPLOT,NLINE,NPTS,Q(16),IPT
   6              COMMON/OUT/ TKOUT,PSIAOT,FOUT(8),FTOTOT
   6              COMMON/POINT/ ID(8)
   6              COMMON/PDATA/ DUM22(990),GF537(45),HF537(45),HCOMB(45),
                 1  ALPHA(45),BETA(45),GAMT2(45),GAMOV2(45)
   6              COMMON/HPASS/ HRX537(3),DELALF(3),DELBET(3),DELGT2(3),DEGOV2(3),
                 1  HI537(3),HO(3),HRXT(3),CPAVG(5),GRX537(3),GI537(3),
                 2  GO(3),GOVT(3),KCHEM(3),LL,RATE1(5),RATE2(5),IER,ILR
   6              COMMON/INDAT/ NUNITS,NSTMS,NTEAR,IORD(15)
   6              COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
   6              COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
```

```
      6         COMMON/UNIT/ NRXR,NHX,NDIV,NMIX,IRXR(5),NCDR,RLNTH(5),IHX(5),
               1             ICDR(5),QCOND(5),QHX(5)
      6         COMMON/PARM/ N,M,TFDSTM,PFDSTM,P(5),IFD,ITR(10),Y(5,8)
      6         COMMON/FLAG/ FLAG1,FLAG2,NFLAG,FLAG3
      6         DIMENSION FSTMOD(25,8),DUMF(8),YDUM(10,8)
      6         DIMENSION ZIL(41), ZTTK(41)
      6         DIMENSION XX1(5,41),XX2(5,41),TTK(5,41),IL(5,41),
               1  YR(5,41,8),DDX1DL(5,41),DDTKDL(5,41),RRATE1(5,41),
               2  RRATE2(5,41),CCPAVG(5,41)
      6      12 CONTINUE
          C
          C      STORE REACTOR INFORMATION
          C
      6         IPT = IPT + 1
     10         DO 100 I = 1, NRXR
     12         XX1(I,IPT) = X1(I)
     20         XX2(I,IPT) = X2(I)
     26         TTK(I,IPT) = TK(I)
     34         IL(I,IPT) = L
     41         IZ = IRXR(I)
     44         JL = NOUT(IZ,1)
     51         DO 31 J = 1, N
     52         YR(I,IPT,J) = Y(I,J)
     63      31 CONTINUE
     66         DDX1DL(I,IPT) = DX1DL(I)
     74         DDTKDL(I,IPT) = DTKDL(I)
    102         RRATE1(I,IPT) = RATE1(I)
    110         RRATE2(I,IPT) = RATE2(I)
    116         CCPAVG(I,IPT) = CPAVG(I)
    124     100 CONTINUE
    126         IF (IPT.LT.NPTS) RETURN
          C      CHECK FOR CONVERGENCE USING TEAR STREAM(S)
          C
    131         IF(NTEAR.EQ.0) GO TO 40
          C
          C           IF NOT CONVERGED STORE OLD VALUES OF TEAR STREAM(S)
          C
    133         DO 20 KI = 1, NTEAR
    135         SUMY = 0.
    136         MM = ITR(KI)
    141         IF (NRUN.EQ.1) GO TO 26
    143         DO 22 M = 1, N
    145         FTOL = 0.005 * FSTM(MM,M)
    152         DELF = ABS(FSTMOD(MM,M) - FSTM(MM,M))
          C
          C        CHECK IF DELF - FTOL IS VERY SMALL, IF SO, BYPASS
          C
    166         DIFF = DELF - FTOL
    170         IF((DIFF.GT.0.).AND.(DIFF.LE.0.01)) GO TO 28
    202         IF(DELF.GT.FTOL) FLAG1 = 1.
    206      28 CONTINUE
    206         YDUM(MM,M) = FSTM(MM,M)/TTFSTM(MM)
    221         SUMY = SUMY + YDUM(MM,M)
    227      22 CONTINUE
    231         CTOL = 0.001
    232         DELY = ABS(SUMY - 1.)
    240         IF(DELY.GE.CTOL) FLAG2 = 1.
    245         IF ((FLAG1.NE.0.).OR.(FLAG2.NE.0.)) GO TO 26
    255         GO TO 40
    256      26 CONTINUE
          C
    256         DO 24 M = 1, N
    260         FSTMOD(MM,M) = FSTM(MM,M)
    270      24 CONTINUE
    272      20 CONTINUE
    275         RETURN
    275      40 CONTINUE
    275         FLAG3 = 1.
          C
          C           WRITE INFORMATION SUBMITTED TO SIMULATION
          C
    277         WRITE(NO,700) (Q(I), I = 1, 16)
    312     700 FORMAT(20X,8A10,/,20X,8A10,///)
    312         WRITE(NO,710)
    316     710 FORMAT (10X,29HPROCESS FLOWSHEET INFORMATION,//,15X,
               1   51HKEY-UNIT TYPE(KT), 1=RXR, 2=HX, 3=DIV, 4=MIX, 5=CDR,//,36X,
               2   6HSTM IN,13X,7HSTM OUT,/,10X,7HUNIT NO,5X,4HTYPE,5X,
```

```
              3    2H 1,5X,2H 2,5X,2H 3,7X,2H 1,5X,2H 2,5X,10HUNIT INFOR,
              4    5X,10HRXR LENGTH,/)
   316          JR = 0
   317          DO 10 J = 1, NUNITS
   322          JJ = IUNIT(J)
   325          IF (KT(J).GT.1) GO TO 8
   331          JR = JR + 1
   333          WRITE(NO,718) (IUNIT(J),KT(J),(IN(J,I),I=1,3),(NOUT(J,I),I=1,2),
              1    DUMDAT(JJ),RLNTH(JR))
   375      718 FORMAT(12X,I2,9X,I2,6X,I2,5X,I2,5X,I2,7X,I2,5X,I2,2(5X,F10.5))
   375          GO TO 10
   377        8 CONTINUE
   377          WRITE(NO,720) (IUNIT(J),KT(J),(IN(J,I),I=1,3),(NOUT(J,I),I=1,2),
              1    DUMDAT(JJ))
   436       10 CONTINUE
   442      720 FORMAT(12X,I2,9X,I2,6X,I2,5X,I2,5X,I2,7X,I2,5X,I2,5X,F10.5)
        C
        C           PRINT INPUT INFORMATION
        C
   442          WRITE(NO,722)
   446      722 FORMAT(//,10X,23HFEED STREAM INFORMATION,//,7X,6HSTREAM,6X,2HTK,
              18X,4HPSIA,20X,21HFLOWRATES(LBMOLES/HR),/,40X,3HCO ,7X,3HH2 ,7X,
              2    3HCH4,7X,3HH2O,7X,3HCO2,7X,3HN2 ,/)
   446          WRITE(NO,724) IFD,TKSTM(IFD),PRSTM(IFD),(FSTM(IFD,I), I=1,N)
   474      724 FORMAT (9X,I2,7X,F7.1,3X,F6.1,2X,6F10.2)
   474          IF (NTEAR.GT.0) GO TO 14
   500          WRITE(NO,725)
   504      725 FORMAT (//,10X,12HSTREAMS TORN,3X,4HNONE)
   504          GO TO 16
   506          CONTINUE
   506       14 WRITE(NO,726) (ITR(I),I = 1, NTEAR)
   522      726 FORMAT(//,10X,12HSTREAMS TORN,3X,10I5)
   522       16 CONTINUE
   522          WRITE(NO,728) (IORD(I),I=1,NUNITS)
   536      728 FORMAT(//,10X,28HUNIT ORDERING OF CALCULATION,3X,15I5)
   536          WRITE(NO,732)
   542      732 FORMAT(1H1)
   542          WRITE(NO,730)
   546      730 FORMAT(10X,23HFLOW STREAM INFORMATION,//,7X,6HSTREAM,6X,2HTK,8X,
              1    4HPSIA,20X,21HFLOWRATES(LBMOLES/HR),/,40X,3HCO ,7X,3HH2 ,7X,
              2    3HCH4,7X,3HH2O,7X,3HCO2,7X,3HN2 ,3X,5HTOTAL)
   546          DO 30 J = 1, NSTMS
   551          WRITE(NO,740) (J,TKSTM(J),PRSTM(J),(FSTM(J,I),I=1,N),TTFSTM(J))
   602      740 FORMAT(6X,I2,9X,F7.1,3X,F6.1,2X,7F10.2)
   602       30 CONTINUE
        C
        C           PRINT HEAT DUTIES OF HX AND COND
        C
   606          IF(NHX.EQ.0) GO TO 1000
   610          WRITE(NO,790)
   614      790 FORMAT(/,10X,29HHEAT EXCHANGER DUTIES, BTU/HR)
   614          DO 1002 J=1, NHX
   617     1002 WRITE(NO,792) J,QHX(J)
   634      792 FORMAT(6X,3HQHX,I1,3H = ,E12.4)
   634     1000 CONTINUE
        C
   634          IF(NCOND.EQ.0) GO TO 1006
   636          WRITE(NO,794)
   642      794 FORMAT(/,10X,24HCONDENSER DUTIES, BTU/HR)
   642          DO 1004 J = 1, NCDR
   645     1004 WRITE(NO,796) J,QCOND(J)
   662      796 FORMAT(6X,5HQCOND,I1,3H = ,E12.4)
   662     1006 CONTINUE
        C
        C           PRINT THE SOLUTION
        C
   662          DO 32 II = 1 , NRXR
   664          WRITE(NO,742) II
   672      742 FORMAT(//,10X,11HREACTOR NO.,I3)
   672          WRITE(NO,750)
   676      750 FORMAT(//,2X,131HLENGTH     XCO        TK        YCO        YH2        YCH4
              1    YH2O       YCO2       DX1DL      DTKDL              RATE1             RATE
              22        CPAVG          )
   676          DO 34 J = 1, NPTS
   701          X = XX1(II,J) + XX2(II,J)
   712          WRITE(NO,760)  IL(II,J),X,TTK(II,J),(YR(II,J,K),K=1,5),
              1    DDX1DL(II,J),CDTKDL(II,J),RRATE1(II,J),RRATE2(II,J),CCPAVG(II,J)
```

```
   776      760 FORMAT(2X,F6.2,F7.5,F8.1,1X,5(F7.5,2X),2(E12.4),2E13.4,1X,F8.4)
   776       34 CONTINUE
          C
          C           PRINT WARNING IF TEMPS IN RXR ARE CUTSIDE RANGE OF KINETICS
          C
  1002          IF(TTK(II,1).LT.547.) GO TO 300
  1011          GO TO 302
  1012      300 WRITE(NO,780)
  1016      780 FORMAT(/,10X,*RXR INLET TEMP BELOW MIN TEMP FOR RATE EQN, 547 K*)
  1016      302 CONTINUE
  1016          IF(TTK(II,NPTS).GT.755.) GO TO 304
  1027          GO TO 306
  1030      304 WRITE(NO,782)
  1034      782 FORMAT(/,10X,*RXR TEMP EXCEEDS MAX TEMP FOR RATE EQN, 755 K*)
  1034      306 CONTINUE
  1034       32 CONTINUE
  1040          WRITE(NO,800) NRUN
  1046      800 FORMAT(10X,*CONVERGENCE OBTAINED AFTER *,I2,*RUNS*)
          C
          C           NOTE - LET HIGHEST STREAM NUMBER ALWAYS BE THE PRODUCT STM
          C
  1046          MPT = NSTMS
  1050          CH4 = FSTM(MPT,3) + FSTM(MPT,1)
  1061          H2 = FSTM(MPT,2) - 3.*FSTM(MPT,1)
  1072          TOTAL = CH4 + H2 + FSTM(MPT,6)
  1101          HHV = (CH4/TOTAL*383033. + H2/TOTAL*122971.)/379.3
  1107          YCO = FSTM(MPT,1)/(FSTM(MPT,1)+FSTM(MPT,2)+FSTM(MPT,3)+FSTM(MPT,5)
               1  +FSTM(MPT,6))
  1144          OUTPUT, HHV,YCO
  1157          PUNCH 200, (Q(I),I=1,16)
  1172      200 FORMAT(8A10,/,8A10)
  1172          DO 42 I = 1, NSTMS
  1175          PUNCH 210, I,TKSTM(I),PRSTM(I),TTFSTM(I),(FSTM(I,J),J=1,N)
  1225      210 FORMAT(I5,3F10.2,/,8F10.2)
  1225       42 CONTINUE
  1231          DO 44 I = 1, NRXR
  1233          DO 46 IPT = 1, NPTS
  1234          PUNCH 220, I,IL(I,IPT),TTK(I,IPT),XX1(I,IPT),XX2(I,IPT),
               1    I,IL(I,IPT),(YR(I,IPT,J),J=1,5),RRATE1(I,IPT)
  1314      220 FORMAT(I5,F6.2,F8.1,2X,2F12.4,/,I5,F6.2,4X,5(F10.5),E13.4)
  1314       46 CONTINUE
  1320       44 CONTINUE
  1323          STOP
  1325          END
```

Appendix C: GRPDYN-Dynamic Program Manual

A USER'S MANUAL FOR THE GENERALIZED REACTOR PROFILE DYNAMIC PROGRAM (GRPDYN)

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1981

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1. Introduction

Dyanmic simulation is becoming a frequently used tool in the development of chemical processes. It is useful in the design of both equipment and controller schemes by predicting the effects of dynamic changes to a particular process or unit. Thus, any adverse effects to the process system could be forseen and corrected for in the rector design.

GRPDYN is a generalized reactor profile dynamic package for simulating an adiabatic, packed-bed reactor system. The program itself was made in conjunction with and is closely similar to the GRPSS steady state package. It is suggested, but not necessary, that GRPSS be used to obtain initial and final steady state conditions for the process under study, while letting GRPDYN calculate the changes with time.

As with GRPSS, GRPDYN is presently configured to study the methanation section of a high-BTU coal gasification plant, employing both the methanation and shift reactions:

$CO + 3H_2 = CH_4 + H_2O$ methanation [1]

$CO + H_2O = CO_2 + H_2$ shift [2]

Its development is also based on a dynamic reactor program prepared by Lehigh University for the U.S. DOE (1), and also uses the DSS/2 method of lines (2) integration system.

Because dynamic simulation is just now beginning to be more widely used and with the ability of this program to study the dynamic effects along the length of the reactor, GRPDYN could be extremely useful in studying reactor dynamics of any reaction and/or process configuration. The generalized approach also permits quick configuration changes as well as the easy addition of other process unit models.

2. System Description

The GRPDYN simulation system consists of a collection of three program sets:

- DSS/2 - A numerical integration package for solving differential equations, with no modification of the original programming necessary as in GRPSS. It is the main calling program for the entire simulation(2).

- Physical Data Base (PDATAB) - A data block containing ideal gas physical properties of 41 chemical species(3).

- DYGEN - A collection of subroutines needed to dynamically simulate the reactor system, including INITAL, DERV, and PRINT called by DSS/2.

The generalized nature of the program requires that all pertinent information be inputed to the program by the user. These sets of information are:

1. DSS/2 input information,
2. process topology,
3. old stream conditions for all streams (initial conditions),
4. new feed stream conditions,
5. order of unit calculations,
6. initial conditions of reactor(s) at each specific point.

All but the first of these sets are read directly by subroutines in DYGEN. Since the process topology is user specified, a total of seven process unit models are available for use (reactor, two heat exchangers, stream divider, stream mixer, and two condensers). These units and their models will be discussed in more detail in the next chapter.

The main focus of GRPDYN is on the internal dynamics of a reactor along a one dimensional grid. In GRPSS, three differential equations were solved for the reactor steady state.

Here, the concentration changes within the reactor are assumed to occur much faster than those relating to temperature changes. This permits the quasi-steady state assumption to be used, thus eliminating any differential equations relating concentration with time. The reactor model is thus simplified to only one differential equation, relating the change in temperature with time, at a given point along the length of the reactor. The numerical solution to this differential equation for each reactor grid point is calculated by DSS/2.

Without going into alot of detail on the workings of GRPDYN, a general outline of each major calculation step is presented below:

1. DSS/2 calls subroutine INITAL in DYGEN to:

   a. identify the compounds being used in the physical data program,

   b. identify the reactions taking place,

   c. calculate the heats of reaction,

   d. read the process topology,

   e. read the old process stream information, such as temperature, pressure, and compositions, of all streams in the system;

   f. read the new feed stream process information,

   g. set the initial conditions for each grid point along the reactor.

2. DSS/2 calls subroutine PRINT, which prints the DSS/2, process topology, and initial condition information;

3. DSS/2 makes multiple calls to DERV, one for each period of time to be calculated, as specified by the user and DSS/2;

   a. at each call, DERV goes through the unit order of calculation sequence, calling in turn each of the unit models being used;

   b. for the reactor model, several subroutines are used to permit the calcuation of the differential equation at each of the reactor grid points;

4. DSS/2 calls PRINT to print the calculated results for the reactor profile(s) and the process streams;

5. DSS/2 continues the calculation until the final time has been reached (user specified);

Table 2-1 gives a listing of all the subroutines found in DYGEN and a brief description of their function.

Table 2-1: DYGEN SUBROUTINE DESCRIPTIONS

- INITAL - Called by DSS/2; sets the initial conditions for the differential equations, and reads other important data by calling subroutines INDENT, STCICH, HPREP, and FLCWST, which are described below.

  * IDENT - States the number of compounds being used and identifies the compound with its corresponding number in PDATAB.

  * STCICH - Gives the stoichiometric coefficients for the reactions taking place involving the compounds specified.

  * HPREP - Calculates heat capacity coefficients and heats of reaction from PDATAB information.

  * FLCWST - Reads the process flowsheet information for the process under study; the old process information of all streams; the new feed stream conditions; and the ordering of unit calculations.

  * INITR1 - Initializes each of the differential equations by reading temperture, pressure, and composition information.

- DERV - Called by DSS/2; calls the individual process unit subroutines in the sequence specified by the user in FLCWST. Units called include a reactor, two heat exchangers, stream divider, stream mixer, and two condensors. Only the reactor contains the differential equations to be solved by DSS/2.

  * DERVR1 - Contains the ODEs being solved, one for each point along the reactor grid, which pertains to the temperature change with respect to time; calls subroutines DSS014 or PDL33, and INTALL.

    - DSS014 - A subroutine which calculates the spatial derivatives of temperature at each reactor grid point; this routine is used only with evenly spaced grids(4).

    - PDL33 - This subroutine uses a Lagrangean method to determine the spatial derivatives of temperature at each reactor grid point; may be used with both even and unevenly spaced grid points (5).

* INTALL - This subroutine integrates all spacial variables from the inlet to the outlet of a reactor. The values of the spatial derivatives are calculated in the subroutine DERVL.

  - DERVL - Called by INTALL, this subroutine calculates the derivatives of all spatial variables at any grid point in a reactor. The spatial variables used here are the fractional conversion of CO due to the methanation and shift reactions. Calls subroutines XADJ, YSFLCW, HRXYCP, and RATE.

  - XADJ - Called by DERVL, XADJ checks to see if any reactant is completely comsumed at any point in a reactor. If one or more of the reactants is completely consumed, the fractional conversions of CO by each reaction is adjusted so that negative flowrates are eliminated.

  - YSFLCW - Called by DERVL, YSFLCW calculates the mole fraction and the outlet vector of temperature, pressure, and flow of each species in moles per hour. The vector is calculated at each point in the reactor and is overwritten such that only the outlet is available for subsequent use.

  - HRXYCP - Called by DERVL, HRXYCP calculates the heat of reaction at each reactor grid point.

  - RATE - Called by DERVL, RATE calculates the rate of reaction at each specified point along the reactor grid, given component partial pressures and temperatures.

* HXT - One of the process unit models called by DERV; simply sets the exit stream temperature to a user specified value and calculates the heat duty required to achieve that temperature; no dynamics involved.

Table 2-1, continued

- HXQ - One of the process unit models called by DERV; similar to HXT, but in this case the heat duty is specified and kept constant and the exit temprature is calculated.

- DIV - One of the process unit models called by DERV; divides a process stream into two uesr specified fractions.

- MIXER - One of the process unit models called by DERV; mixes together two or three process streams and determines the composition and temperature of the resulting stream. Calls subroutines HGAS, HILC, and TCALC to assist in the calculation.

  * HGAS - Calculates the specific enthalpy of a gas using CPMEAN.

  * CPMEAN - Calculates average heat capacity using PDATAB.

  * HILO - Keeps track of high and low temperature values during the mixer calculation.

  * TCALC - Calculates the temperature of a mixed stream.

- CONDQ - One of the process unit models called by DERV; simulates a combined heat exchanger-water condensate separation system. Given the required heat duty (Q) to be removed by cooling, an exit temperature and fraction of water removal are calculated. No dynamics are involved. Calls subroutines FALPCS, HGAS, and HWATER to assist in the calculation.

- CONDF - One of the process unit models called by DERV; similar to CONDQ except that the fraction of water removal is specified and the exit temperature and heat duty are calculated.

  * FALPOS - Uses the false-position method for determining the next value of the independent variable to be tried in an iteration.

  * HWATER - Determines the enthalpy of liquid water.

- <u>PRINT</u> - Called by DSS/2 to print the inputed information and calculation results.

3. Process Topology

The "generalized" programming of CRPDYN requires that the process topology be entered into the program through the data deck. This chapter will describe the functions of the seven possible process units available for simulation.

The topological data required in GRPDYN falls under four catagories; process, unit, stream, and reactor.

The process data give an overall view of the process being simulated. The total number of each type of process unit, the total number of streams, and the number of reactor grid points are all submitted together. The notation in the program are:

- NRXR = number of reactors,
- NHX = number of heat exchangers,
- NDIV = number of stream dividers,
- NMIX = number of stream mixers,
- NCDR = number of condensers,
- NSTMS = total number of process streams,
- NPTS = total number of grid points in each reactor.

The unit data describe each process unit used in the model with the individual number of the unit, its type (i.e. reactor, etc.), the stream numbers entering and leaving the unit, and some additional data depending on the unit's function. The program uses the notation below:

- IUNIT = individual unit number (note: some units will have their own unit number, ICDR, the individual condenser number);
- KT = unit type where: 1 = RXR1, 2 = HXQ, 3 = MIX, 4 = DIV, 5 = CDRF, 6 = RXR2, 7 = HXT, 8 CDRQ;
- IN(I) = stream number(s) entering the unit (I = max of 3),

- NOUT(J) = stream number(s) exiting the unit (J = max of 2),

- DUMDAT = data which are characteristic of the unit (i.e. reactor area, condenser duty, etc.);

- RLNTH = length of reactor (used for reactors only).

The only criteria for naming the individual stream numbers is that the major product stream is given the highest stream number available (i.e. NSTMS).

The stream data require that the stream number, temperature, pressure and composition be specified for <u>all</u> streams. The user must specify the old feed-stream conditions, the new feed-stream conditions and the original conditions in <u>all</u> of the remaining streams. In providing all of the above information, the initial conditions for the simulation are specified as well as the desired feed stream changes. The nomenclature used in DYGEN are:

- IFD = feed stream number,

- TKFDOD = old feed stream temperature, K;

- TKSTM(J) = temperature of stream J, K;

- PRFDOD = old feed stream pressure, psia;

- PRSTM(J) = pressure of stream J, psia;

- FDOD(I) = molar flowrate per hour of compound I in the old feed stream, where: 1 = CO, 2 = H2, 3 = CH4, 4 = H2O, 5 = CO2, 6 = N2;

- FSTM(J,I) = molar flowrate per hour of compound I in stream J.

Note the stream data must be presented in ascending order to the program.

Finally, the initial conditions in each reactor must be stated to initialize the reactor differential equations being solved. These are most readily produced by running the GRPSS program at the desired conditions. The nomenclature used in

DYGEN are:

- L(I) = percent length of reactor at point I,
- TK(I,K) = temperature at point I in Reactor K, K;
- X1(I,K) = fractional conversion of CO by methanation reaction [Equation 1] at Point I in Reactor K;
- X2(I,K) = fractional conversion of CO by shift reaction [Equation 2] at Point I in Reactor K;
- YCOMP(I,J,K) = composition of Compound J at Point I in Reactor K, in molar fraction;
- RATE1(I,K) = rate of methanation reaction at Point I in Reactor K.

Note that only one reactor grid may be specified for the entire simulation. Thus, if 41 reactor grid points are specified, all reactors will have 41 points.

The following is a discussion of the process unit subroutines available. Please remember that K is defined as the individual unit number which is specified by the user.

3.1. Chemical Reactor - DERVR(K,JR,TK,DTKDT,X1,X2,RTE1,YDUM)

This subroutine simulates a dynamic adiabatic, packed-bed chemical reactor. When DERVR is called by the subroutine DERV, the values of K, the unit number, and JR, the individual reactor number, are supplied to the subroutine. This enables the routine to find the correct stream and reactor information.

Initially, DERVR numerically estimates the change in temperature with respect to length using the present values in the temperature array, TK. This is accomplished using a three-point upwind approximation method such as DSS014 (4) or PDL33 (5). The fractional conversion for each reaction at every point in the reactor is calculated starting with Point 1 (which has the inlet stream conditions) and proceeding towards the final point, NPTS (which will contain the exit stream conditions). The above information is used to numerically calculate the temperature change with respect to time (DTKDT) for every point in the reactor grid array, L, at a given time, T. DSS/2 utilizes the estimate of DTKDT to numerically integrate the differential equation and calculate a temperature profile, TK. The following arrays (data at each reactor grid point) are transferred out of the subroutine to be stored for printout:

- TK = temperature, K;
- DTKDT = first derivative of temperature with respect to time,
- X1, X2 = fractional conversion of methanation (shift) reaction,
- RTE1 = rate of methanation reaction, lbmoles/hr;
- YDUM = molar fractional composition of each component except N2.

Additional information is required for the calculation. Catalyst data, specifically the void fraction, specific heat, and the bulk ratio, are already included in the DERVR subroutine for a Harshaw catalyst. Both the reactor cross-sectional area, DUMDAT(K), in square feet, and the length of the reactor, RLNTH(JR), in feet, are also required to be inputed by the user.

The reactor grid used may be of either equal or unequal spacings, which are specified by the user. DERVR requires that an estimate of the change in temperature with respect to length (DTKDT) at a particular time be made to calculate TK. To calculate this first derivative, a spatial differentiation routine is used. FOr evenly spaced grids, the suggested routine is DSS014 (4) and for unevenly spaced grids, PDL33 (5) is suggested, although the latter may also be used for evenly spaced points. DSS014 is a simplier calculation, and thus, uses less time for a calculation.

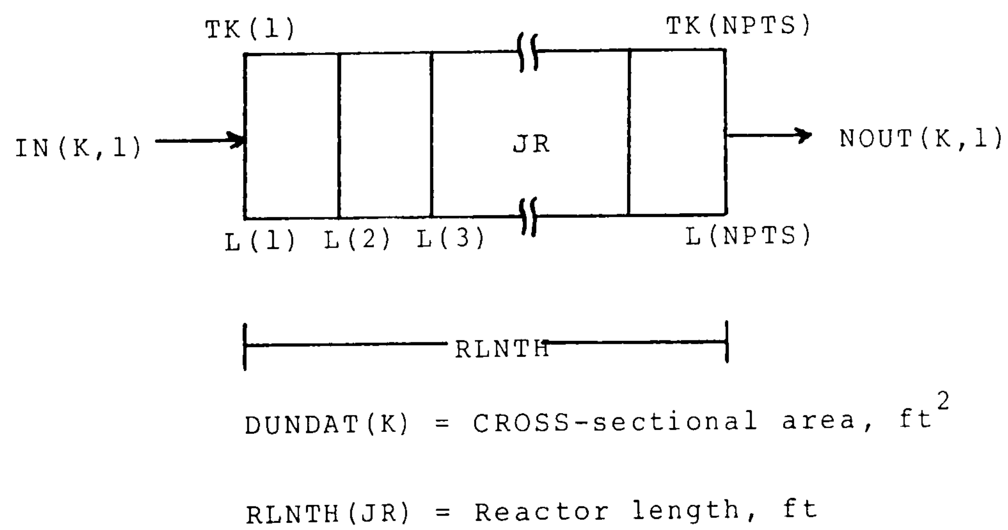
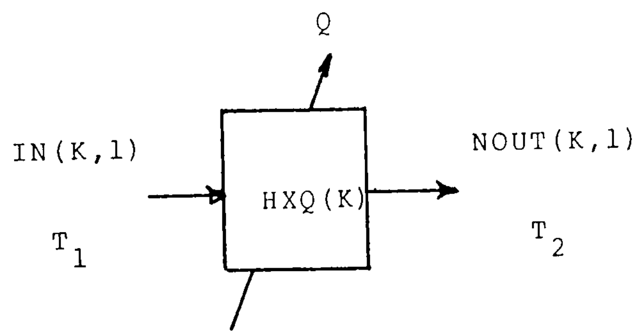


Figure 3-1: Chemical Reactor Topology

3.2. Heat Exchanger with Constant Heat Duty - HXQ(K)

This subroutine describes a heat exchanger by removing (or adding) a quantity of heat from an inlet stream, and then calculating a new exit stream temperature. Because heat exchanger dynamics were found to be much faster than reactor dynamics, no differential equations pertaining to the heat exchangers were included in the model. The exclusion of these differential equations also alleiviates any stiffness problems which might be created by the different calculations. The heat duty, Q, is user-specified and remains constant throughout the entire simulation calculation. A positive Q represents heat addition to the system, and a negative Q indicates heat removal. The basic assumption for the use of this subroutine is a heat exchanger unit entirely without control.



where:

DUMDAT(K) = Desired heat duty, Q, in BTU/lbmole

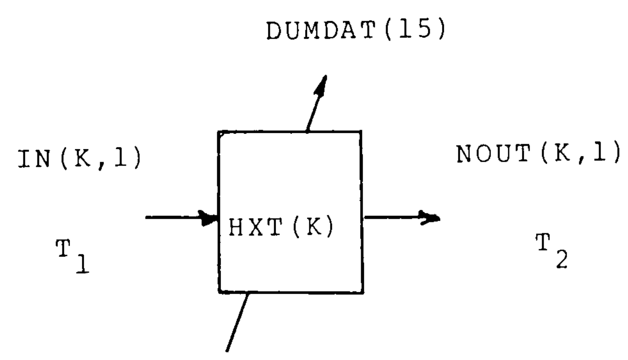
NOTE: +Q = heat addition

-Q = heat removal

Figure 3-2: Heat Exchanger with Constant Heat Duty Topology

3.3. Heat Exchanger with Constant Outlet Temperature-HXT(K)

This subroutine describes a heat exchanger by changing the temperature of an inlet stream to a user specified outlet temperature. This subroutine is almost identical to the steady state heat exchanger routine found in SSGEN. A heat duty, DUMDAT(15), is also calculated for the exchanger [note: only one HXT may be used because of this limitation].



where:

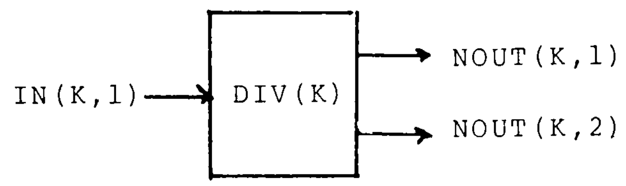
DUMDAT(K) = Desired outlet temperature, T_2, in K

DUMDAT(15) = Calculated heat duty, BTI/lbmole

Figure 3-3: Heat Exchanger with Constant Cutlet Temperature

3.4. Stream Divider - DIV(K)

This subroutine separates a stream into two parts, by a fraction specified by DUMDAT(K). It is identical to the stream divider routine found in SSGEN. Because any changes in the unit occur instantaneously, no dynamics are involved with this unit.



where:

DUMDAT(K) = Fraction of input stream going to output stream 1, 0 < DUMDAT < 1

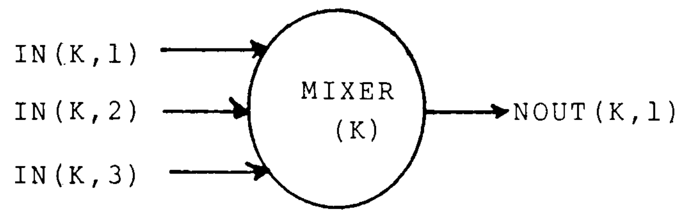
NOUT(K,1) = IN(K,1) * DUMDAT(K)

NOUT(K,2) = IN(K,1) * (1. - DUMDAT(K))

Figure 3-4: Stream Divider Topology

3.5. Stream Mixer - MIXFR(K)

This subroutine simulates a mixer for up to three streams by summing the flows for each compound in all the streams. The exit temperature is also calculated by summing the enthalpies of each stream, and then performing an iteration to find the new temperature. Like the stream divider, any changes are considered to occur instantaneously, and therefore involve no dynamics with the unit. This routine is identical to the mixer routine found in SSGEN.



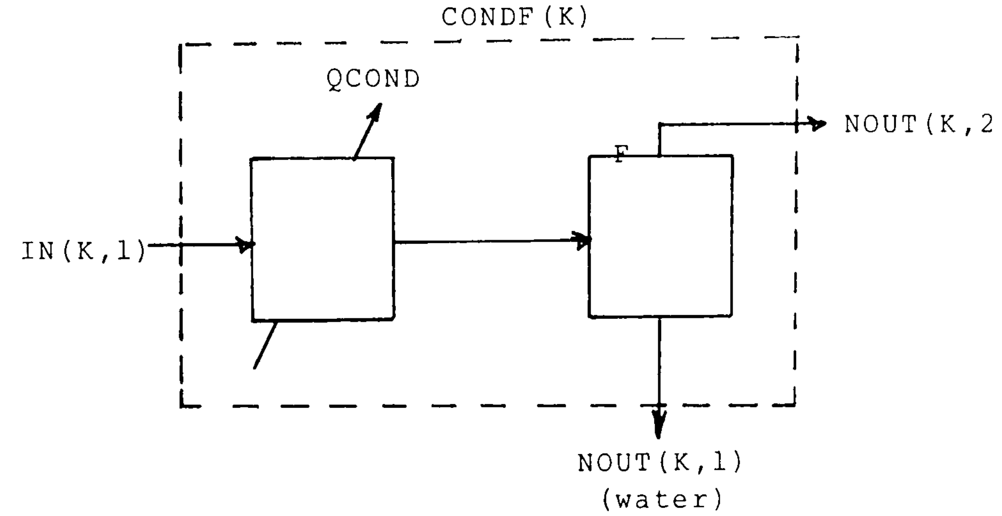
where:

DUMDAT(K) = 0.; No specific data required

Figure 3-5: Stream Mixer Topology

3.6. Condenser with Constant Water Removal - CCNDF(K)

This subroutine simulates of condenser system consisting of a heat exchanger and a liquid separation unit. The routine is almost identical to the steady state routine found in SSCEN. DUMDAT is specified as the desired fraction of water removal from the system. The amount of steam condensing is calculated via a false-position iteration using the Antoine Equation to calculate a vapor pressure at an assumed temperature. An enthalpy balance is performed using the estimated condenser temperature just iterated for and the HGAS and HWATER routines to calculate the enthalpies. If the water removal is specified as zero, then the inlet stream is cooled to the saturation temperature. Of course, the second output stream being calculated is the flowrate of the condensed water leaving the unit. A heat duty is also calculated, QCOND, in BTU per hour, for the system.

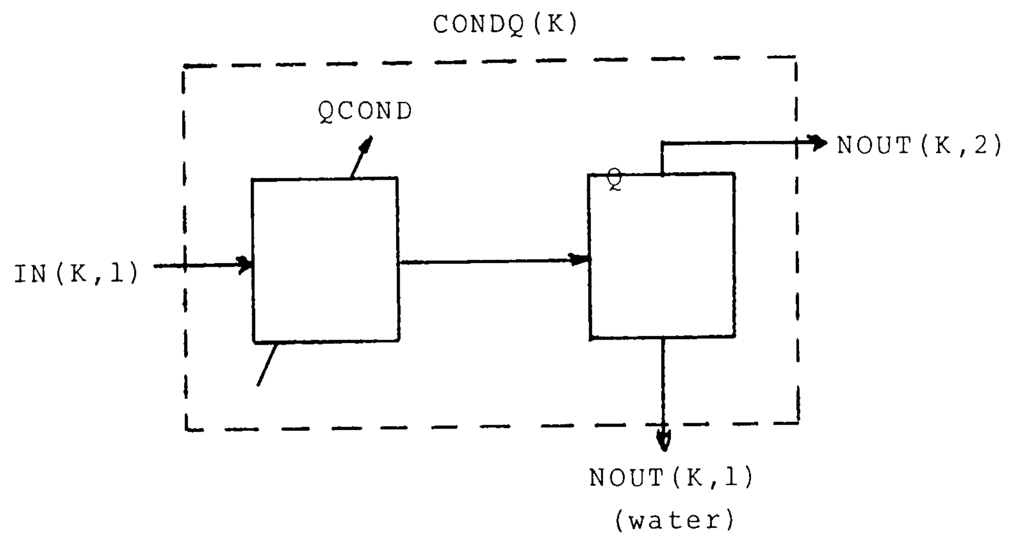


where:
DUMDAT(K) = Fraction of water being removed from inlet stream
QCOND = Amount of heat removed from inlet stream, BTU/hr
for the water component only:
NOUT(K,2) = IN(K,1) * DUMDAT(K)
NOUT(K,1) = IN(K,1) * (1. - DUMDAT(K))
NOTE: TEMPERATURE OF CONDENSER IS THE TEMPERATURE OF THE TWO OUTLET STREAMS

Figure 3-6: Constant Fraction Condenser Topology

3.7. Condenser with Constant Heat Duty - CONDQ(K)

This subroutine simulates a condenser system utilizing a constant level of heat removal. DUMDAT(K) is specified as the desired heat removal from the process stream. The subroutine first checks to see if condensation takes place by comparing the vapor pressure of water at the assumed condenser temperature with the partial pressure of water in the stream. In either case, an enthalpy balance is performed to determine the new exit stream temperature, and the amount of water condensing (if occuring).



where:

DUMDAT(K)=QCOND(ICDR) = Amount of heat removal BTU/hr

ICDR = Individual condenser number

for the water component only:

NOUT(K,2) = IN(K,1) * DUMDAT(K)

NOUT(K,1) = IN(K,1) * (1. - DUMDAT(K))

NOTE: TEMPERATURE OF CONDENSER IS THE TEMPERATURE OF THE TWO OUTLET STREAMS

Figure 3-7: Constant Heat Duty Condenser Topology

3.8. Comments on Topology

The set-up of the topology for the dynamic program, GRPDYN, is almost identical to that used in CRPSS, the steady state program. The only difference between the two is the addition of the two unit subroutines to provide the user with a choice of heat exchange and condenser systems. The proceedure for determining the ordering of the calculations in GRPDYN is also identical to that described in GRPSS. The user is refered to that manual for more details and examples.

4. Additional Information for Using CRPDYN

4.1. Present Simulation Capabilities

The following information gives an indication of the dimensional capacity of GRPDYN. Use beyond these limits would, of course, require dimensional changes in some of the subroutines found in GRPDYN. Listed below are the variable names and nomenclature of some quantities that might require changing.

- 8 Compounds - ID(8)
- 3 Reactions in the reactor - A(3,10)
- Topology Limits
  * 2 Reactors - IRXR(2), RLNTH(2), AREA(2)
  * 5 Heat exchangers - HX(5)
  * 2 Condensers - ICR(2)
  * 15 Units (total) - IUNIT(15)
  * 25 Streams - FSTM(25,8)

41 Reactor grid points - L(41), TK1(41), TK2(41)

In the present configuration, the entire package, DSS/2 (shortened, but not modified as done for the steady state program), PDATAB, and DYGEN programs require approximately 110K memory on the CDC6400 computer.

Note: When changing unit and stream limits, all variables pertaining to those elements must be changed along with the varibale listed.

4.2. Summary of Data Cards

CARD NO.	FORMAT	VARIABLE NAMES	USE
DSS/2 Cards			
1	20A4	TITLE	Documentation
2	3E10.0	TO,TF,TP	Initial, final, and print increment values of the independent variable (time)
3	4I5,2X, A3,E10.0	N,NMAX, NTYPE,NPRINT IRRTYP,ERROR	Number of ODE'S, ratio of print interval to minimum integration interval, integration algorithm,print option, type of error, max allowable integration error
DYGEN Cards			
4	8A10	TEXT	Documentation for program run
5	8A10	TEXT	Documentation for program run
6	7I5	NRXR,NHX,NDIV, NMIX,NCDR,NSTMS, NPTS	No. of reactors, heat exch'grs, dividers, mixers, condensers, streams and reactor points
ONE SET OF CARDS 7 & 8 FOR EACH UNIT			
7	7I5	IUNIT,KT, IN(3),NOUT(2)	Unit no., unit type, stream numbers entering (3), stream numbers exiting (2)
8	F10.5	DUMDAT	Extra unit data
FOR REACTORS ONLY			
8A	2F10.5	DUMDAT,RLNTH	Cross-sectional area, reactor length

CARD NO.	FORMAT	VARIABLE NAMES	USE
ONE SET OF CARDS 9 & 10 FOR THE OLD FEED STREAM CONDITIONS			
9	I5,3F10.3	IFD,TKFDOD, PRFDOD,TTFDOD	Feed stream number, temp (K), pressure (psia), total molar flowrate of old feed stream
10	8F10.5	FDOD(6)	Old feed stream molar flowrates per hour of the 6 compounds in system in order of: CO H2 CH4 H2O CO2 N2
ONE SET OF CARDS 11 & 12 GIVING THE NEW FEED STEAM CONDITIONS AND INITIAL CONDITIONS OF ALL OTHER STREAMS IN SYSTEM			
11	3F10.3	TKSTM,PRSTM TTFSTM	Temperature (K), pressure(psia) total molar flow rate
12	8F10.5	FSTM(6)	Molar flow per hour of the six compounds in system CO H2 CH4 H2O CO2 N2
13	20I5	IORD(I)	order of unit calculation for Ith unit
ONE SET OF CARDS 14 & 15 FOR EVERY POINT IN EACH REACTOR SPECIFYING THE INITIAL REACTOR CONDITIONS			
14	F6.2,F8.1 2F12.4	L(I),TK(I,K), X1(I,K),X2(I,K)	Reactor length(percent),temp(K), reaction conversions of reactor K, at grid point I
15	5F10.5, E13.4	YCOMP(I,5,K) RATE1(I,K)	mole fraction of five componds: CO H2 CH4 H2O CO2 N2, and rate of methanation rxn at point I for reactor K

<u>DSS/2 Cards</u>

16	All	END OF RUNS	Tells DSS/2 no further computations are necessary

4.3. Comments on Reactor Grid Specification

In the course of developing and using this program package, it was discovered that using different numbers of reactor grid points and intervals could substantially change the entire calculation. Too few points could not show rapid temperature changes along the length of the reactor. Many points could easily detect temperature changes, but also create storage problems for the computer and extremely lengthly computation times.

After some study, the following recommendations for the specification of reactor grid points are listed below.

1. Reactor grid points should be placed at evenly spaced of semi-evenly spaced intervals (such as, two different intervals at the front and rear of the reactor, or even three intervals in the front, middle and rear).

2. When two or more different intervals are employed, the closer spacings should be concentrated toward the front of the reactor, in the region of the largest temperature gradient.

3. Grid point intervals of less than 2 %length tend to increase the total number of points without actually helping the final calculation result.

4. Grid point intervals greater than 5 %length create distortions with the reactor temperature peaks (i.e. draws them out).

4.4. Comments Cn the Use of Spatial Differentiators

In studying the reactor grid point problem, several types of spatial differentiators were also tested. While the specific details of the investigation are reserved for the body of the thesis for which this manual is an appendix to, the general results concerning the routines are summarized below.

- Three-point upwind routines provide the best results, from both the standpoint of realistic profiles and numerical stability.

- The two-point upwind routine (equivalant to the stirred tank reactor) tested gave very gradual and unrealistic dynamic temperature peaks.

- The four-and-five-point upwind routines introduced alot of numerical oscillation at points directly in front of dynamic temperature peaks, again, making the profiles unrealistc.

Appendix A: Dynamic Program Sample Cutput

```
RUN NO.  1 - DYNAMIC METHANATOR WITH RECYCLE

INITIAL VALUE OF TIME =  0.

FINAL VALUE OF TIME =  6.0000E-01

PRINT INTERVAL OF TIME =  2.5000E-02

NUMBER OF FIRST-ORDER DIFFERENTIAL EQUATIONS =  82

PRINT INTERVAL/MINIMUM INTEGRATION INTERVAL =  1000

INTEGRATION ALGORITHM =  8
       1 - RUNGE KUTTA EULER
       2 - RUNGE KUTTA NIESSE
       3 - RUNGE KUTTA MERSON
       4 - RUNGE KUTTA TANAKA - 4
       5 - RUNGE KUTTA TANAKA - 5
       6 - RUNGE KUTTA CHAI
       7 - RUNGE KUTTA ENGLAND
       8 - RUNGE KUTTA WES  - 4/1
       9 - RUNGE KUTTA WES  - 4/2
      10 - RUNGE KUTTA WES  - 4/3
      11 - RUNGE KUTTA WES  - 4/4
      12 - RUNGE KUTTA WES  - 4/5
      13 - RUNGE KUTTA WES  - 5/1
      14 - RUNGE KUTTA WES  - 5/2

PRINT OPTION = 1
      NO INTEGRATION ERROR DIAGNOSTICS - 0
      SUMMARY OF INTEGRATION ERRORS    - 1

TYPE OF INTEGRATION ERROR = REL

MAXIMUM INTEGRATION ERROR =  5.000E-03
```

HYGAS PILOT PLANT - DYNAMIC STUDY
25 PERCENT RISE IN THE CO CONCENTRATION AT CONST TOTAL FLOW

TIME 0. HRS

INITIAL CONDITIONS FOR REACTOR SYSTEM
PROCESS FLOWSHEET INFORMATION

KEY-UNIT TYPE(KT),1=RXR1, 2=HXQ, 3=DIV, 4=MIX, 5=CDRF, 6=RXR2, 7=HXT, 8=CDRQ

UNIT NO	TYPE	STM IN 1	STM IN 2	STM IN 3	STM OUT 1	STM OUT 2	UNIT INFOR	RXR LENGTH
1	1	4	0	0	5	0	3.14200	5.00000
2	6	8	0	0	9	0	3.14200	10.00000
3	5	9	0	0	10	14	9.9000E-01	
4	3	1	0	0	2	6	.53300	
5	4	6	13	0	7	0	0.00000	
6	4	7	5	0	8	0	0.00000	
7	4	2	12	0	3	0	0.00000	
8	3	11	0	0	12	13	.73600	
9	7	3	0	0	4	0	5.5900E+02	
10	3	10	0	0	11	15	.78400	

FEED STREAM INFORMATION

STREAM	TK	PSIA	FLOWRATES(LBMOLES/HR) CO	H2	CH4	H2O	CO2	N2	TOTAL
INITIAL	310.0	834.0	9.60	38.70	18.83	0.00	0.00	7.88	75.[illegible]
NEW	310.0	834.0	12.00	36.30	18.83	0.00	0.00	7.88	75.[illegible]

UNIT ORDERING OF CALCULATION 3 10 8 4 5 6 7 9 1 2

TIME 0. HRS

FLOW STREAM INFORMATION FOR DYNAMIC SIMULATION

STREAM	TK	PSIA	FLOWRATES(LBMOLES/HR) CO	H2	CH4	H2O	CO2	N2	TOTAL
1	310.0	834.0	12.00	36.30	18.83	0.00	0.00	7.88	75.0
2	310.0	834.0	5.12	20.63	10.03	0.00	0.00	4.20	39.9
3	302.1	834.0	5.12	48.20	93.16	.08	0.00	26.93	173.4
4	559.0	834.0	5.12	48.20	93.16	.08	0.00	26.93	173.4
5	708.8	834.0	0.00	32.85	98.27	5.20	0.00	26.93	163.2
6	310.0	834.0	4.48	18.07	8.79	0.00	0.00	3.68	35.0
7	304.9	834.0	4.48	25.14	30.09	.02	0.00	9.50	69.2
8	607.9	834.0	4.48	57.83	128.51	5.22	0.00	36.43	232.4
9	703.1	834.0	0.00	44.38	133.00	9.70	0.00	36.43	223.5
10	300.0	834.0	0.00	44.18	133.20	.13	0.00	36.43	213.9
11	300.0	834.0	0.00	34.54	104.43	.10	0.00	28.56	167.7
12	300.0	834.0	0.00	27.57	83.12	.08	0.00	22.74	133.5
13	300.0	834.0	0.00	7.07	21.30	.02	0.00	5.83	34.2
14	300.0	834.0	0.00	0.00	0.00	9.57	0.00	0.00	9.5
15	300.0	834.0	0.00	9.54	28.77	.03	0.00	7.87	46.2

REACTOR NO. 1

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
0.00	559.00	0.0000	0.0000	1.2792E+00	.02949
2.50	574.70	.1015	0.0000	1.3622E+00	.02666
5.00	591.10	.2084	0.0000	1.4190E+00	.02364
7.50	607.80	.3183	0.0000	1.4356E+00	.02049
10.00	624.30	.4275	0.0000	1.4005E+00	.01732
12.50	640.00	.5319	0.0000	1.3100E+00	.01425
15.00	654.20	.6274	0.0000	1.1710E+00	.01141
17.50	666.50	.7108	0.0000	1.0005E+00	.00890
20.00	676.80	.7807	0.0000	8.1963E-01	.00678
22.50	685.10	.8369	0.0000	6.4718E-01	.00506
25.00	691.40	.8806	0.0000	4.9567E-01	.00371
27.50	696.30	.9137	0.0000	3.7057E-01	.00269
30.00	699.80	.9382	0.0000	2.7197E-01	.00193
32.50	702.40	.9560	0.0000	1.9686E-01	.00137
35.00	704.30	.9689	0.0000	1.4106E-01	.00097
37.50	705.60	.9780	0.0000	1.0033E-01	.00069
40.00	706.60	.9846	0.0000	7.0994E-02	.00048
42.50	707.20	.9892	0.0000	5.0048E-02	.00034
45.00	707.70	.9924	0.0000	3.5189E-02	.00024
47.50	708.00	.9947	0.0000	2.4695E-02	.00017
50.00	708.30	.9963	0.0000	1.7309E-02	.00012
52.50	708.40	.9974	0.0000	1.2120E-02	.00008
55.00	708.50	.9982	0.0000	8.4816E-03	.00006
57.50	708.60	.9987	0.0000	5.9327E-03	.00004
60.00	708.70	.9991	0.0000	4.1485E-03	.00003
62.50	708.70	.9994	0.0000	2.9003E-03	.00002
65.00	708.70	.9996	0.0000	2.0273E-03	.00001
67.50	708.80	.9997	0.0000	1.4169E-03	.00001
70.00	708.80	.9998	0.0000	9.9024E-04	.00001
72.50	708.80	.9998	0.0000	6.9202E-04	0.00000
75.00	708.80	.9999	0.0000	4.8359E-04	0.00000
77.50	708.80	.9999	0.0000	3.3793E-04	0.00000
80.00	708.80	.9999	0.0000	2.3614E-04	0.00000
82.50	708.80	1.0000	0.0000	1.6500E-04	0.00000
85.00	708.80	1.0000	0.0000	1.1530E-04	0.00000

87.50	708.80	1.0000	0.0000	8.0567E-05	0.00000
90.00	708.80	1.0000	0.0000	5.6296E-05	0.00000
92.50	708.80	1.0000	0.0000	3.9337E-05	0.00000
95.00	708.80	1.0000	0.0000	2.7487E-05	0.00000
97.50	708.80	1.0000	0.0000	1.9207E-05	0.00000
100.00	708.80	1.0000	0.0000	1.3421E-05	0.00000

REACTOR NO. 2

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
1.00	607.90	0.0000	0.0000	1.3559E+00	.01928
2.50	630.30	.2319	0.0000	1.2739E+00	.01495
5.00	650.40	.4407	0.0000	1.0959E+00	.01097
7.50	666.70	.6127	0.0000	8.6245E-01	.00765
10.00	679.00	.7429	0.0000	6.2736E-01	.00510
12.50	687.60	.8347	0.0000	4.2898E-01	.00329
15.00	693.40	.8962	0.0000	2.8056E-01	.00207
17.50	697.10	.9358	0.0000	1.7806E-01	.00129
20.00	699.40	.9606	0.0000	1.1083E-01	.00079
22.50	700.80	.9760	0.0000	6.8143E-02	.00048
25.00	701.70	.9854	0.0000	4.1580E-02	.00029
27.50	702.30	.9912	0.0000	2.5254E-02	.00018
30.00	702.60	.9947	0.0000	1.5295E-02	.00011
32.50	702.80	.9968	0.0000	9.2472E-03	.00006
35.00	702.90	.9980	0.0000	5.5850E-03	.00004
37.50	703.00	.9988	0.0000	3.3710E-03	.00002
40.00	703.00	.9993	0.0000	2.0339E-03	.00001
42.50	703.00	.9996	0.0000	1.2269E-03	.00001
45.00	703.00	.9997	0.0000	7.4000E-04	.00001
47.50	703.10	.9998	0.0000	4.4628E-04	0.00000
50.00	703.10	.9999	0.0000	2.6913E-04	0.00000
52.50	703.10	.9999	0.0000	1.6230E-04	0.00000
55.00	703.10	1.0000	0.0000	9.7869E-05	0.00000
57.50	703.10	1.0000	0.0000	5.9017E-05	0.00000
60.00	703.10	1.0000	0.0000	3.5588E-05	0.00000
62.50	703.10	1.0000	0.0000	2.1460E-05	0.00000
65.00	703.10	1.0000	0.0000	1.2941E-05	0.00000
67.50	703.10	1.0000	0.0000	7.8034E-06	0.00000
70.00	703.10	1.0000	0.0000	4.7056E-06	0.00000
72.50	703.10	1.0000	0.0000	2.8375E-06	0.00000
75.00	703.10	1.0000	0.0000	1.7110E-06	0.00000
77.50	703.10	1.0000	0.0000	1.0318E-06	0.00000
80.00	703.10	1.0000	0.0000	6.2217E-07	0.00000
82.50	703.10	1.0000	0.0000	3.7518E-07	0.00000
85.00	703.10	1.0000	0.0000	2.2623E-07	0.00000
87.50	703.10	1.0000	0.0000	1.3642E-07	0.00000
90.00	703.10	1.0000	0.0000	8.2264E-08	0.00000
92.50	703.10	1.0000	0.0000	4.9606E-08	0.00000
95.00	703.10	1.0000	0.0000	2.9913E-08	0.00000
97.50	703.10	1.0000	0.0000	1.8038E-08	0.00000
100.00	703.10	1.0000	0.0000	1.0877E-08	0.00000

QCOND(1) = I

TIME 5.0000E-02 HRS

FLOW STREAM INFORMATION FOR DYNAMIC SIMULATION

STREAM	TK	PSIA	FLOWRATES(LBMOLES/HR) CO	H2	CH4	H2O	CO2	N2	TOTAL
1	310.0	834.0	12.00	36.30	18.83	0.00	0.00	7.88	75.0
2	310.0	834.0	6.40	19.35	10.03	0.00	0.00	4.20	39.9
3	302.4	834.0	6.63	20.91	98.86	.07	0.00	26.95	153.4
4	559.0	834.0	6.63	20.91	98.86	.07	0.00	26.95	153.4
5	709.0	834.0	.27	1.94	105.22	6.43	0.00	26.95	140.7
6	310.0	834.0	5.60	16.35	8.79	0.00	0.00	3.68	35.0
7	305.2	834.0	5.66	17.35	31.56	.02	0.00	9.51	64.1
8	607.3	834.0	5.93	19.19	136.78	6.44	0.00	36.46	204.8
9	703.1	834.0	.37	2.50	142.34	12.01	0.00	36.46	193.6
10	300.0	834.0	.37	2.50	142.34	.11	0.00	36.46	181.7
11	300.0	834.0	.29	1.96	111.59	.09	0.00	28.58	142.5
12	300.0	834.0	.23	1.56	88.83	.07	0.00	22.75	113.4
13	300.0	834.0	.06	.40	22.76	.02	0.00	5.83	29.0
14	300.0	834.0	0.00	0.00	0.00	11.90	0.00	0.00	11.9
15	300.0	834.0	.08	.54	30.75	.02	0.00	7.87	39.2

REACTOR NO. 1

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
0.00	559.00	0.0000	0.0000	1.5569E+00	.04319
2.50	580.09	.0976	0.0000	1.7234E+00	.03931
5.00	602.40	.2037	0.0000	1.8445E+00	.03501
7.50	625.29	.3144	0.0000	1.8882E+00	.03044
10.00	647.71	.4244	0.0000	1.8314E+00	.02580
12.50	668.55	.5276	0.0000	1.6757E+00	.02138
15.00	686.82	.6191	0.0000	1.4502E+00	.01738
17.50	701.83	.6962	0.0000	1.1964E+00	.01396
20.00	713.20	.7584	0.0000	9.5014E-01	.01116
22.50	720.81	.8071	0.0000	7.3203E-01	.00896
25.00	724.89	.8441	0.0000	5.5060E-01	.00726
27.50	726.01	.8717	0.0000	4.0764E-01	.00599
30.00	725.13	.8922	0.0000	3.0095E-01	.00505
32.50	723.23	.9073	0.0000	2.2423E-01	.00434
35.00	721.32	.9187	0.0000	1.6897E-01	.00382
37.50	719.73	.9272	0.0000	1.2831E-01	.00342
40.00	718.93	.9337	0.0000	9.6404E-02	.00311
42.50	718.19	.9386	0.0000	7.2670E-02	.00289
45.00	717.99	.9422	0.0000	5.3241E-02	.00272
47.50	717.04	.9450	0.0000	4.2113E-02	.00259
50.00	716.77	.9471	0.0000	3.1278E-02	.00249
52.50	715.17	.9489	0.0000	2.9212E-02	.00241
55.00	715.01	.9503	0.0000	2.1665E-02	.00234
57.50	713.09	.9517	0.0000	2.3679E-02	.00227
60.00	713.45	.9528	0.0000	1.5643E-02	.00222
62.50	711.38	.9539	0.0000	1.9786E-02	.00217
65.00	712.30	.9547	0.0000	1.0660E-02	.00213
67.50	710.26	.9555	0.0000	1.6062E-02	.00209
70.00	711.41	.9562	0.0000	7.0451E-03	.00206
72.50	709.58	.9568	0.0000	1.2584E-02	.00204
75.00	710.65	.9572	0.0000	4.8718E-03	.00201
77.50	709.27	.9577	0.0000	9.1510E-03	.00199
80.00	709.92	.9581	0.0000	4.0958E-03	.00198
82.50	709.28	.9583	0.0000	5.6000E-03	.00196
85.00	709.29	.9586	0.0000	4.0508E-03	.00195

87.50	709.39	.9588	0.0000	2.5785E-03	.00194
90.00	708.89	.9590	0.0000	3.8861E-03	.00193
92.50	709.39	.9591	0.0000	8.1228E-04	.00192
95.00	708.79	.9593	0.0000	3.0414E-03	.00192
97.50	709.15	.9594	0.0000	7.4930E-04	.00191
100.00	709.01	.9594	0.0000	1.1453E-03	.00191

REACTOR NO. 2

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
0.00	606.60	0.0000	0.0000	1.5183E+00	.02896
2.50	634.64	.1970	0.0000	1.4665E+00	.02353
5.00	658.75	.3767	0.0000	1.2871E+00	.01845
7.50	679.37	.5274	0.0000	1.0469E+00	.01412
10.00	696.03	.6459	0.0000	8.0322E-01	.01065
12.50	708.96	.7345	0.0000	5.8978E-01	.00803
15.00	717.17	.7976	0.0000	4.1094E-01	.00615
17.50	721.43	.8398	0.0000	2.7003E-01	.00488
20.00	722.03	.8669	0.0000	1.7130E-01	.00406
22.50	720.32	.8842	0.0000	1.1220E-01	.00353
25.00	717.43	.8962	0.0000	8.0068E-02	.00317
27.50	714.47	.9052	0.0000	6.1047E-02	.00290
30.00	711.95	.9121	0.0000	4.7871E-02	.00269
32.50	710.02	.9175	0.0000	3.7557E-02	.00252
35.00	708.55	.9218	0.0000	2.9466E-02	.00239
37.50	707.35	.9252	0.0000	2.3321E-02	.00229
40.00	706.35	.9279	0.0000	1.8718E-02	.00221
42.50	705.53	.9301	0.0000	1.5130E-02	.00214
45.00	704.89	.9318	0.0000	1.2152E-02	.00209
47.50	704.42	.9332	0.0000	9.6167E-03	.00205
50.00	704.08	.9343	0.0000	7.4936E-03	.00201
52.50	703.83	.9351	0.0000	5.7914E-03	.00199
55.00	703.63	.9358	0.0000	4.4725E-03	.00197
57.50	703.48	.9363	0.0000	3.4633E-03	.00195
60.00	703.37	.9367	0.0000	2.6764E-03	.00194
62.50	703.29	.9370	0.0000	2.0437E-03	.00193
65.00	703.24	.9372	0.0000	1.5245E-03	.00192
67.50	703.20	.9374	0.0000	1.1063E-03	.00192
70.00	703.19	.9375	0.0000	7.8946E-04	.00191
72.50	703.17	.9376	0.0000	5.6897E-04	.00191
75.00	703.16	.9376	0.0000	4.2622E-04	.00191
77.50	703.14	.9377	0.0000	3.3284E-04	.00191
80.00	703.13	.9377	0.0000	2.6403E-04	.00191
82.50	703.12	.9378	0.0000	2.0513E-04	.00191
85.00	703.11	.9378	0.0000	1.5367E-04	.00191
87.50	703.11	.9378	0.0000	1.1147E-04	.00191
90.00	703.11	.9378	0.0000	8.0429E-05	.00190
92.50	703.11	.9378	0.0000	5.8725E-05	.00190
95.00	703.10	.9378	0.0000	4.3905E-05	.00190
97.50	703.10	.9378	0.0000	3.2985E-05	.00190
100.00	703.10	.9378	0.0000	2.4720E-05	.00190

QCOND(1) = 1436235

TIME 1.0000E-01 HRS

FLOW STREAM INFORMATION FOR DYNAMIC SIMULATION

STREAM	TK	PSIA	FLOWRATES(LBMOLES/HR) CO	H2	CH4	H2O	CO2	N2	TOTAL
1	310.0	834.0	12.00	36.30	18.83	0.00	0.00	7.88	75.0
2	310.0	834.0	6.40	19.35	10.03	0.00	0.00	4.20	39.9
3	302.4	834.0	6.63	20.91	98.86	.07	0.00	26.95	153.4
4	559.0	834.0	6.63	20.91	98.86	.07	0.00	26.95	153.4
5	709.8	834.0	.29	1.90	105.20	6.41	0.00	26.95	140.7
6	310.0	834.0	5.60	16.95	8.79	0.00	0.00	3.68	35.0
7	305.2	834.0	5.66	17.35	31.56	.02	0.00	9.51	64.1
8	609.2	834.0	5.95	19.25	136.75	6.42	0.00	36.46	204.8
9	703.1	834.0	.37	2.50	142.34	12.01	0.00	36.46	193.6
10	300.0	834.0	.37	2.50	142.34	.11	0.00	36.46	181.7
11	300.0	834.0	.29	1.96	111.59	.09	0.00	28.58	142.5
12	300.0	834.0	.23	1.56	88.83	.07	0.00	22.75	113.4
13	300.0	834.0	.06	.40	22.76	.02	0.00	5.83	29.0
14	300.0	834.0	0.00	0.00	0.00	11.90	0.00	0.00	11.9
15	300.0	834.0	.08	.54	30.74	.02	0.00	7.87	39.2

REACTOR NO. 1

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
0.00	559.00	0.0000	0.0000	1.5572E+00	.04320
2.50	580.10	.0976	0.0000	1.7239E+00	.03931
5.00	602.45	.2037	0.0000	1.8455E+00	.03502
7.50	625.38	.3145	0.0000	1.8898E+00	.03044
10.00	647.87	.4246	0.0000	1.8333E+00	.02580
12.50	668.80	.5279	0.0000	1.6779E+00	.02137
15.00	687.30	.6195	0.0000	1.4534E+00	.01737
17.50	702.92	.6968	0.0000	1.2022E+00	.01394
20.00	715.62	.7595	0.0000	9.5938E-01	.01112
22.50	725.62	.8087	0.0000	7.4300E-01	.00888
25.00	733.25	.8461	0.0000	5.5561E-01	.00717
27.50	738.80	.8731	0.0000	3.9372E-01	.00593
30.00	742.60	.8913	0.0000	2.5795E-01	.00509
32.50	745.00	.9024	0.0000	1.5441E-01	.00457
35.00	746.35	.9088	0.0000	8.5604E-02	.00428
37.50	746.99	.9122	0.0000	4.5800E-02	.00412
40.00	747.11	.9140	0.0000	2.5768E-02	.00403
42.50	746.80	.9152	0.0000	1.7844E-02	.00398
45.00	746.06	.9163	0.0000	1.7280E-02	.00393
47.50	744.83	.9175	0.0000	2.1398E-02	.00387
50.00	743.03	.9190	0.0000	2.8541E-02	.00380
52.50	740.62	.9211	0.0000	3.7110E-02	.00371
55.00	737.67	.9236	0.0000	4.5447E-02	.00359
57.50	734.34	.9265	0.0000	5.1759E-02	.00345
60.00	730.93	.9297	0.0000	5.5030E-02	.00330
62.50	727.72	.9330	0.0000	5.4717E-02	.00315
65.00	724.99	.9361	0.0000	5.1565E-02	.00300
67.50	722.82	.9389	0.0000	4.6112E-02	.00287
70.00	721.20	.9415	0.0000	4.0083E-02	.00275
72.50	719.93	.9436	0.0000	3.3713E-02	.00265
75.00	718.90	.9454	0.0000	2.9032E-02	.00257
77.50	717.86	.9470	0.0000	2.4609E-02	.00249
80.00	716.88	.9484	0.0000	2.2924E-02	.00243
82.50	715.76	.9496	0.0000	1.9919E-02	.00237
85.00	714.83	.9508	0.0000	2.0225E-02	.00231

87.50	713.76	.9519	0.0000	1.6533E-02	.00226
90.00	713.12	.9529	0.0000	1.8118E-02	.00222
92.50	712.18	.9538	0.0000	1.2379E-02	.00217
95.00	711.93	.9547	0.0000	1.6103E-02	.00213
97.50	711.02	.9553	0.0000	7.4880E-03	.00210
100.00	711.16	.9560	0.0000	1.5021E-02	.00207

REACTOR NO. 2

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
0.00	607.35	0.0000	0.0000	1.5528E+00	.02906
2.50	635.74	.1994	0.0000	1.4823E+00	.02354
5.00	660.54	.3805	0.0000	1.3029E+00	.01841
7.50	681.40	.5319	0.0000	1.0538E+00	.01404
10.00	697.35	.6500	0.0000	8.0060E-01	.01057
12.50	708.86	.7377	0.0000	5.8322E-01	.00797
15.00	717.09	.7998	0.0000	4.0560E-01	.00610
17.50	722.61	.8411	0.0000	2.6480E-01	.00486
20.00	726.21	.8662	0.0000	1.5768E-01	.00410
22.50	728.20	.8799	0.0000	8.4084E-02	.00368
25.00	729.39	.8866	0.0000	4.1319E-02	.00347
27.50	730.07	.8897	0.0000	1.8489E-02	.00338
30.00	730.42	.8911	0.0000	7.5977E-03	.00334
32.50	730.33	.8918	0.0000	4.7710E-03	.00332
35.00	729.59	.8927	0.0000	7.4445E-03	.00329
37.50	728.03	.8943	0.0000	1.4182E-02	.00324
40.00	725.63	.8970	0.0000	2.2384E-02	.00316
42.50	722.60	.9007	0.0000	2.9749E-02	.00305
45.00	719.27	.9050	0.0000	3.4299E-02	.00291
47.50	716.05	.9096	0.0000	3.5503E-02	.00277
50.00	713.25	.9142	0.0000	3.3778E-02	.00263
52.50	711.00	.9183	0.0000	3.0175E-02	.00251
55.00	709.28	.9219	0.0000	2.5771E-02	.00240
57.50	707.97	.9249	0.0000	2.1430E-02	.00231
60.00	706.94	.9274	0.0000	1.7629E-02	.00223
62.50	706.10	.9295	0.0000	1.4493E-02	.00217
65.00	705.41	.9312	0.0000	1.1922E-02	.00211
67.50	704.85	.9326	0.0000	9.7637E-03	.00207
70.00	704.43	.9337	0.0000	7.9123E-03	.00204
72.50	704.10	.9346	0.0000	6.3304E-03	.00201
75.00	703.86	.9353	0.0000	5.0117E-03	.00199
77.50	703.67	.9359	0.0000	3.9437E-03	.00197
80.00	703.53	.9363	0.0000	3.0928E-03	.00196
82.50	703.42	.9367	0.0000	2.4145E-03	.00195
85.00	703.34	.9370	0.0000	1.8690E-03	.00194
87.50	703.28	.9372	0.0000	1.4303E-03	.00193
90.00	703.24	.9373	0.0000	1.0837E-03	.00193
92.50	703.21	.9375	0.0000	8.1897E-04	.00192
95.00	703.19	.9375	0.0000	6.2348E-04	.00192
97.50	703.16	.9376	0.0000	4.8124E-04	.00192
100.00	703.15	.9377	0.0000	3.7568E-04	.00192

QCOND(1) = 1436410

TIME 1.5000E-01 HRS

FLOW STREAM INFORMATION FOR DYNAMIC SIMULATION

STREAM	TK	PSIA	FLOWRATES(LBMOLES/HR) CO	H2	CH4	H2O	CO2	N2	TOTAL
1	310.0	834.0	12.00	36.30	18.83	0.00	0.00	7.88	75.0
2	310.0	834.0	6.40	19.35	10.03	0.00	0.00	4.20	39.9
3	302.4	834.0	6.63	20.93	98.85	.07	0.00	26.95	153.4
4	559.0	834.0	6.63	20.93	98.85	.07	0.00	26.95	153.4
5	730.0	834.0	.39	2.21	105.10	6.31	0.00	26.95	140.9
6	310.0	834.0	5.60	16.35	8.79	0.00	0.00	3.68	35.0
7	305.2	834.0	5.66	17.36	31.55	.02	0.00	9.51	64.1
8	623.6	834.0	6.06	19.56	136.65	6.33	0.00	36.46	205.0
9	703.7	834.0	.38	2.53	142.33	12.00	0.00	36.46	193.7
10	300.0	834.0	.38	2.53	142.33	.11	0.00	36.46	181.8
11	300.0	834.0	.30	1.99	111.58	.09	0.00	28.58	142.5
12	300.0	834.0	.24	1.58	88.82	.07	0.00	22.75	113.4
13	300.0	834.0	.06	.41	22.76	.02	0.00	5.83	29.0
14	300.0	834.0	0.00	0.00	0.00	11.59	0.00	0.00	11.8
15	300.0	834.0	.08	.55	30.74	.02	0.00	7.87	39.2

REACTOR NO. 1

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
0.00	559.00	0.0000	0.0000	1.5590E+00	.04324
2.50	580.12	.0976	0.0000	1.7262E+00	.03935
5.00	602.49	.2038	0.0000	1.8482E+00	.03504
7.50	625.44	.3147	0.0000	1.8927E+00	.03046
10.00	647.94	.4248	0.0000	1.8359E+00	.02582
12.50	668.98	.5281	0.0000	1.6800E+00	.02138
15.00	687.38	.6198	0.0000	1.4548E+00	.01737
17.50	703.00	.6971	0.0000	1.2031E+00	.01394
20.00	715.68	.7597	0.0000	9.5983E-01	.01112
22.50	725.70	.8089	0.0000	7.4329E-01	.00888
25.00	733.32	.8462	0.0000	5.5563E-01	.00717
27.50	738.88	.8732	0.0000	3.9352E-01	.00593
31.00	742.78	.8913	0.0000	2.5714E-01	.00509
32.50	745.11	.9024	0.0000	1.5391E-01	.00457
35.00	746.74	.9086	0.0000	8.2989E-02	.00429
37.50	747.38	.9119	0.0000	4.3994E-02	.00413
40.00	747.98	.9135	0.0000	2.0144E-02	.00406
42.50	748.06	.9143	0.0000	1.0826E-02	.00402
45.00	748.27	.9147	0.0000	4.1268E-03	.00401
47.50	748.23	.9148	0.0000	2.7500E-03	.00400
50.00	748.32	.9149	0.0000	6.2816E-04	.00399
52.50	748.24	.9150	0.0000	1.1455E-03	.00399
55.00	748.30	.9150	0.0000	8.0937E-06	.00399
57.50	748.15	.9151	0.0000	1.4099E-03	.00399
60.00	748.20	.9151	0.0000	3.1565E-04	.00399
62.50	747.90	.9153	0.0000	3.1060E-03	.00398
65.00	747.94	.9154	0.0000	1.4649E-03	.00397
67.50	747.28	.9157	0.0000	7.2638F-03	.00396
70.00	747.25	.9160	0.0000	4.4428E-03	.00394
72.50	745.85	.9167	0.0000	1.5796E-02	.00391
75.00	745.69	.9175	0.0000	1.0774E-02	.00388
77.50	743.05	.9189	0.0000	2.9905E-02	.00381
80.00	742.73	.9203	0.0000	2.0613E-02	.00374
82.50	738.37	.9226	0.0000	4.7464E-02	.00364
85.00	738.33	.9247	0.0000	2.9825E-02	.00354

87.50	732.00	.9277	0.0000	6.2170E-02	.00340
90.00	733.52	.9301	0.0000	3.0812E-02	.00329
92.50	724.91	.9334	0.0000	6.9903E-02	.00313
95.00	730.18	.9355	0.0000	1.7911E-02	.00303
97.50	717.68	.9386	0.0000	7.4571E-02	.00289
100.00	730.02	.9408	0.0000	0.	.00279

REACTOR NO. 2

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
0.00	603.29	0.0000	0.0000	1.8110E+00	.02954
2.50	645.15	.2177	0.0000	1.5924E+00	.02341
5.00	668.30	.4043	0.0000	1.3441E+00	.01803
7.50	688.05	.5553	0.0000	1.0585E+00	.01358
10.00	701.42	.6698	0.0000	7.7991E-01	.01016
12.50	712.83	.7530	0.0000	5.6036E-01	.00764
15.00	719.21	.8108	0.0000	3.8196E-01	.00587
17.50	723.66	.8486	0.0000	2.4511E-01	.00471
20.00	727.20	.8709	0.0000	1.4137E-01	.00402
22.50	727.72	.8835	0.0000	8.0569E-02	.00363
25.00	731.16	.8887	0.0000	2.3711E-02	.00347
27.50	729.38	.8918	0.0000	2.4231E-02	.00337
30.00	732.39	.8934	0.0000	0.	.00333
32.50	730.23	.8938	0.0000	4.5185E-03	.00331
35.00	731.82	.8941	0.0000	0.	.00330
37.50	730.41	.8942	0.0000	6.5369E-04	.00330
40.00	731.05	.8942	0.0000	0.	.00330
42.50	730.41	.8943	0.0000	2.4562E-04	.00330
45.00	730.62	.8943	0.0000	0.	.00330
47.50	730.36	.8943	0.0000	4.0018E-04	.00330
50.00	730.13	.8945	0.0000	1.7574E-03	.00329
52.50	729.58	.8950	0.0000	4.6414E-03	.00327
55.00	728.59	.8961	0.0000	8.9794E-03	.00324
57.50	727.09	.8978	0.0000	1.4330E-02	.00319
60.00	725.00	.9002	0.0000	2.0508E-02	.00311
62.50	722.42	.9034	0.0000	2.6069E-02	.00302
65.00	719.57	.9071	0.0000	2.9941E-02	.00290
67.50	716.68	.9112	0.0000	3.1641E-02	.00277
70.00	714.04	.9152	0.0000	3.0993E-02	.00265
72.50	711.77	.9190	0.0000	2.8671E-02	.00253
75.00	709.96	.9224	0.0000	2.5229E-02	.00242
77.50	708.55	.9254	0.0000	2.1511E-02	.00233
80.00	707.45	.9279	0.0000	1.7924E-02	.00225
82.50	706.57	.9299	0.0000	1.4841E-02	.00219
85.00	705.85	.9317	0.0000	1.2254E-02	.00214
87.50	705.25	.9331	0.0000	1.0138E-02	.00209
90.00	704.77	.9342	0.0000	8.3525E-03	.00206
92.50	704.39	.9352	0.0000	6.8356E-03	.00203
95.00	704.09	.9360	0.0000	5.5338E-03	.00200
97.50	703.86	.9366	0.0000	4.4379E-03	.00198
100.00	703.69	.9371	0.0000	3.5318E-03	.00197

QCON)(1) = 1438868

TIME 2.0000E-01 HRS

FLOW STREAM INFORMATION FOR DYNAMIC SIMULATION

STREAM	TK	PSIA	FLOWRATES(LBMOLES/HR) CO	H2	CH4	H2O	CO2	N2	TOTAL
1	310.0	834.0	12.00	36.30	18.83	0.00	0.00	7.88	75.0
2	310.0	834.0	6.40	19.35	10.03	0.00	0.00	4.20	39.9
3	302.4	834.0	6.67	21.03	98.82	.07	0.00	26.95	153.5
4	559.0	834.0	6.67	21.03	98.82	.07	0.00	26.95	153.5
5	742.6	834.0	.53	2.53	104.96	6.20	0.00	26.95	141.2
6	310.0	834.0	5.60	16.35	8.79	0.00	0.00	3.68	35.0
7	305.2	834.0	5.67	17.38	31.55	.02	0.00	9.51	64.1
8	637.0	834.0	6.22	20.05	136.49	6.21	0.00	36.46	205.4
9	707.9	834.0	.44	2.71	142.27	11.99	0.00	36.46	193.8
10	300.0	834.0	.44	2.70	142.27	.11	0.00	36.46	181.9
11	300.0	834.0	.34	2.12	111.54	.09	0.00	28.58	142.6
12	300.0	834.0	.27	1.58	88.79	.07	0.00	22.75	113.5
13	300.0	834.0	.07	.43	22.75	.02	0.00	5.83	29.1
14	300.0	834.0	0.00	0.00	0.00	11.88	0.00	0.00	11.8
15	300.0	834.0	.09	.58	30.73	.02	0.00	7.87	39.3

REACTOR NO. 1

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
0.00	559.00	0.0000	0.0000	1.5686E+00	.04343
2.50	580.25	.0978	0.0000	1.7392E+00	.03952
5.00	602.76	.2042	0.0000	1.8636E+00	.03519
7.50	625.84	.3155	0.0000	1.9090E+00	.03057
10.00	648.44	.4259	0.0000	1.8510E+00	.02589
12.50	669.44	.5295	0.0000	1.6922E+00	.02142
15.00	687.96	.6213	0.0000	1.4632E+00	.01739
17.50	703.55	.6985	0.0000	1.2082E+00	.01394
20.00	716.20	.7611	0.0000	9.6231E-01	.01111
22.50	726.12	.8101	0.0000	7.4384E-01	.00887
25.00	733.69	.8472	0.0000	5.5489E-01	.00717
27.50	739.18	.8739	0.0000	3.9189E-01	.00593
30.00	742.96	.8918	0.0000	2.5556E-01	.00509
32.50	745.35	.9028	0.0000	1.5175E-01	.00458
35.00	746.78	.9089	0.0000	8.3104E-02	.00430
37.50	747.56	.9121	0.0000	4.2392E-02	.00415
40.00	747.98	.9137	0.0000	2.1244E-02	.00407
42.50	748.17	.9145	0.0000	9.8273E-03	.00404
45.00	748.29	.9149	0.0000	5.1492E-03	.00402
47.50	748.31	.9150	0.0000	2.0189E-03	.00401
50.00	748.35	.9151	0.0000	1.4965E-03	.00401
52.50	748.33	.9152	0.0000	1.2811E-05	.00400
55.00	748.36	.9152	0.0000	9.6505E-04	.00400
57.50	748.32	.9152	0.0000	0.	.00400
60.00	748.39	.9153	0.0000	1.3752E-03	.00400
62.50	748.28	.9153	0.0000	0.	.00400
65.00	748.45	.9154	0.0000	2.3340E-03	.00399
67.50	748.21	.9155	0.0000	0.	.00399
70.00	748.55	.9157	0.0000	3.8206E-03	.00398
72.50	748.09	.9158	0.0000	0.	.00397
75.00	748.67	.9160	0.0000	5.3706E-03	.00396
77.50	747.92	.9162	0.0000	0.	.00396
80.00	748.79	.9164	0.0000	6.7007E-03	.00394
82.50	747.69	.9166	0.0000	0.	.00393
85.00	748.86	.9170	0.0000	8.0838E-03	.00392

87.50	747.37	.9172	0.0000	0.	.00391
90.00	748.81	.9176	0.0000	1.0125E-02	.00389
92.50	746.85	.9179	0.0000	0.	.00387
95.00	748.51	.9186	0.0000	1.5079E-02	.00384
97.50	745.84	.9190	0.0000	0.	.00382
100.00	747.76	.9201	0.0000	2.6184E-02	.00377

REACTOR NO. 2

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
0.00	634.96	0.0000	0.0000	2.1056E+00	.03029
2.50	671.77	.2516	0.0000	1.9270E+00	.02302
5.00	697.99	.4614	0.0000	1.5213E+00	.01678
7.50	715.35	.6171	0.0000	1.0819F+00	.01205
10.00	725.41	.7242	0.0000	7.2742E-01	.00874
12.50	730.73	.7938	0.0000	4.6553E-01	.00656
15.00	733.10	.8364	0.0000	2.8294E-01	.00522
17.50	733.78	.8608	0.0000	1.6251E-01	.00445
20.00	733.77	.8746	0.0000	9.3510E-02	.00401
22.50	733.25	.8824	0.0000	5.2997E-02	.00376
25.00	732.76	.8871	0.0000	3.2964E-02	.00361
27.50	732.24	.8900	0.0000	2.0232F-02	.00352
30.00	731.89	.8919	0.0000	1.3869E-02	.00346
32.50	731.57	.8932	0.0000	8.9467E-03	.00342
35.00	731.33	.8941	0.0000	7.0941E-03	.00339
37.50	731.07	.8948	0.0000	4.9445E-03	.00337
40.00	730.92	.8953	0.0000	4.1121E-03	.00335
42.50	730.85	.8957	0.0000	2.3422E-03	.00334
45.00	730.91	.8959	0.0000	1.1073E-03	.00334
47.50	731.02	.8959	0.0000	0.	.00333
50.00	731.14	.8959	0.0000	0.	.00333
52.50	731.16	.8959	0.0000	0.	.00333
55.00	731.07	.8959	0.0000	0.	.00333
57.50	730.91	.8959	0.0000	2.8910E-04	.00333
60.00	730.75	.8961	0.0000	1.3161E-03	.00333
62.50	730.58	.8963	0.0000	1.7499E-03	.00332
65.00	730.40	.8966	0.0000	2.2094E-03	.00331
67.50	730.13	.8969	0.0000	2.9562E-03	.00330
70.00	729.69	.8974	0.0000	4.5472E-03	.00328
72.50	728.99	.8983	0.0000	7.0381E-03	.00326
75.00	727.94	.8995	0.0000	1.0665E-02	.00322
77.50	726.46	.9013	0.0000	1.5049E-02	.00316
80.00	724.54	.9036	0.0000	1.9793E-02	.00309
82.50	722.25	.9065	0.0000	2.4083E-02	.00300
85.00	719.71	.9098	0.0000	2.7275E-02	.00289
87.50	717.10	.9134	0.0000	2.8838E-02	.00278
90.00	714.63	.9170	0.0000	2.8699E-02	.00266
92.50	712.43	.9205	0.0000	2.7074E-02	.00255
95.00	710.60	.9237	0.0000	2.4433E-02	.00245
97.50	709.12	.9265	0.0000	2.1286E-02	.00236
100.00	707.95	.9290	0.0000	1.8093E-02	.00228

QCOND(1) = 1456142

TIME 2.5000E-01 HRS

FLOW STREAM INFORMATION FOR DYNAMIC SIMULATION

STREAM	TK	PSIA	FLOWRATES(LBMOLES/HR) CO	H2	CH4	H2O	CO2	N2	TOTAL
1	310.0	834.0	12.00	36.30	18.83	0.00	0.00	7.88	75.0
2	310.0	834.0	6.40	19.35	10.03	0.00	0.00	4.20	39.9
3	302.4	834.0	6.77	21.33	98.72	.07	0.00	26.95	153.8
4	559.0	834.0	6.77	21.33	98.72	.07	0.00	26.95	153.8
5	748.5	834.0	.57	2.73	104.92	6.27	0.00	26.95	141.4
6	310.0	834.0	5.60	16.95	8.79	0.00	0.00	3.68	35.0
7	305.2	834.0	5.70	17.46	31.52	.02	0.00	9.51	64.2
8	637.9	834.0	6.27	20.19	136.44	6.29	0.00	36.46	205.6
9	724.2	834.0	.60	3.18	142.11	11.96	0.00	36.46	194.3
10	300.0	834.0	.60	3.18	142.11	.11	0.00	36.46	182.4
11	300.0	834.0	.47	2.49	111.42	.09	0.00	28.58	143.0
12	300.0	834.0	.37	1.98	88.69	.07	0.00	22.75	113.8
13	300.0	834.0	.10	.51	22.73	.02	0.00	5.83	29.1
14	300.0	834.0	0.00	0.00	0.00	11.85	0.00	0.00	11.8
15	300.0	834.0	.13	.59	30.70	.02	0.00	7.87	39.4

REACTOR NO. 1

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
0.00	559.00	0.0000	0.0000	1.5961E+00	.04399
2.50	580.65	.0982	0.0000	1.7762E+00	.04002
5.00	603.61	.2055	0.0000	1.9090E+00	.03560
7.50	627.17	.3179	0.0000	1.9584E+00	.03087
10.00	650.20	.4295	0.0000	1.8980E+00	.02608
12.50	671.52	.5340	0.0000	1.7305E+00	.02151
15.00	690.20	.6262	0.0000	1.4901E+00	.01740
17.50	705.81	.7035	0.0000	1.2237E+00	.01390
20.00	718.36	.7657	0.0000	9.6900E-01	.01105
22.50	728.10	.8141	0.0000	7.4377E-01	.00881
25.00	735.41	.8504	0.0000	5.4971E-01	.00711
27.50	740.63	.8763	0.0000	3.8322E-01	.00590
30.00	744.13	.8934	0.0000	2.4602E-01	.00509
32.50	746.29	.9037	0.0000	1.4429E-01	.00460
35.00	747.52	.9094	0.0000	7.8439E-02	.00433
37.50	748.16	.9123	0.0000	4.0622E-02	.00419
40.00	748.47	.9139	0.0000	2.0639E-02	.00412
42.50	748.59	.9146	0.0000	1.0610E-02	.00408
45.00	748.63	.9151	0.0000	5.6956E-03	.00406
47.50	748.62	.9153	0.0000	3.3089E-03	.00405
50.00	748.60	.9154	0.0000	2.1152E-03	.00405
52.50	748.57	.9155	0.0000	1.5028E-03	.00404
55.00	748.54	.9156	0.0000	1.1456E-03	.00404
57.50	748.51	.9156	0.0000	9.3005E-04	.00404
61.00	748.49	.9157	0.0000	7.5764E-04	.00403
62.50	748.47	.9157	0.0000	6.4292E-04	.00403
65.00	748.45	.9158	0.0000	5.2247E-04	.00403
67.50	748.44	.9158	0.0000	4.6131E-04	.00403
70.00	748.43	.9158	0.0000	3.6933E-04	.00403
72.50	748.41	.9158	0.0000	3.3772E-04	.00403
75.00	748.41	.9159	0.0000	2.4245E-04	.00403
77.50	748.40	.9159	0.0000	2.2134E-04	.00403
80.00	748.40	.9159	0.0000	1.1467E-04	.00403
82.50	748.39	.9159	0.0000	1.0174E-04	.00403
85.00	748.41	.9159	0.0000	0.	.00402

87.50	748.41	.9159	0.0000	0.	.00402
90.00	748.44	.9159	0.0000	0.	.00402
92.50	748.44	.9159	0.0000	0.	.00402
95.00	748.49	.9159	0.0000	0.	.00402
97.50	748.47	.9159	0.0000	0.	.00402
100.00	748.52	.9159	0.0000	0.	.00402

REACTOR NO. 2

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
0.00	637.69	0.0000	0.0000	2.1414E+00	.03048
2.50	676.61	.2569	0.0000	1.9992E+00	.02301
5.00	707.33	.4733	0.0000	1.5897E+00	.01653
7.50	729.92	.6332	0.0000	1.1280E+00	.01163
10.00	745.23	.7377	0.0000	7.2024E-01	.00837
12.50	754.36	.7926	0.0000	3.9364E-01	.00664
15.00	758.60	.8173	0.0000	1.7177E-01	.00586
17.50	759.66	.8281	0.0000	6.4386E-02	.00552
20.00	758.93	.8326	0.0000	3.9422E-02	.00538
22.50	757.08	.8372	0.0000	3.6879E-02	.00523
25.00	754.43	.8425	0.0000	4.2408E-02	.00506
27.50	751.26	.8487	0.0000	4.9010E-02	.00487
30.00	747.83	.8553	0.0000	5.3346E-02	.00465
32.50	744.46	.8620	0.0000	5.3931E-02	.00444
35.00	741.41	.8685	0.0000	5.0772E-02	.00423
37.50	738.87	.8742	0.0000	4.4885E-02	.00405
40.00	736.87	.8791	0.0000	3.7692E-02	.00389
42.50	735.35	.8831	0.0000	3.0471E-02	.00377
45.00	734.21	.8863	0.0000	2.4051E-02	.00367
47.50	733.33	.8887	0.0000	1.8758E-02	.00359
50.00	732.67	.8907	0.0000	1.4563E-02	.00352
52.50	732.15	.8922	0.0000	1.1283E-02	.00348
55.00	731.76	.8933	0.0000	8.7055E-03	.00344
57.50	731.46	.8942	0.0000	6.6437E-03	.00341
60.00	731.26	.8949	0.0000	4.9417E-03	.00339
62.50	731.13	.8953	0.0000	3.4904E-03	.00337
65.00	731.07	.8957	0.0000	2.2558E-03	.00336
67.50	731.06	.8958	0.0000	1.2857E-03	.00336
70.00	731.06	.8959	0.0000	6.7039E-04	.00336
72.50	731.05	.8960	0.0000	4.6646E-04	.00335
75.00	730.99	.8961	0.0000	6.3439E-04	.00335
77.50	730.89	.8962	0.0000	1.0505E-03	.00335
80.00	730.74	.8964	0.0000	1.5883E-03	.00334
82.50	730.54	.8967	0.0000	2.2081E-03	.00333
85.00	730.27	.8970	0.0000	2.9975E-03	.00332
87.50	729.89	.8975	0.0000	4.1455E-03	.00331
90.00	729.35	.8982	0.0000	5.8690E-03	.00328
92.50	728.56	.8992	0.0000	8.3207E-03	.00325
95.00	727.47	.9005	0.0000	1.1508E-02	.00321
97.50	726.03	.9023	0.0000	1.5245E-02	.00315
100.00	724.23	.9046	0.0000	1.9146E-02	.00308

QCOND(1) = 1529169

TIME 3.0000E-01 HRS

FLOW STREAM INFORMATION FOR DYNAMIC SIMULATION

STREAM	TK	PSIA	FLOWRATES(LBMOLES/HR) CO	H2	CH4	H2O	CO2	N2	TOTAL
1	310.0	834.0	12.00	36.30	18.83	0.00	0.00	7.88	75.0
2	310.0	834.0	6.40	19.35	10.03	0.00	0.00	4.20	39.9
3	302.4	834.0	6.80	21.43	98.69	.07	0.00	26.95	153.9
4	559.0	834.0	6.80	21.43	98.69	.07	0.00	26.95	153.9
5	748.6	834.0	.57	2.74	104.92	6.30	0.00	26.95	141.4
6	310.0	834.0	5.60	16.95	8.79	0.00	0.00	3.68	35.0
7	305.2	834.0	5.71	17.49	31.51	.02	0.00	9.51	64.2
8	637.9	834.0	6.28	20.23	136.43	6.32	0.00	36.46	205.7
9	730.7	834.0	.65	3.34	142.06	11.95	0.00	36.46	194.4
10	300.0	834.0	.65	3.34	142.06	.11	0.00	36.46	182.6
11	300.0	834.0	.51	2.62	111.37	.09	0.00	28.58	143.1
12	300.0	834.0	.41	2.08	88.65	.07	0.00	22.75	113.9
13	300.0	834.0	.10	.53	22.72	.02	0.00	5.83	29.2
14	300.0	834.0	0.00	0.00	0.00	11.84	0.00	0.00	11.8
15	300.0	834.0	.14	.72	30.68	.02	0.00	7.87	39.4

REACTOR NO. 1

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
1.00	559.00	0.0000	0.0000	1.6054E+00	.04418
2.50	580.79	.0984	0.0000	1.7889E+00	.04019
5.00	603.98	.2060	0.0000	1.9258E+00	.03573
7.50	627.86	.3189	0.0000	1.9788E+00	.03097
10.00	651.29	.4312	0.0000	1.9197E+00	.02613
12.50	673.03	.5364	0.0000	1.7503E+00	.02150
15.00	692.12	.6291	0.0000	1.5054E+00	.01735
17.50	708.08	.7067	0.0000	1.2334E+00	.01382
20.00	720.90	.7689	0.0000	9.7292E-01	.01096
22.50	730.82	.8170	0.0000	7.4189E-01	.00871
25.00	738.18	.8528	0.0000	5.4140E-01	.00704
27.50	743.35	.8777	0.0000	3.6890E-01	.00586
30.00	746.69	.8937	0.0000	2.2920E-01	.00510
32.50	748.65	.9030	0.0000	1.2979E-01	.00466
35.00	749.68	.9080	0.0000	6.8769E-02	.00442
37.50	750.13	.9105	0.0000	3.5581E-02	.00430
40.00	750.28	.9119	0.0000	1.8910E-02	.00423
42.50	750.25	.9126	0.0000	1.0981E-02	.00420
45.00	750.15	.9131	0.0000	7.2299E-03	.00418
47.50	750.01	.9135	0.0000	5.5247E-03	.00416
50.00	749.87	.9137	0.0000	4.5903E-03	.00415
52.50	749.71	.9140	0.0000	4.1659E-03	.00413
55.00	749.58	.9142	0.0000	3.7260E-03	.00412
57.50	749.44	.9144	0.0000	3.5621E-03	.00411
60.00	749.33	.9146	0.0000	3.1466E-03	.00411
62.50	749.20	.9148	0.0000	3.0789E-03	.00410
65.00	749.12	.9149	0.0000	2.5959E-03	.00409
67.50	749.00	.9151	0.0000	2.6352E-03	.00408
70.00	748.95	.9152	0.0000	2.0487E-03	.00408
72.50	748.84	.9153	0.0000	2.2503E-03	.00407
75.00	748.82	.9154	0.0000	1.5174E-03	.00407
77.50	748.71	.9155	0.0000	1.9483E-03	.00406
80.00	748.72	.9156	0.0000	9.9427E-04	.00406
82.50	748.60	.9157	0.0000	1.7517E-03	.00405
85.00	748.65	.9158	0.0000	4.3209E-04	.00405

87.50	748.51	.9158	0.0000	1.6390E-03	.00405
90.00	748.62	.9159	0.0000	0.	.00404
92.50	748.44	.9159	0.0000	1.4913E-03	.00404
95.00	748.60	.9160	0.0000	0.	.00404
97.50	748.38	.9160	0.0000	1.3094E-03	.00404
100.00	748.61	.9161	0.0000	0.	.00403

REACTOR NO. 2

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
1.00	637.62	0.0000	0.0000	2.1460E+00	.03052
2.50	676.25	.2567	0.0000	1.9987E+00	.02305
5.00	707.29	.4730	0.0000	1.5936E+00	.01656
7.50	730.53	.6332	0.0000	1.1341E+00	.01165
10.00	746.36	.7377	0.0000	7.2216E-01	.00838
12.50	755.94	.7911	0.0000	3.9023E-01	.00670
15.00	760.78	.8155	0.0000	1.4938E-01	.00593
17.50	762.73	.8249	0.0000	2.7896E-02	.00563
20.00	763.38	.8266	0.0000	0.	.00557
22.50	763.53	.8266	0.0000	0.	.00557
25.00	763.43	.8266	0.0000	0.	.00557
27.50	763.19	.8267	0.0000	2.7621E-04	.00557
30.00	762.86	.8272	0.0000	3.3038E-03	.00556
32.50	762.42	.8280	0.0000	5.9621E-03	.00553
35.00	761.80	.8292	0.0000	9.0073E-03	.00549
37.50	750.91	.8309	0.0000	1.3074E-02	.00544
40.00	759.65	.8333	0.0000	1.8529E-02	.00536
42.50	757.96	.8366	0.0000	2.5285E-02	.00526
45.00	755.78	.8407	0.0000	3.2742E-02	.00512
47.50	753.18	.8457	0.0000	3.9834E-02	.00497
50.00	750.25	.8513	0.0000	4.5360E-02	.00479
52.50	747.19	.8574	0.0000	4.8354E-02	.00459
55.00	744.19	.8634	0.0000	4.8406E-02	.00440
57.50	741.45	.8692	0.0000	4.5735E-02	.00422
60.00	739.10	.8744	0.0000	4.1044E-02	.00405
62.50	737.18	.8790	0.0000	3.5247E-02	.00390
65.00	735.66	.8828	0.0000	2.9216E-02	.00378
67.50	734.49	.8858	0.0000	2.3598E-02	.00368
70.00	733.59	.8883	0.0000	1.8748E-02	.00360
72.50	732.89	.8903	0.0000	1.4756E-02	.00354
75.00	732.35	.8918	0.0000	1.1542E-02	.00349
77.50	731.94	.8930	0.0000	8.9542E-03	.00346
80.00	731.64	.8939	0.0000	6.8482E-03	.00343
82.50	731.43	.8946	0.0000	5.1236E-03	.00340
85.00	731.28	.8951	0.0000	3.7297E-03	.00339
87.50	731.18	.8954	0.0000	2.6528E-03	.00338
90.00	731.11	.8957	0.0000	1.8973E-03	.00337
92.50	731.05	.8959	0.0000	1.4648E-03	.00336
95.00	730.96	.8960	0.0000	1.3420E-03	.00336
97.50	730.85	.8962	0.0000	1.5010E-03	.00335
100.00	730.69	.8965	0.0000	1.9158E-03	.00334

QCOND(1) = 1559131

TIME 3.5000E-01 HRS

FLOW STREAM INFORMATION FOR DYNAMIC SIMULATION

STREAM	TK	PSIA	CO	H2	CH4	H2O	CO2	N2	TOTAL
			FLOWRATES(LBMOLES/HR)						
1	310.0	834.0	12.00	36.30	18.83	0.00	0.00	7.88	75.0
2	310.0	834.0	6.40	19.35	10.03	0.00	0.00	4.20	39.9
3	302.4	834.0	6.81	21.47	98.67	.07	0.00	26.95	153.9
4	559.0	834.0	6.81	21.47	98.67	.07	0.00	26.95	153.9
5	743.3	834.0	.55	2.67	104.94	6.34	0.00	26.95	141.4
6	310.0	834.0	5.60	16.95	8.79	0.00	0.00	3.68	35.0
7	305.2	834.0	5.71	17.50	31.51	.02	0.00	9.51	64.2
8	639.9	834.0	6.28	20.24	136.43	6.33	0.00	36.46	205.7
9	732.1	834.0	.67	3.41	142.03	11.34	0.00	36.46	194.5
10	300.0	834.0	.67	3.40	142.04	.11	0.00	36.46	182.6
11	300.0	834.0	.53	2.67	111.36	.09	0.00	28.58	143.2
12	300.0	834.0	.42	2.12	88.64	.07	0.00	22.75	114.0
13	300.0	834.0	.11	.54	22.72	.02	0.00	5.83	29.2
14	300.0	834.0	0.00	0.00	0.00	11.83	0.00	0.00	11.8
15	300.0	834.0	.14	.73	30.68	.02	0.00	7.87	39.4

REACTOR NO. 1

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
0.00	559.00	0.0000	0.0000	1.6091E+00	.04426
2.50	580.83	.0985	0.0000	1.7938E+00	.04025
5.00	604.08	.2062	0.0000	1.9317E+00	.03579
7.50	628.02	.3192	0.0000	1.9853E+00	.03101
10.00	651.52	.4317	0.0000	1.9258E+00	.02615
12.50	673.32	.5370	0.0000	1.7557E+00	.02152
15.00	692.48	.6298	0.0000	1.5034E+00	.01735
17.50	708.51	.7074	0.0000	1.2362E+00	.01382
20.00	721.42	.7696	0.0000	9.7454E-01	.01094
22.50	731.44	.8177	0.0000	7.4227E-01	.00870
25.00	738.93	.8533	0.0000	5.4000E-01	.00702
27.50	744.21	.8780	0.0000	3.6520E-01	.00585
30.00	747.67	.8936	0.0000	2.2364E-01	.00511
32.50	749.75	.9025	0.0000	1.2351E-01	.00469
35.00	750.90	.9071	0.0000	6.2921E-02	.00447
37.50	751.48	.9093	0.0000	3.0268E-02	.00436
40.00	751.76	.9104	0.0000	1.4526E-02	.00431
42.50	751.85	.9109	0.0000	6.8526E-03	.00429
45.00	751.87	.9112	0.0000	4.0022E-03	.00428
47.50	751.82	.9113	0.0000	2.2975E-03	.00427
50.00	751.77	.9115	0.0000	2.4029E-03	.00426
52.50	751.66	.9116	0.0000	1.7753E-03	.00426
55.00	751.58	.9117	0.0000	2.7683E-03	.00425
57.50	751.42	.9118	0.0000	1.9277E-03	.00424
60.00	751.35	.9120	0.0000	3.7006E-03	.00424
62.50	751.12	.9122	0.0000	1.9408E-03	.00423
65.00	751.07	.9124	0.0000	4.9784E-03	.00422
67.50	750.77	.9126	0.0000	1.3005E-03	.00421
70.00	750.80	.9129	0.0000	6.6601E-03	.00420
72.50	750.36	.9130	0.0000	0.	.00419
75.00	750.55	.9134	0.0000	8.5237E-03	.00417
77.50	749.91	.9137	0.0000	0.	.00416
80.00	750.39	.9141	0.0000	1.0780E-02	.00414
82.50	749.38	.9144	0.0000	0.	.00412
85.00	750.38	.9150	0.0000	1.3778E-02	.00409

87.50	748.75	.9154	0.0000	0.	.00408
90.00	750.58	.9161	0.0000	1.8226E-02	.00404
92.50	747.93	.9167	0.0000	0.	.00401
95.00	751.10	.9176	0.0000	2.4390E-02	.00397
97.50	746.87	.9184	0.0000	0.	.00393
100.00	751.98	.9196	0.0000	3.2152E-02	.00387

REACTOR NO. 2

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
0.00	637.62	0.0000	0.0000	2.1832E+00	.03054
2.50	676.80	.2584	0.0000	2.0012E+00	.02301
5.00	707.57	.4749	0.0000	1.5964E+00	.01651
7.50	730.96	.6346	0.0000	1.1279E+00	.01161
10.00	746.48	.7384	0.0000	7.1923E-01	.00837
12.50	756.29	.7914	0.0000	3.8800E-01	.00669
15.00	760.83	.8156	0.0000	1.4656E-01	.00592
17.50	762.70	.8248	0.0000	2.9945E-02	.00563
20.00	763.22	.8267	0.0000	0.	.00557
22.50	763.42	.8267	0.0000	0.	.00557
25.00	763.53	.8267	0.0000	0.	.00557
27.50	763.62	.8267	0.0000	0.	.00557
30.00	763.69	.8267	0.0000	0.	.00557
32.50	763.70	.8267	0.0000	0.	.00557
35.00	763.70	.8267	0.0000	0.	.00557
37.50	763.64	.8267	0.0000	0.	.00557
40.00	763.57	.8267	0.0000	0.	.00557
42.50	763.43	.8267	0.0000	0.	.00557
45.00	763.24	.8267	0.0000	0.	.00557
47.50	763.03	.8269	0.0000	1.6898E-03	.00557
50.00	762.75	.8274	0.0000	3.2375E-03	.00555
52.50	762.38	.8282	0.0000	5.6864E-03	.00553
55.00	761.83	.8292	0.0000	7.6745E-03	.00549
57.50	761.07	.8307	0.0000	1.1613E-02	.00545
60.00	759.99	.8328	0.0000	1.5898E-02	.00538
62.50	758.59	.8356	0.0000	2.1469E-02	.00529
65.00	756.79	.8391	0.0000	2.7490E-02	.00518
67.50	754.63	.8433	0.0000	3.3628E-02	.00505
70.00	752.14	.8481	0.0000	3.8994E-02	.00489
72.50	749.42	.8535	0.0000	4.2915E-02	.00472
75.00	746.62	.8591	0.0000	4.4757E-02	.00454
77.50	743.90	.8646	0.0000	4.4358E-02	.00436
80.00	741.39	.8699	0.0000	4.1894E-02	.00420
82.50	739.20	.8747	0.0000	3.7893E-02	.00404
85.00	737.37	.8789	0.0000	3.2990E-02	.00391
87.50	735.89	.8825	0.0000	2.7827E-02	.00379
90.00	734.72	.8855	0.0000	2.2892E-02	.00370
92.50	733.81	.8879	0.0000	1.8492E-02	.00362
95.00	733.09	.8899	0.0000	1.4746E-02	.00356
97.50	732.54	.8914	0.0000	1.1647E-02	.00351
100.00	732.12	.8926	0.0000	9.1144E-03	.00347

QCOND(1) = 1564815

TIME 4.0000E-01 HRS

FLOW STREAM INFORMATION FOR DYNAMIC SIMULATION

STREAM	TK	PSIA	FLOWRATES(LBMOLES/HR) CO	H2	CH4	H2O	CO2	N2	TOTAL
1	310.0	834.0	12.00	36.30	18.83	0.00	0.00	7.88	75.0
2	310.0	834.0	6.40	19.35	10.03	0.00	0.00	4.20	39.9
3	302.4	834.0	6.92	21.79	98.57	.07	0.00	26.95	154.2
4	553.0	834.0	6.92	21.79	98.57	.07	0.00	26.95	154.2
5	750.7	834.0	.60	2.82	104.89	6.39	0.00	26.95	141.6
6	310.0	834.0	5.60	16.95	8.79	0.00	0.00	3.68	35.0
7	305.2	834.0	5.74	17.58	31.48	.02	0.00	9.51	64.3
8	640.2	834.0	6.34	20.40	136.37	6.41	0.00	36.46	205.9
9	743.6	834.0	.85	3.33	141.86	11.90	0.00	36.46	195.0
10	300.0	834.0	.84	3.31	141.87	.11	0.00	36.46	183.1
11	300.0	834.0	.66	3.06	111.23	.09	0.00	28.58	143.6
12	300.0	834.0	.52	2.44	88.54	.07	0.00	22.75	114.3
13	300.0	834.0	.13	.62	22.69	.02	0.00	5.83	29.3
14	300.0	834.0	0.00	0.00	0.00	11.79	0.00	0.00	11.7
15	300.0	834.0	.18	.84	30.64	.02	0.00	7.87	39.5

REACTOR NO. 1

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
1.00	559.00	0.0000	0.0000	1.6380E+00	.04485
2.50	581.23	.0989	0.0000	1.8331E+00	.04077
5.00	604.89	.2075	0.0000	1.9789E+00	.03621
7.50	629.22	.3216	0.0000	2.0353E+00	.03133
10.00	653.00	.4351	0.0000	1.9719E+00	.02636
12.50	674.96	.5410	0.0000	1.7920E+00	.02163
15.00	694.13	.6341	0.0000	1.5341E+00	.01740
17.50	710.07	.7115	0.0000	1.2503E+00	.01382
20.00	722.80	.7733	0.0000	9.8082E-01	.01092
22.50	732.61	.8208	0.0000	7.4298E-01	.00867
25.00	739.87	.8558	0.0000	5.3681E-01	.00700
27.50	744.95	.8799	0.0000	3.5989E-01	.00585
30.00	748.23	.8949	0.0000	2.1838E-01	.00513
32.50	750.18	.9034	0.0000	1.1982E-01	.00472
35.00	751.25	.9077	0.0000	6.0825E-02	.00451
37.50	751.79	.9099	0.0000	2.9303E-02	.00440
40.00	752.06	.9109	0.0000	1.3835E-02	.00435
42.50	752.17	.9113	0.0000	6.4694E-03	.00433
45.00	752.21	.9116	0.0000	3.1805E-03	.00432
47.50	752.22	.9117	0.0000	1.6085E-03	.00431
50.00	752.22	.9117	0.0000	9.9616E-04	.00431
52.50	752.21	.9118	0.0000	6.0137E-04	.00431
55.00	752.20	.9118	0.0000	5.4657E-04	.00431
57.50	752.18	.9118	0.0000	3.8872E-04	.00431
60.00	752.16	.9119	0.0000	5.1720E-04	.00430
62.50	752.14	.9119	0.0000	4.2327E-04	.00430
65.00	752.11	.9119	0.0000	6.7077E-04	.00430
67.50	752.07	.9120	0.0000	5.8634E-04	.00430
70.00	752.04	.9120	0.0000	9.3577E-04	.00430
72.50	751.99	.9121	0.0000	8.2977E-04	.00430
75.00	751.94	.9121	0.0000	1.2934E-03	.00429
77.50	751.86	.9122	0.0000	1.1296E-03	.00429
80.00	751.80	.9123	0.0000	1.7503E-03	.00428
82.50	751.71	.9124	0.0000	1.4574E-03	.00428
85.00	751.63	.9125	0.0000	2.3170E-03	.00427

87.50	751.51	.9126	0.0000	1.7587E-03	.00427
90.00	751.42	.9127	0.0000	2.9857E-03	.00426
92.50	751.27	.9129	0.0000	1.9263E-03	.00426
95.00	751.17	.9131	0.0000	3.7721E-03	.00425
97.50	750.98	.9132	0.0000	1.8721E-03	.00424
100.00	750.89	.9134	0.0000	4.9184E-03	.00423

REACTOR NO. 2

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
0.00	639.85	0.0000	0.0000	2.2121E+00	.03077
2.50	679.42	.2616	0.0000	2.0536E+00	.02309
5.00	710.29	.4799	0.0000	1.6177E+00	.01649
7.50	732.87	.6395	0.0000	1.1354E+00	.01155
10.00	748.16	.7415	0.0000	7.1263E-01	.00833
12.50	757.37	.7919	0.0000	3.7982E-01	.00673
15.00	761.76	.8155	0.0000	1.4021E-01	.00598
17.50	763.29	.8242	0.0000	3.0061E-02	.00570
20.00	763.61	.8260	0.0000	4.2932E-03	.00564
22.50	763.60	.8263	0.0000	2.2418E-03	.00563
25.00	763.60	.8264	0.0000	5.9691E-04	.00563
27.50	763.67	.8265	0.0000	0.	.00562
30.00	763.75	.8265	0.0000	0.	.00562
32.50	763.78	.8265	0.0000	0.	.00562
35.00	763.74	.8265	0.0000	0.	.00562
37.50	763.67	.8265	0.0000	0.	.00562
40.00	763.59	.8265	0.0000	1.7672E-04	.00562
42.50	753.56	.8266	0.0000	4.2449E-04	.00562
45.00	753.57	.8266	0.0000	0.	.00562
47.50	763.62	.8266	0.0000	0.	.00562
50.00	763.66	.8266	0.0000	0.	.00562
52.50	763.67	.8266	0.0000	0.	.00562
55.00	763.64	.8266	0.0000	0.	.00562
57.50	763.56	.8266	0.0000	8.3543E-05	.00562
60.00	763.45	.8268	0.0000	1.1183E-03	.00562
62.50	763.31	.8270	0.0000	1.8546E-03	.00561
65.00	763.16	.8273	0.0000	2.4150E-03	.00560
67.50	762.98	.8277	0.0000	2.9990E-03	.00558
70.00	762.74	.8282	0.0000	3.8613E-03	.00557
72.50	762.40	.8289	0.0000	5.2328E-03	.00555
75.00	761.92	.8299	0.0000	7.2967E-03	.00552
77.50	761.25	.8312	0.0000	1.0156E-02	.00547
80.00	760.34	.8330	0.0000	1.3843E-02	.00542
82.50	759.15	.8353	0.0000	1.8303E-02	.00534
85.00	757.65	.8383	0.0000	2.3360E-02	.00525
87.50	755.82	.8419	0.0000	2.8678E-02	.00513
90.00	753.68	.8461	0.0000	3.3770E-02	.00500
92.50	751.29	.8508	0.0000	3.8054E-02	.00484
95.00	748.73	.8559	0.0000	4.0978E-02	.00468
97.50	746.13	.8611	0.0000	4.2164E-02	.00451
100.00	743.61	.8662	0.0000	4.1501E-02	.00435

QCOND(1) = 1615398

TIME 4.5000E-01 HRS

FLOW STREAM INFORMATION FOR DYNAMIC SIMULATION

STREAM	TK	PSIA	FLOWRATES(LBMOLES/HR) CO	H2	CH4	H2O	CO2	N2	TOTAL
1	310.0	834.0	12.00	36.30	18.83	0.00	0.00	7.88	75.0
2	310.0	834.0	6.40	19.35	10.03	0.00	0.00	4.20	39.9
3	302.4	834.0	7.06	22.21	98.43	.07	0.00	26.95	154.7
4	559.0	834.0	7.06	22.21	98.43	.07	0.00	26.95	154.7
5	752.4	834.0	.61	2.86	104.88	6.52	0.00	26.95	141.8
6	310.0	834.0	5.60	16.95	8.79	0.00	0.00	3.68	35.0
7	305.2	834.0	5.77	17.59	31.44	.02	0.00	9.51	64.4
8	642.5	834.0	6.37	20.50	136.34	6.55	0.00	36.46	206.2
9	760.7	834.0	1.07	4.59	141.64	11.86	0.00	36.46	195.6
10	300.0	834.0	1.07	4.59	141.64	.11	0.00	36.46	183.8
11	300.0	834.0	.84	3.50	111.05	.09	0.00	28.58	144.1
12	300.0	834.0	.67	2.86	88.39	.07	0.00	22.75	114.7
13	300.0	834.0	.17	.73	22.65	.02	0.00	5.83	29.4
14	300.0	834.0	0.00	0.00	0.00	11.74	0.00	0.00	11.7
15	300.0	834.0	.23	.99	30.59	.02	0.00	7.87	39.7

REACTOR NO. 1

REACTOR LENGTH	TEMP (K)	FPACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
0.00	559.00	0.0000	0.0000	1.6773E+00	.04564
2.50	581.81	.0996	0.0000	1.8872E+00	.04147
5.00	606.25	.2094	0.0000	2.0481E+00	.03679
7.50	631.49	.3254	0.0000	2.1138E+00	.03173
10.00	656.20	.4409	0.0000	2.0488E+00	.02659
12.50	678.95	.5485	0.0000	1.8555E+00	.02169
15.00	698.68	.6425	0.0000	1.5776E+00	.01733
17.50	714.87	.7201	0.0000	1.2736E+00	.01367
20.00	727.59	.7813	0.0000	9.8719E-01	.01075
22.50	737.14	.8276	0.0000	7.3506E-01	.00851
25.00	743.96	.8609	0.0000	5.1671E-01	.00689
27.50	748.46	.8830	0.0000	3.3302E-01	.00581
30.00	751.16	.8962	0.0000	1.9384E-01	.00516
32.50	752.57	.9033	0.0000	1.0391E-01	.00481
35.00	753.23	.9070	0.0000	5.3354E-02	.00463
37.50	753.42	.9089	0.0000	2.7964E-02	.00453
40.00	753.45	.9100	0.0000	1.5387E-02	.00448
42.50	753.31	.9106	0.0000	9.8519E-03	.00445
45.00	753.24	.9110	0.0000	6.5540E-03	.00443
47.50	753.03	.9113	0.0000	5.4602E-03	.00442
50.00	753.00	.9116	0.0000	3.9009E-03	.00440
52.50	752.77	.9118	0.0000	3.9635E-03	.00439
55.00	752.82	.9119	0.0000	2.5824E-03	.00438
57.50	752.56	.9121	0.0000	3.1907E-03	.00438
60.00	752.71	.9122	0.0000	1.3606E-03	.00437
62.50	752.39	.9123	0.0000	2.7992E-03	.00436
65.00	752.65	.9124	0.0000	2.0203E-04	.00436
67.50	752.24	.9125	0.0000	2.4408E-03	.00436
70.00	752.64	.9126	0.0000	0.	.00435
72.50	752.11	.9127	0.0000	2.0707E-03	.00435
75.00	752.67	.9127	0.0000	0.	.00434
77.50	751.97	.9128	0.0000	1.7572E-03	.00434
80.00	752.72	.9129	0.0000	0.	.00434
82.50	751.83	.9129	0.0000	1.6350E-03	.00434
85.00	752.78	.9130	0.0000	0.	.00433

87.50	751.66	.9130	0.0000	1.6826E-03	.00433
90.00	752.85	.9131	0.0000	0.	.00433
92.50	751.45	.9132	0.0000	1.9863E-03	.00432
95.00	752.93	.9132	0.0000	0.	.00432
97.50	751.17	.9133	0.0000	2.6347E-03	.00432
100.00	753.02	.9134	0.0000	0.	.00431

REACTOR NO. 2

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
0.00	641.66	0.0000	0.0000	2.2698E+00	.03090
2.50	680.69	.2644	0.0000	2.0760E+00	.02311
5.00	712.72	.4840	0.0000	1.6391E+00	.01643
7.50	736.52	.6439	0.0000	1.1456E+00	.01146
10.00	751.70	.7435	0.0000	7.0288E-01	.00831
12.50	760.70	.7888	0.0000	3.6665E-01	.00686
15.00	764.74	.8114	0.0000	1.1673E-01	.00613
17.50	766.13	.8186	0.0000	1.5881E-02	.00590
20.00	766.31	.8196	0.0000	7.6680E-04	.00587
22.50	766.20	.8199	0.0000	1.6300E-03	.00586
25.00	765.86	.8205	0.0000	4.0492E-03	.00584
27.50	765.51	.8212	0.0000	5.5816E-03	.00582
30.00	765.15	.8220	0.0000	6.3724E-03	.00579
32.50	764.84	.8228	0.0000	6.3381E-03	.00577
35.00	764.57	.8235	0.0000	5.8910E-03	.00575
37.50	764.35	.8241	0.0000	5.2614E-03	.00573
40.00	764.16	.8247	0.0000	4.5463E-03	.00571
42.50	764.00	.8251	0.0000	3.9018E-03	.00569
45.00	763.88	.8255	0.0000	3.1932E-03	.00568
47.50	763.80	.8258	0.0000	2.4482E-03	.00567
50.00	763.76	.8260	0.0000	1.7092E-03	.00567
52.50	763.73	.8261	0.0000	1.1223E-03	.00566
55.00	763.72	.8262	0.0000	7.4366E-04	.00566
57.50	763.70	.8262	0.0000	6.0543E-04	.00566
60.00	763.67	.8263	0.0000	5.8620E-04	.00566
62.50	763.64	.8264	0.0000	5.6394E-04	.00565
65.00	763.62	.8264	0.0000	4.6557E-04	.00565
67.50	763.62	.8265	0.0000	2.9839E-04	.00565
70.00	763.62	.8265	0.0000	9.2779E-05	.00565
72.50	763.61	.8265	0.0000	9.3622E-05	.00565
75.00	763.59	.8265	0.0000	2.6905E-04	.00565
77.50	763.54	.8266	0.0000	5.8758E-04	.00565
80.00	763.47	.8267	0.0000	1.0241E-03	.00564
82.50	763.37	.8270	0.0000	1.5258E-03	.00563
85.00	763.23	.8272	0.0000	2.1041E-03	.00563
87.50	763.05	.8276	0.0000	2.8139E-03	.00561
90.00	762.81	.8281	0.0000	3.7499E-03	.00560
92.50	762.49	.8287	0.0000	5.0339E-03	.00558
95.00	762.05	.8296	0.0000	6.7962E-03	.00555
97.50	761.47	.8308	0.0000	9.1491E-03	.00551
100.00	750.68	.8324	0.0000	1.2165E-02	.00546

QCOND(1) = 1696736

TIME 4.7500E-01 HRS

FLOW STREAM INFORMATION FOR DYNAMIC SIMULATION

STREAM	TK	PSIA	CO	H2	CH4	H2O	CO2	N2	TOTAL
			FLOWRATES(LBMOLES/HR)						
1	310.0	834.0	12.00	36.30	18.83	0.00	0.00	7.88	75.0
2	310.0	834.0	6.40	19.35	10.03	0.00	0.00	4.20	39.9
3	302.4	834.0	7.08	22.27	98.41	.07	0.00	26.95	154.7
4	559.0	834.0	7.08	22.27	98.41	.07	0.00	26.95	154.7
5	752.4	834.0	.62	2.88	104.87	6.53	0.00	26.95	141.8
6	310.0	834.0	5.60	16.35	8.79	0.00	0.00	3.68	35.0
7	305.2	834.0	5.78	17.70	31.44	.02	0.00	9.51	64.4
8	641.6	834.0	6.39	20.56	136.32	6.56	0.00	36.46	206.2
9	762.9	834.0	1.10	4.58	141.61	11.85	0.00	36.46	195.7
10	300.0	834.0	1.10	4.68	141.61	.11	0.00	36.46	183.9
11	300.0	834.0	.86	3.57	111.02	.09	0.00	28.58	144.2
12	300.0	834.0	.68	2.32	88.38	.07	0.00	22.75	114.8
13	300.0	834.0	.18	.75	22.65	.02	0.00	5.83	29.4
14	300.0	834.0	0.00	0.00	0.00	11.74	0.00	0.00	11.7
15	300.0	834.0	.24	1.01	30.59	.02	0.00	7.87	39.7

REACTOR NO. 1

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATE1	YCO
0.00	559.00	0.0000	0.0000	1.6824E+00	.04574
2.50	581.89	.0997	0.0000	1.8943E+00	.04156
5.00	606.46	.2097	0.0000	2.0579E+00	.03686
7.50	631.91	.3260	0.0000	2.1261E+00	.03178
10.00	656.89	.4419	0.0000	2.0623E+00	.02661
12.50	679.95	.5500	0.0000	1.8680E+00	.02168
15.00	699.99	.6443	0.0000	1.5873E+00	.01729
17.50	716.49	.7220	0.0000	1.2797E+00	.01361
20.00	729.46	.7833	0.0000	9.8905E-01	.01068
22.50	739.22	.8294	0.0000	7.3177E-01	.00845
25.00	746.14	.8621	0.0000	5.0716E-01	.00685
27.50	750.64	.8833	0.0000	3.1872E-01	.00581
30.00	753.27	.8955	0.0000	1.7951E-01	.00521
32.50	754.61	.9019	0.0000	9.3105E-02	.00489
35.00	755.17	.9052	0.0000	4.6935E-02	.00473
37.50	755.28	.9068	0.0000	2.4745E-02	.00465
40.00	755.19	.9078	0.0000	1.4698E-02	.00460
42.50	754.98	.9084	0.0000	1.0377E-02	.00457
45.00	754.74	.9089	0.0000	8.4087E-03	.00455
47.50	754.47	.9093	0.0000	7.5684E-03	.00452
50.00	754.23	.9097	0.0000	6.9344E-03	.00450
52.50	753.97	.9101	0.0000	6.6093E-03	.00449
55.00	753.77	.9104	0.0000	6.0180E-03	.00447
57.50	753.54	.9108	0.0000	5.7476E-03	.00445
60.00	753.39	.9110	0.0000	5.0008E-03	.00444
62.50	753.18	.9113	0.0000	4.8056E-03	.00443
65.00	753.10	.9115	0.0000	3.9026E-03	.00441
67.50	752.90	.9118	0.0000	3.8976E-03	.00440
70.00	752.88	.9119	0.0000	2.8484E-03	.00440
72.50	752.69	.9121	0.0000	3.0611E-03	.00439
75.00	752.75	.9122	0.0000	1.8583E-03	.00438
77.50	752.52	.9124	0.0000	2.5097E-03	.00437
80.00	752.67	.9124	0.0000	9.5920E-04	.00437
82.50	752.39	.9125	0.0000	2.1545E-03	.00437
85.00	752.63	.9126	0.0000	0.	.00436

87.50	752.28	.9127	0.0000	1.8797E-03	.00436
90.00	752.62	.9127	0.0000	0.	.00436
92.50	752.18	.9128	0.0000	1.5796E-03	.00435
95.00	752.61	.9128	0.0000	0.	.00435
97.50	752.06	.9129	0.0000	1.5115E-03	.00435
100.00	752.60	.9129	0.0000	0.	.00435

REACTOR NO. 2

REACTOR LENGTH	TEMP (K)	FRACTIONAL CONVERSION OF CO METH	SHIFT	RATEL	YCO
0.00	639.89	0.0000	0.0000	2.2613E+00	.03098
2.50	681.39	.2647	0.0000	2.0948E+00	.02316
5.00	713.25	.4850	0.0000	1.6468E+00	.01645
7.50	736.62	.6448	0.0000	1.1470E+00	.01146
10.00	752.04	.7441	0.0000	7.0340E-01	.00831
12.50	761.33	.7885	0.0000	3.6579E-01	.00689
15.00	765.59	.8109	0.0000	1.0722E-01	.00617
17.50	767.09	.8175	0.0000	6.8674E-03	.00596
20.00	767.41	.8179	0.0000	0.	.00594
22.50	767.33	.8179	0.0000	0.	.00594
25.00	767.09	.8181	0.0000	8.2091E-04	.00594
27.50	766.84	.8185	0.0000	2.9005E-03	.00592
30.00	766.58	.8191	0.0000	4.0364E-03	.00591
32.50	766.31	.8197	0.0000	4.7666E-03	.00589
35.00	766.01	.8204	0.0000	5.3784E-03	.00586
37.50	765.70	.8211	0.0000	5.8955E-03	.00584
40.00	765.37	.8219	0.0000	6.2124E-03	.00581
42.50	765.07	.8227	0.0000	6.2298E-03	.00579
45.00	764.79	.8234	0.0000	5.9718E-03	.00577
47.50	764.54	.8240	0.0000	5.4910E-03	.00574
50.00	764.33	.8246	0.0000	4.8880E-03	.00573
52.50	764.16	.8251	0.0000	4.2319E-03	.00571
55.00	764.02	.8255	0.0000	3.5592E-03	.00570
57.50	763.91	.8259	0.0000	2.8846E-03	.00569
60.00	763.84	.8261	0.0000	2.2390E-03	.00568
62.50	763.79	.8263	0.0000	1.6707E-03	.00567
65.00	763.75	.8264	0.0000	1.2266E-03	.00567
67.50	763.72	.8266	0.0000	9.2586E-04	.00566
70.00	763.69	.8266	0.0000	7.4433E-04	.00566
72.50	763.67	.8267	0.0000	6.2853E-04	.00566
75.00	763.65	.8268	0.0000	5.2693E-04	.00566
77.50	763.63	.8268	0.0000	4.2093E-04	.00566
80.00	763.62	.8269	0.0000	3.3150E-04	.00565
82.50	763.61	.8269	0.0000	3.0566E-04	.00565
85.00	763.58	.8269	0.0000	3.8797E-04	.00565
87.50	763.54	.8270	0.0000	5.9899E-04	.00565
90.00	763.48	.8272	0.0000	9.3507E-04	.00564
92.50	763.38	.8273	0.0000	1.3847E-03	.00564
95.00	763.26	.8276	0.0000	1.9501E-03	.00563
97.50	763.08	.8279	0.0000	2.6635E-03	.00562
100.00	762.86	.8284	0.0000	3.5920E-03	.00560

QCOND(1) = 1707246

```
 07/01/81 LEHIGH U. NOS/BE-1.4   L530     05/31/81
20.26.58.SWIMOH2  FROM
20.25.58.SWIM,B****,T250,*OBIE,CM120000,STOFF.
20.27.00.ACCOUNT(***)
20.27.00.PAGES(N,100)
20.27.01.MAP(PART)
20.27.01.ATTACH(DSS,DSSDYN,ID=JEO)
20.27.01.AT CY= 002 SN=SYSTEM
20.27.01.ATTACH(PDATAB,PDATAB,ID=WES)
20.27.02.AT CY= 001 SN=SYSTEM
20.27.02.ATTACH(OLDPL,DYGEN,ID=JEO)
20.27.02.AT CY= 002 SN=SYSTEM
20.27.03.UPDATE(F,D,L=12)
20.27.13. UPDATE COMPLETE.
20.27.14.OLD(RUNT)
20.27.14.RUNT(S6,,,COMPILE)
20.28.26.   21700  OCTAL REQUIRED
20.28.27.      8.922 CP SECONDS COMPILATION
20.28.27.LOAD(DSS)
20.28.28.LOAD(PDATAB)
20.28.28.LOAD(LGO)
20.28.28.EXECUTE.
20.29.24.      NON-FATAL LOADER ERRORS - SEE MAP
21.29.34.SS TIME LIMIT
21.29.34.P=062307,FL=074100
21.29.34.OP  00046848 WORDS - FILE OUTPUT , DC 40
21.29.36.SYSTEM SECONDS USED BY THIS JOB = 250.0
21.29.36.EXECUTION COST OF THIS JOB, NOT INCL I/O COST, IS $ 16.00
21.29.36.CURRENT AUTHORIZATION BALANCE IS $  272.07
21.29.36.NR. OF NON-STANDARD (DISK) CIO CALLS =      117
21.29.36.NR. OF SYSTEM REQUESTS =     1129
21.29.40.MAXIMUM 114000 CM WORDS USED.
21.29.40.CP      531.789 SEC.
21.29.40.PP       43.136 SEC.
21.29.40.CM        7.237 SEC.

****** 21.34.31.    SWIMOH2 005558 LINES PRINTED  /// END OF LIST ///   LQ  23
```
****** 21.34.31.   SWIMOH2 005558 LINES PRINTED /// END OF LIST ///   LQ 23

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3. Stein, F. P., "DSS/2 Ideal Gas Physical Properties Package," Tech. report DCE4, Lehigh University, 1979.

4. Schiesser, W. E., "DSS/2-An Introductory to the Numerical Methods of Lines Integration of Partial Differential Equations," Tech. report, Lehigh University, 1977.

5. Hu, S. S. and W. E. Schiesser, "Partial Differentiator-Lagrange, PDL33," 1980. Developed at Lehigh University, program to be published with other work later.

Appendix D: Listing of Dynamic Program Portion (DYGEN) of GRPDYN

```
            SUBROUTINE INITAL
      C...
      C...
            COMMON/T/ T,NRUN,NFIN
  2         COMMON/Y/ TK1(41),TK2(41)
  2         COMMON/F/ DTK1(41),DTK2(41)
  2   C...
      C...
            COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
  2         COMMON/INDAT/ NUNITS,NSTMS,IORD(15)
  2         COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
  2         COMMON/UNIT/ NRXR,NHX,NDIV,NMIX,NCDR,IRXR(2),RLNTH(2),
  2        1            IHX(5),ICDR(2),AREA(2)
             COMMON/ODFEED/ TKFDOD,PRFDOD,FDOD(8),TTFDOD
  2         COMMON/MEP/ X1(41,2),X2(41,2),NC,NFLAG,NFLAG1,NPTS,ND,L(41)
  2         COMMON/HPASS/ HRX537(3),DELALF(3),DELBET(3),DELGT2(3),
  2        1 DEGOV2(3),HI537(3),HO(3),GRX537(3),GI537(3),GO(3)
            COMMON/STOICH/ A(3,8), DELA(3)
  2         COMMON/POINT/ ID(8)
  2         REAL L
  2   C...
      C
      C     NOTATION
      C
      C        DTK1(I) = FIRST DERIVATIVE OF TK1(I) W/R TO TIME
      C        DTK2(I) = FIRST DERIVATIVE OF TK2(I) W/R TO TIME
      C        NC = NUMBER OF COMPONENTS
      C        ND = MAXIMUM NUMBER OF REACTOR POINTS WHICH MAY BE USED
      C        T = TIME (HR)
      C        TK1(I) = TEMPERATURE (K) AT POINT I IN REACTOR 1
      C        TK2(I) = TEMPERATURE (K) AT POINT I IN REACTOR 2
      C
  2         NC = 6
  4         ND = 41
      C...
      C...  THE COMPONENTS ARE IDENTIFIED IN SUBROUTINE IDENT.
      C...
  5         CALL IDENT
  6         CALL STOICH
  7         CALL HPREP
 10         CALL FLOWST
      C...
      C...
      C...  THE TEMPERATURE PROFILE IN THE REACTOR IS TK(41).
      C...  TK1 IS CALCULATED FROM DIFFERENTIAL EQUATIONS DEFINED IN DERVR1
      C...  AND INITIALIZED IN INITR1.
      C...
 11         CALL INITR(NRXR)
 13         NFLAG=0
 14         NFLAG1 = 0
 15         NFLAG1 = NFLAG1 + 1
      C...
 17         RETURN
 17         END


            SUBROUTINE FLOWST
      C
      C        SUBROUTINE FLOWST READS THE PROCESS FLOWSHEET
      C        INFORMATION FOR THE PROCESS UNDER STUDY
      C
            COMMON/INDAT/ NUNITS,NSTMS,IORD(15)
  2         COMMON/UNIT/ NRXR,NHX,NDIV,NMIX,NCDR,IRXR(2),RLNTH(2),
  2        1            IHX(5),ICDR(2),AREA(2)
            COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
  2         COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
  2          COMMON/ODFEED/ TKFDOD,PRFDOD,FDOD(8),TTFDOD
  2         COMMON/MEP/ DUM(164),NC,NFLAG,NFLAG1,NPTS,ND,L(41)
  2         COMMON/PRT/ Q(16),RATE1(41,2),RATE2(41,2),YCOMP(41,8,2)
  2
      C
      C     NOTATION
      C
      C              CALLED FROM INITAL
      C
      C        DUMDAT(  ) = DUMMY ARRAY CONTAINING REQUIRED DATA
      C
```

```
C                  FOR UNIT J
C       FDOD(I) = MOLAR FLOWRATE OF OLD FEED STREAM CONDITIONS FOR
C            COMPONENT I
C       FSTM(J,I) = FLOWRATE OF COMPONENT I IN STREAM J, LBMOLE PER HR
C       IFD = FEED STREAM NUMBER
C       IHX = INDIVIDUAL HEAT EXCHANGER NUMBER
C       IN(J,I) = STREAM NUMBER ENTERING UNIT J FROM INLET POSITION I
C       IORD(I) = ORDER IN WHICH WHICH UNIT I IS CALCULATED
C       IUNIT(J) = INDIVIDUAL UNIT NUMBER FOR J-TH UNIT
C       JCDR = CONDENSER COUNTER
C       JHX = HEAT EXCHNAGER COUNTER
C       JR = REACTOR COUNTER
C       KT(J) = TYPE OF INDIVIDUAL UNIT FOR J-TH UNIT, WHERE -
C                   1 = REACTOR 1
C                   2 = HEAT EXCHANGER WITH CONSTANT HEAT DUTY
C                   3 = STREAM DIVIDER
C                   4 = STREAM MIXER
C                   5 = CONDENSER WITH CONSTANT FRACTION OF WATER REMOVAL
C                   6 = REACTOR 2
C                   7 = HEAT EXCHANGER WITH CONSTANT OUTLET TEMPERATURE
C                   8 = CONDENSER WITH CONSTANT HEAT DUTY
C       NCDR = TOTAL NUMBER OF CONDENSERS
C       NHX = TOTAL NUMBER OF HEAT EXCHANGERS
C       NMIX = TOTAL NUMBER OF MIXERS
C       NOUT(J,I) = STREAM NUMBER EXITING UNIT J FROM OUTLET POSITION 1
C       NPTS = TOTAL NUMBER OF POINTS BEING USED FOR ALL REACTOR GRIDS
C       NRXR = TOTAL NUMBER OF REACTORS
C       NSTMS = TOTAL NUMBER OF STREAMS BEING USED IN THE PROCESS
C       NUNITS = TOAL NUMBER OF UNITS BEING SIMULATED
C       PRFDOD = PRESSURE IN PSIA OF THE OLD FEED STREAM CONDITIONS
C       PRSTM(J) = PRESSURE (PSIA) OF STREAM J
C       Q(I) = ARRAY FOR TEXT CARDS
C       RLNTH(I) = LENGTH IN FEET OF REACTOR I
C       TKFDOD = TEMPERATURE (K) OF OLD FEED STREAM CONDITIONS
C       TKSTM(J) = TEMPERATURE (K) OF STREAM J
C         TTFDOD = TOTAL MOLAR FLOW OF THE OLD FEED STREAM CONDITIONS
C       TTFSTM(J) = TOTAL MOLAR FLOW OF STRAM J IN LBMOLES PER HR
C
C
C             READ TEXT CARDS
      READ 105,(Q(I),I=1,16)
  105 FORMAT (8A10)
C
      READ 100,  NRXR,NHX,NDIV,NMIX,NCDR,NSTMS,NPTS
  100 FORMAT(7I5)
C
      NUNITS = NRXR + NHX + NDIV + NMIX + NCDR
C
C            READ PROCESS FLOWSHEET
C
      JR = 0
      JHX = 0
      JCDR = 0
      DO 10 J = 1, NUNITS
      READ 110,      (IUNIT(J),KT(J),(IN(J,I),I = 1,3),(NOUT(J,I),I=1,2))
  110 FORMAT (7I5)
C
C            DETERMINE HX NUMBER FOR FUTURE USE
C
      IF(JHX.EQ.NHX) GO TO 70
      IF(KT(J).EQ.2) GO TO 75
      GO TO 70
   75 CONTINUE
      JHX = JHX + 1
      IHX(JHX) = IUNIT(J)
   70 CONTINUE
C
C            DETERMINE COND NUMBER FOR FUTURE USE
C
      IF(JCDR.EQ.NCDR) GO TO 80
      IF(KT(J).EQ.5) GO TO 85
      GO TO 80
   85 CONTINUE
      JCDR = JCDR + 1
      ICDR(JCDR) = IUNIT(J)
   80 CONTINUE
C
```

```
C        READ OTHER REQUIRED DATA FOR UNIT TYPE, FOR A REACTOR,
C        ALSO READ THE LENGTH OF REACTOR
C
      JJ = IUNIT(J)
      IF (KT(J).EQ.1) GO TO 60
      IF (KT(J).EQ.6) GO TO 62
      IF ((KT(J).EQ.2).OR.(KT(J).EQ.5)) GO TO 64
      READ 112,      DUMDAT(JJ)
  112 FORMAT (F10.5)
      GO TO 65
   60 CONTINUE
      READ 111, DUMDAT(JJ), RLNTH(1)
      GO TO 65
   62 CONTINUE
      READ 111, DUMDAT(JJ), RLNTH(2)
  111 FORMAT(2F10.5)
      GO TO 65
   64 CONTINUE
      READ 113, DUMDAT(JJ)
  113 FORMAT(E12.4)
   65 CONTINUE
   10 CONTINUE
C
C           READ OLD FEED STREAM CONDITIONS
C
      READ 120,  IFD,TKFDOD,PRFDOD,TTFDOD,(FDOD(I),I=1, NC)
  120 FORMAT(I5,3F10.3,/,8F10.5)
C
C           READ NEW FEED CONDITIONS AS WELL AS ALL OTHER STREAM CONDITIO
C
      DO 33 J = 1, NSTMS
      READ 125,   TKSTM(J),PRSTM(J),TTFSTM(J),(FSTM(J,I),I=1,NC)
  125 FORMAT(5X,3F10.3,/,8F10.5)
   33 CONTINUE
C
C            READ ORDER OF UNIT CALCULATION
C
      READ 130,    (IORD(I), I=1,NUNITS)
  130 FORMAT (20I5)
      RETURN
      END


      SUBROUTINE INITR(NRXR)
C
C           THIS SUBROUTINE IS CALLED BY INITAL TO READ THE INITIAL
C                REACTOR TEMPERATURE PROFILES
C
C...  INITIALIZATION OF REACTOR 1 DIFFERENTIAL EQUATIONS
C
      COMMON/Y/ TK(41,2)
      COMMON/MEP/ X1(41,2),X2(41,2),NC,NFLAG,NFLAG1,NPTS,ND,L(41)
      COMMON/PRT/ Q(16),RATE1(41,2),RATE2(41,2),YCOMP(41,8,2)
      REAL L
C
C     NOTATION
C
C        I = GRID POINT COUNTER
C        K = REACTOR COUNTER
C        L(I) PERCENT OF REACTOR LENGTH AT ITH POINT IN REACTOR GRID
C        TK(I,K) = TEMPERATURE (K) AT POINT I IN REACTOR K
C        X1(I,K) = FRACTIONAL CONVERSION BY REACTION 1 AT POINT I
C                  REACTOR K
C        YCOMP(I,J,K) = FRACTIONAL COMPOSITION OF COMPONENT J AT POINT I
C                    IN REACTOR K(EXCLUDING N2)
C
C          READ INITIAL TEMP AND CONVERSION PROFILES OBTAINED BY
C           STEADY STATE METHANATION ROUTINE, WHERE IPTS IS THE
C           NUMBER OF REACTOR GRID POINTS.
C
      DO 10 K = 1, NRXR
      DO 20 I = 1, NPTS
      READ 100, L(I),TK(I,K),X1(I,K),X2(I,K)
      READ 102, (YCOMP(I,J,K),J=1,5),RATE1(I,K)
  100 FORMAT(5X,F6.2,F8.1,2X,2F12.4)
  102 FORMAT(15X,5F10.5,E13.4)
```

```
   20 CONTINUE
      IF (NPTS.EQ.ND) GO TO 10
      J = NPTS + 1
      DO 30 I = J, ND
      TK(I,K) = 0.
      X1(I,K) = 0.
      X2(I,K) = 0.
   30 CONTINUE
   10 CONTINUE
      RETURN
      END


      SUBROUTINE DERV
C
C        SUBROUTINE DERV CALLS THE INDIVIDUAL PROCESS SUBROUTINES
C        IN THE SEQUENCE SPECIFIED BY THE ORDER OF UNIT CALCULATIONS
C
C
      COMMON /T/ T,NFIN,NRUN
      COMMON/Y/ TK1(41),TK2(41)
      COMMON/F/ DTK1(41),DTK2(41)
      COMMON/INDAT/ NUNITS,NSTMS,IORD(15)
      COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
      COMMON/UNIT/ NRXR,NHX,NDIV,NMIX,NCDR,IRXR(2),RLNTH1,RLNTH2,
     1             IHX(5),ICDR(2)
      COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
      COMMON/MEP/ X11(41),X21(41),X12(41),X22(41),NC,NFLAG
      COMMON/STOICH/ A(3,8), DELA(3)
      COMMON/HPASS/ HRX537(3),DELALF(3),DELBET(3),DELGT2(3),
     1 DEGOV2(3),HI537(3),HO(3),GRX537(3),GI537(3),GO(3)
      COMMON/POINT/ ID(8)
      COMMON/PRT/ Q(16),RTE11(41),RTE21(41),DUM(82),YCOMP1(41,8),
     1   YCOMP2(41,8)
C
C
      DO 100 I = 1, NUNITS
      J = 0
   90 CONTINUE
      J = J + 1
      IF(IORD(I).EQ.IUNIT(J)) GO TO 95
      GO TO 90
   95 CONTINUE
      K = IUNIT(J)
      JKT = KT(J)
C
C
      GO TO (1,2,3,4,5,6,7,8),JKT
    1 CALL DERVR (K,1,TK1,DTK1,X11,X12,RTE11,YCOMP1)
      GO TO 100
    2 CALL HXQ(K)
      GO TO 100
    3 CALL DIV(K)
      GO TO 100
    4 CALL MIXER(K)
      GO TO 100
    5 CALL CONCF(K)
      GO TO 100
    6 CALL DERVR(K,2,TK2,DTK2,X21,X22,RTE21,YCOMP2)
      GO TO 100
    7 CALL HTX(K)
      GO TO 100
    8 CALL CONDQ(K)
  100 CONTINUE
      RETURN
      END


      SUBROUTINE DERVR (KK,JR,TK,DTKDT,X1,X2,RTE1,YDUM)
C
C        THIS SUBROUTINE CONTAINS THE DIFFERENTIAL EQUATIONS TO
C        BE SOLVED FOR EACH POINT ALONG THE REACTOR BEING CALCULATED
C
C
C
      COMMON/UNIT/ NRXR,NHX,NDIV,NMIX,NCDR,IRXR(2),RLNTH(2),
```

```
                 1        IHX(5),ICDR(2)
    13             COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
    13             COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
    13             COMMON/MEP/ DUM(164),NC,NFLAG,NFLAG1,NPTS,ND,L(41)
    13             COMMON/STOICH/ A(3,8), DELA(3)
    13             COMMON/HPASS/ HRX537(3),DELALF(3),DELBET(3),DELGT2(3),
                 1 DEGOV2(3),HI537(3),HO(3),GRX537(3),GI537(3),GO(3)
          C...
          C...
          C...     COMMON BLOCK /STORL/ CONTAINS ALL VARIABLES NEEDED BY
          C...     SUBROUTINE DERVL TO CALCULATE THE DERIVATIVES OF ALL SPATIAL
          C...     VARIABLES AT ANY GRID POINT IN A REACTOR.  IN THIS MODEL, THE
          C...     SPATIAL VARIABLES ARE THE FRACTIONAL CONVERSIONS OF CO DUE TO THE
          C...     METHANATION AND SHIFT REACTIONS.
    13             COMMON/STORL/ FINL(8),FOUTL(8),TKL(41),P,TOTMIN,TOTMOL,
                 1              TKOUTL,PSIAOL,FTOTOT(41),Y(8),HRXT(41,3),
                 2              HRX(3),GOVT(3),KCHEM(3),CPAVG(41),RATE1(41),
                 3              RATE2(41),AREAL,RELIN(8),YCOMP(41,8)
    13             DIMENSION FIN(8),FOUT(8)
    13             DIMENSION II(41),DTKDL(41),DTKDL2(41),DXDL(41,2)
    13             DIMENSION TK(41),DTKDT(41),X(41,2),X1(41),X2(41),RTE1(41),
                 1    YDUM(41,8)
    13             REAL KCHEM,LTOT,L
          C
          C            CALLED FROM DERV
          C
          C            AREA = CROSS-SECTIONAL AREA OF REACTOR IN SQ. FT.
          C            BLKRHO = BULK RATIO OF THE CTALYST
          C            CCAT = HEAT CAPCITY OF THE CATALYST
          C            DTKDT(I) = FIRST DERIVATIVE OF TEMP. W/R TO TIME AT POINT I
          C            DTKDL2 = SECOND DERIVATIVE OF TEMP. W/R TO TIME
          C            DXDL = DIRST DERIVATIVE OF FRACTIONAL CONVERION W/R TO LENGTH
          C            FIN(I) FLOWRATE OF COMPONENT I( IN LBMOLES PER HR)
          C            IER = STREAM NUMBER ENTERING REACTOR
          C            ILR = STREAM NUMBER LEAVING THE REACTOR
          C            LTOT = TOTAL PERCENT LENGTH OF THE REACTOR BEING STUDIED
          C            REACL = REACTOR LENGTH OF REACTOR IN QUESTION
          C            TKIN = TEMPERATURE ENTERING THE REACTOR (ALOS AT POINT 1)
          C            VOID = VOID FRACTION IN THE REACTOR BED
          C
    13             VOID = 0.37
    14             CCAT = 0.258
    16             BLKRHO = 88.0
    17             LTOT = 100.
          C
          C               DETERMINE THE STREAM NUMBERS BEING USED
          C
    21             IER = IN(KK,1)
    26             ILR = NOUT(KK,1)
    32             AREA = DUMDAT(KK)
    35             REACL = RLNTH(JR)
    40             TKIN = TKSTM(IER)
    43             DO 18 J = 1, NC
    45          18 FIN(J) = FSTM(IER,J)
    57             FTOTIN = TTFSTM(IER)
          C...
          C...     SET CONDITIONS AT INLET FACE OF REACTOR.
          C...
    62             TK(1) = TKIN
    66             X(1,1) = 0.0
    74             X(1,2) = 0.0
   101             DTKDT(1) = 0.
          C...
          C...
          C...     REACTOR PRESSURE CONSTANT THROUGHOUT THE REACTOR.
          C...
   104             P = PRSTM(IER)
          C...
          C...
          C...     CLAMP TO PREVENT EXCESS NEGATIVE TEMPERATURE EXCURSIONS.
          C...
   107             DO 1 J=2,NPTS
   111             IF(TK(J).GT.(TKIN-10.)) GO TO 1
   120             TK(J)=TKIN-10.
   125             DTKDT(J)=0.
   131           1 CONTINUE
          C...
```

```
          C...   CLAMP TO PREVENT EXCESS POSITIVE EXCURSIONS.
          C...
 134             DO 2 J=2,NPTS
 135             IF(TK(J).LT.1500.) GO TO 2
 141             TK(J)=1500.
 145             DTKDT(J)=0.
 151      2      CONTINUE
          C...
          C...
          C...   CONSTANTS REQUIRED IN EVALUATION OF TEMPORAL DERIVATIVES.
          C...
 154             TERM1 = VOID * P / 19.3158
 156             TERM2 = BLKRHO*CCAT
          C...
          C...
          C...
          C...   COMPUTE THE 1ST AND 2ND SPATIAL DERIVATIVES OF TEMPERATURE.
          C...
 160             CALL DSS014 (0.,LTOT,NPTS,TK,DTKDL,1.)
 165             CALL DSS014 (0.,LTOT,NPTS,DTKDL,DTKDL2,1.)
          C...
          C...
          C...   IF NO CO IN FEEC THEN NO REACTIONS OCCUR.
          C...
 171             IF(FIN(1).LE.0.) GO TO 15
          C...
          C...
          C...   NORMALIZE TOTAL FLOW WITH RESPECT TO FIRST COMPONENT FLOW.
          C...
 201             TOTMIN    = FTOTIN/FIN(1)
          C...
          C...
          C...   NORMALIZE COMPONENT FLOWS WITH RESPECT TO FIRST COMPONENT FLOW.
          C...
 205             DO 14 I=1,NC
 206             RELIN(I) = FIN(I)/FIN(1)
 216          14 CONTINUE
          C...
          C...
 221             DO 10 K=1,NC
 222             FINL(K) = FIN(K)
 227          10 CONTINUE
 232             AREAL = AREA
 233             DO 11 J=1,NPTS
 235             TKL(J) = TK(J)
 242          11 CONTINUE
          C...
          C...
          C...   COMPUTE THE FRACTIONAL CONVERSION OF CO BY EACH REACTION AT EACH
          C...   SPATIAL POINT.
          C...
 245             CALL INTALL (X,DXDL,2,NPTS,L,REACL)
          C...
          C...
 251             TTFSTM(ILR) = 0.
 255             DO 12 K=1,NC
 262             FOUT(K) = FOUTL(K)
 267             FSTM(ILR,K) = FOUTL(K)
 277             TTFSTM(ILR) = TTFSTM(ILR) + FSTM(ILR,K)
 311          12 CONTINUE
 314             TKOUT = TKOUTL
 315             TKSTM(ILR) = TKOUTL
 321             PSIAOT = PSIAOL
 323             PRSTM(ILR) = PSIAOL
          C...
          C...
          C...   COMPUTE TEMPORAL DERIVATIVES OF TEMPERATURE TK.
          C...
 327             DO 20 J=2,NPTS
 330             TERM3 = FTOTOT(J) * 100./AREA/REACL
 335             DTKDT(J) = ( -HRXT(J,1)*RATE1(J) - HRXT(J,2)*RATE2(J) -
                1 TERM3*CPAVG(J)*DTKDL(J))/( TERM1/TK(J)*CPAVG(J) +
                2 TERM2 ) + 1.02*DTKDL2(J)
 407          20 CONTINUE
          C
          C        RESTORE X VALUES FOR TRANSFER BACK TO DERV
          C
```

```
      DO 30 I = 1, NPTS
      X1(I) = X(I,1)
      X2(I) = X(I,2)
      RTE1(I) = RATE1(I)
      DO 22 J = 1, NC
   22 YDUM(I,J) = YCOMP(I,J)
   30 CONTINUE
      RETURN
C...
C...
C...  SPECIAL CODING EXECUTED ONLY IN UNUSUAL CASE OF NO CO IN FEED IN
C...  WHICH CASE NO REACTIONS OCCUR.  FLOWS, COMPOSITIONS, AND TOTAL
C...  FLOW ARE THE SAME AS INLET VALUES.
C...
C...
   15 CONTINUE
      DO 32 I=1,NC
      FOUT(I)=FIN(I)
      FSTM(ILR) = FIN(I)
   32 Y(I)=FIN(I)/FTOTIN
      TKOUT = TK(NPTS)
      TKSTM(ILR) = TK(NPTS)
      PSIAOT=P
      PRSTM(ILR) = P
C...
C...
C...  SET VALUES OF X AND CALCULATE TEMPORAL DERIVATIVES. NOTE THAT
C...  THERE COULD BE TEMPERATURE CHANGES IN ABSENCE OF CHEMICAL
C...  REACTIONS.
C...
C...
      DO 31 J=1,NPTS
      IP=J
      X(IP,1) = 0.0
      X(IP,2) = 0.0
      CALL HRXYCP(TK,HRX,GOVT,KCHEM,CPAV,Y,IP)
      IF(J.EQ.1) GO TC 31
      TERM4 = FTOTIN * 100./AREA/REACL
      DTKDT(J) = ( -TERM4*CPAVG(J)/DTKDL(J) ) / (TERM1/TK(J)*CPAVG(J) +
     1 TERM2 ) + 1.02*DTKDL2(J)
   31 CONTINUE
C
C      RESTORE X VALUES FOR TRANSFER BACK TO DERV
C
      DO 33 I = 1, NPTS
      X1(I) = X(I,1)
      X2(I) = X(I,2)
   33 CONTINUE
      RETURN
      END


      SUBROUTINE INTALL (Y,F,NVARL,NPTS,L,REACL)
C...
C...
C...  SUBROUTINE INTALL INTEGRATES ALL SPATIAL VARIABLES FROM THE INLET
C...  TO THE OUTLET OF A REACTOR. THE VALUES OF THE SPATIAL DERIVATIVES
C...  ARE CALCULATED IN SUBROUTINE DERVL.
C...
C...
      DIMENSION Y(41,2),F(41,2),E(2)
      DIMENSION L(41)
      REAL L
C...
C...
C...
C...  ALL SPATIAL VARIABLES ARE INTEGRATED TO THE NEXT GRID POINT USING
C...  THE EXPLICIT EULER PREDICTOR-CORRECTOR METHOD.
C...
      J = 1
      CALL DERVL (Y,F,NVARL,NPTS,J,REACL)
   20 CONTINUE
      H = L(J+1) - L(J)
      DO 10 I = 1, NVARL
      Y(J+1,I) = Y(J,I) + F(J,I)*H
   10 CONTINUE
C...
C...
C...  THE VALUES OF ALL SPATIAL VARIABLES AT THE ADVANCED GRID POINT ARE
```

```
          C...   CORRECTED BY CALCULATING AN ERROR TERM.
          C...
 50              J = J + 1
 52              CALL DERVL (Y,F,NVARL,NPTS,J,REACL)
 53              DO 11 I=1,NVARL
 60              E(I) = (F(J,I) - F(J-1,I))*H/2.
 77              Y(J,I) = Y(J,I) + E(I)
112         11   CONTINUE
          C...
          C...
          C...   THE DERIVATIVES OF ALL SPATIAL VARIABLES AT THE ADVANCED GRID
          C...   POINT ARE CALCULATED. THE SUBROUTINE RETURNS ONLY AFTER THE LAST
          C...   GRID POINT IS REACHED.
          C...
115              CALL DERVL (Y,F,NVARL,NPTS,J,REACL)
116              IF (J.EQ.NPTS) RETURN
124              GO TO 20
125              END


                 SUBROUTINE DERVL (X,DXDL,NVARL,NPTS,IP,REACL)
          C...
          C...
          C...   SUBROUTINE DERVL CALCULATES THE DERIVATIVES OF ALL SPATIAL
          C...   VARIABLES AT ANY GRID POINT IN A REACTOR. IN THIS CASE, THE
          C...   SPATIAL VARIABLES ARE THE FRACTIONAL CONVERSION OF CO DUE TO THE
          C...   METHANATION AND SHIFT REACTIONS.
          C...
 11              COMMON/MEP/ DUM(164),NC
 11              COMMON/STOICH/ A(3,8), DELA(3)
 11              COMMON/HPASS/ HRX537(3),DELALF(3),DELBET(3),DELGT2(3),
               1  DEGOV2(3),HI537(3),HO(3),GRX537(3),GI537(3),GO(3)
 11              COMMON/STORL/ FIN(8),FOUT(8),TK(41),P,TOTMIN,TOTMOL,TKOUT,
               1               PSIAOT,FTOTOT(41),Y(8),HRXT(41,3),HRX(3),
               2               GOVT(3),KCHEM(3),CPAVG(41),RATE1(41),RATE2(41),
               3               AREA,RELIN(8),YCOMP(41,8)
 11              DIMENSION X(41,2),DXDL(41,2)
          C...
          C...
          C...   XADJ IS CALLED TO ADJUST THE FRACTIONAL CONVERSION OF EACH
          C...   REACTION IF ANY REACTANTS ARE TOTALLY CONSUMED.
          C...
 11              CALL XADJ (X,NPTS,RELIN,P,IP)
          C...
          C...
          C...   THE MOLE FRACTIONS ARE CALCULATED AT A GIVEN GRID POINT.
          C...
 13              TERM3 = FIN(1) * 100./AREA/REACL
 24              CALL YSFLOW (IP,TK,P,X,TOTMIN,TOTMOL,FIN,TKOUT,PSIAOT,FTOT,FOUT,Y)
 40              FTOTOT(IP) = FTOT
          C...
          C...
          C...   THE HEAT CAPACITY OF THE GAS STREAM AND THE HEATS OF REACTION
          C...   ARE CALCULATED AT A GIVEN GRID POINT.
          C...
 50              CALL HRXYCP (TK,HRX,GOVT,KCHEM,CPAV,Y,IP)
 57              CPAVG(IP) = CPAV
 67              DO 10 I=1,3
 71              HRXT(IP,I) = HRX(I)
100         10   CONTINUE
          C...
          C...
          C...   THE RATE OF REACTION FOR EACH REACTION IS CALCULATED.
          C...
102              CALL RATE (TK,P,Y,R1,R2,KCHEM,IP)
111              RATE1(IP) = R1
121              RATE2(IP) = R2
          C...
          C...
          C...   THE SPATIAL DERIVATIVES ARE CALCULATED.
          C...
125              DXDL(IP,1) = RATE1(IP)/TERM3
135              DXDL(IP,2) = RATE2(IP)/TERM3
145              RETURN
146              END
```

```
      SUBROUTINE HXQ(KK)
      COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
      COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
      COMMON/UNIT/ NRXR,NHX,NDIV,NMIX,NCOR,IRXR(2),RLNTH1,RLNTH2,
     1        IHX(5),ICOR(2),AREA(2)
      COMMON/MEP/ DUM(164),NC
      COMMON/POINT/ ID(8)
      DIMENSION YY(8),T(26)
C
C          THIS SUBROUTINE ASSUMES A CONSTANT HEAT DUTY, Q,
C          PROCEEDING THROUGH THE EXCHANGER AT ALL TIMES,
C          ASSUMING NO CONTROL IS ON THE UNIT.
C
C
C        CALLED FROM DERV
C
C
C
C     NOTATION
C
C        IEH = STREAM NUMBER ENTERING HEAT EXCHANGER
C        ILH = STREAM NUMBER EXITING THE HEAT EXCHANGER
C        QHX = HEAT DUTY BEING USED IN THE EXCHANGER, FROM DUMDAT
C        YY(J) = FRACTION OF COMPOSITION OF COMPOUND J
C        HIEH(HILH) = ENTHALPY (BTU/LBMOLE) OF STREAM ENTERING HEAT E
C                  (LEAVING ) HEAT EXCHANGER
C        TIEH (TILH) = TEMPERATURE OF STREAM ENTERING
C                   (LEAVING) HEAT EXCHANGER
C
      IEH = IN(KK,1)
      ILH = NOUT(KK,1)
C
C           NOTE-  POS Q - HEAT ADDITION,
C                  NEG Q - HEAT REMOVAL
C
      QHX = DUMDAT(KK)
      PRSTM(ILH) = PRSTM(IEH)
      DO 10 K = 1, NHX
   10 IF(IHX(K).EQ.IUNIT(KK)) LL=K
      DO 2 J = 1, NC
      YY(J) = FSTM(IEH,J)/TTFSTM(IEH)
    2 FSTM(ILH,J) = FSTM(IEH,J)
      TTFSTM(ILH) = TTFSTM(IEH)
C
C          CALCULATE THE EXIT TEMPERATURE FOR THE EXCHANGER
C
      TIEH = TKSTM(IEH) * 1.8
C
C          CALCULATE THE ENTHALPY IN BTU/(LBMOLE) FOR ENTERING STREAM
C
      CALL HGAS (ID,NC,TIEH,YY,CPAVG,HIEH)
      HILH = (HIEH*TTFSTM(IEH) + QHX)/TTFSTM(ILH)
C
      TOL = 10.
      LOOP = 1
      T(LOOP) = 1200.
   20 CONTINUE
      CALL HGAS(ID,NC,T(LOOP),YY,CPIMG,TAHILH)
      DEL = HILH - TAHILH
      ADEL = ABS(DEL)
      IF(ADEL.LE.TOL) GO TO 30
      CALL FALPOS(T(LOOP),DEL,LOOP,TNEW)
      LOOP = LOOP + 1
      T(LOOP) = TNEW
      IF (LOOP.EQ.26) GO TO 40
      GO TO 20
   30 CONTINUE
      TKSTM(ILH) = T(LOOP)/1.8
      RETURN
   40 WRITE(NO,100)
  100 FORMAT(/,10X,*HX IN TROUBLE*)
      OUTPUT,LOOP,T(LOOP),DEL,TNEW
      RETURN
      END
```

```
              SUBROUTINE HXT(KK)
      6       COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
      6       COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
      6       COMMON/UNIT/ NRXR,NHX,NDIV,NMIX,NCDR,IRXR(2),RLNTH1,RLNTH2,
             1           IHX(5),ICDR(2),AREA(2)
      6       COMMON/MEP/ DUM(164),NC
      6       COMMON/PCINT/ ID(8)
      6       DIMENSION YY(8),T(26)
        C
        C          THIS SUBROUTINE MAINTAINS A CONSTANT EXIT
        C          TEMPERATURE, ASSUMING PERFECT CONTROL
        C
        C          CALLLED FORM DERV
        C
        C     NOTATION
        C         IEH = STREAM NUMBER ENTERING HEAT EXCHANGER
        C         ILH = STREAM NUMBER LEAVING THE HEAT EXCHANGER
        C         DUMDAT = NEW TEMPERATUE OF STREAM (K)
        C         DUMDAT(15) = HEAT DUTY CALCULATED FOR THE EXCHANGER
      6       IEH = IN(KK,1)
     13       ILH = NOUT(KK,1)
     17       TKSTM(ILH) = DUMDAT(KK)
     24       PRSTM(ILH) = PRSTM(IEH)
     31       DO 10 K = 1, NHX
     32    10 IF(IHX(K).EQ.IUNIT(KK)) LL=K
     43       DO 2 J = 1, NC
     44       YY(J) = FSTM(IEH,J)/TTFSTM(IEH)
     55     2 FSTM(ILH,J) = FSTM(IEH,J)
     70       TTFSTM(ILH) = TTFSTM(IEH)
        C
        C          CALCULATE THE HEAT DUTY FOR THE EXCHANGER
        C
     75       TIEH = TKSTM(IEH) * 1.8
    101       TILH = TKSTM(ILH) * 1.8
        C
        C          CALCULATE CPAVG IN BTU/(LBMOLE)(DEG R)
        C
    105       CALL CPMEAN (ID, NC,TILH,TIEH,YY,CPAVG)
        C
        C          CALCULATE QHX IN BTU/(HR)
        C
    111       DUMDAT(15) = CPAVG * (TILH - TIEH) * TTFSTM(IEH)
    121       RETURN
    122       END


              SUBROUTINE DIV(I)
      6       COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
      6       COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
      6       COMMON/MEP/ DUM(164),NC
        C
        C          THIS SUBROUTINE ACTS AS A STREAM DIVIDER
        C
        C
        C
        C     NOTATION
        C          DUMDAT = FRACTION OF INLET STREAM BEING
        C                   DIVERTED TO OUTLET STREAM NI
        C                   DIVERTED TO OUTLET STREAM NO. 1 (DIVFRC)
        C        FSUM1 (FSUM2) = TOTAL FLOWRATE OF STREAM LEAVING
        C                   FROM POSITION 1 (2)
        C        IED = STREAM NUMBER ENTERING DIVIDER
        C        IOD1 = STREAM NUMBER LEAVING DIVIDER FROM POSITION 1
        C        IOD2 = STREAM NUMBER LEAVING DIVIDER FROM POSITION 2
        C
      6       DIVFRC = DUMDAT(I)
     11       IED = IN(I,1)
     16       IOD1 = NOUT(I,1)
     22       IOD2 = NOUT(I,2)
     27       FSUM1 = 0.
     30       FSUM2 = 0.
     31       DO 2 J = 1, NC
     33       FSTM(IOD1,J) = FSTM(IED,J) * DIVFRC
     44       FSTM(IOD2,J) = FSTM(IED,J) * (1. - DIVFRC)
     57       FSUM1 = FSUM1 + FSTM(IOD1,J)
     64       FSUM2 = FSUM2 + FSTM(IOD2,J)
```

```
  71       2 CONTINUE
  73         TTFSTM(IOD1) = FSUM1
  76         TTFSTM(IOD2) = FSUM2
 101         TKSTM(IOD1) = TKSTM(IED)
 106         PRSTM(IOD1) = PRSTM(IED)
 113         TKSTM(IOD2) = TKSTM(IED)
 120         PRSTM(IOD2) = PRSTM(IED)
 125         RETURN
 126         END


             SUBROUTINE MIXER(I)
       C
       C        SUBROUTINE MIXER COMBINES THE CONTENTS OF TWO OR THREE
       C        STREAMS, AND THEN DETERMINES THE NEW STREAM TEMPERATURE
   6         COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
   6         COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
   6         COMMON/UNIT/ NRXR,NHX,NDIV,NMIX
   6         COMMON/MEP/ DUM(164),NC
   6         COMMON/POINT/ ID(8)
   6         DIMENSION DMCOMP(8),IEM(4),SUMF(8)
       C        NOTATION
       C
       C        DMCOMP(J) = DUMMY VARIABLE FOR THE MOLEFRACTION  OF
       C                COMPOUND J IN STREAM ILM
       C        HOUT = ENTHALPY OF OUTLET STREAM, CAL
       C        HSUM = SUM OF INLET STREAM ENTHALPIES, CAL
       C        IEM(K) = STREAM NUMBER ENTERING MIXER FROM POSITION K
       C        ILM = STREAM NUMBER LEAVING MIXER
       C        K = COUNTER FOR THE INLET STREAM POSITIONS, NUMBERED 1, 2, OR3
       C        SUMF(J) = SUM OF EACH COMPOUND J IN NEW STREAM(LBMOL/HR
       C        TKDUM = DUMMY VARIABLE FOR THE TEMP OF ONE OF THE ENTERING
       C                STREAMS, (K)
       C        TNEW = TEMPERATURE OF OUTLET STREAM DEG R
       C        TSUMF = TOTAL FLOW OF NEW STREAM, LBMOL/HR
       C
       C          DETERMINE STREAM NUMBERS ENTERING AND LEAVING MIXER
       C
   6         DO 1 K = 1, 3
   7         IEM(K) = IN(I,K)
  15       1 CONTINUE
  17         ILM = NOUT(I,1)
       C
       C          SUM COMPONENT FLOWS OF ALL STREAMS AND GET NEW TOTAL FLOW
       C
  24         TSUMF = 0.
  25         DO 3 J = 1, NC
  26         SUMF(J) = 0.
  30         DO 5 K = 1, 3
  32         IED = IEM(K)
  35         IF(IED.EQ.0) GO TO 5
  36         SUMF(J) = SUMF(J) + FSTM(IED,J)
  50       5 CONTINUE
  52         TSUMF = TSUMF + SUMF(J)
  56         FSTM(ILM,J) = SUMF(J)
  65       3 CONTINUE
  67         TTFSTM(ILM) = TSUMF
       C
       C          CALCULATE INDIVIDUAL STREAM ENTHALPIES
       C          CALCULATE NEW OUTLET STREAM TEMPERATURE
       C
  72         THI = 0.
  73         TLO = 0.
  74         HSUM = 0.
  75         DO 7 K = 1, 4
  77         IF (K.EQ.4) GO TO 6
 101         IED = IEM(K)
 104         IF(IED.EQ.0) GO TO 7
 106         TKDUM = TKSTM(IED)*1.8
 112         GO TO 8
 112       6 CONTINUE
 112         IED = ILM
 114       8 CONTINUE
 114         DO 9 J = 1, NC
       C
       C          CALCULATE STREAM COMPOSITION
```

```
C
      DMCOMP(J) = FSTM(IED,J)/TTFSTM(IED)
    9 CONTINUE
C
C          CALCULATE INDIVIDUAL STREAM ENTHALPIES
C
      IF (K.EQ.4) GO TO 7
      CALL HGAS (ID,NC,TKDUM,DMCOMP,CPIGM,HDUM)
      CALL HILO (K,TKDUM,THI,TLO,HDUM,HHI,HLO)
      HSUM = HSUM + HDUM*TTFSTM(IED)
    7 CONTINUE
      HOUT = HSUM/TSUMF
      CALL TCALC(ID,NC,DMCOMP,THI,TLO,HHI,HLO,TNEW,HOUT)
      TKSTM(ILM) = TNEW/1.8
      IEDD = IN(I,1)
      PRSTM (ILM) = PRSTM(IEDD)
      RETURN
      END


      SUBROUTINE HILC(K,XDUM,XHI,XLO,YDUM,YHI,YLO)
C
C          THIS SUBROUTINE KEEPS TRACK OF PRESENT HI AND LO TEMP VALUES
C
      IF(K.GT.1) GO TO 12
      XLO = XDUM
      YLO = YDUM
      GO TO 18
   12 CONTINUE
      IF (K.GT.2) GO TO 16
      IF (XDUM.GE.XLO) GO TO 13
      GO TO 15
   13 CONTINUE
      XHI = XDUM
      YHI = YDUM
   15 CONTINUE
      IF (XDUM.LT.XLO) GO TO 14
      GO TO 18
   14 CONTINUE
      XHI = XLC
      YHI = YLC
      XLO = XDUM
      YLO = YDUM
      GO TO 18
   16 CONTINUE
      IF (XDUM.GE.XHI) GO TO 17
      GO TO 19
   17 CONTINUE
      XHI = XDUM
      YHI = YDUM
   19 CONTINUE
      IF (XDUM.LE.XLO) GO TO 21
      GO TO 18
   21 CONTINUE
      XLO = XDUM
      YLO = YDUM
   18 CONTINUE
      RETURN
      END


      SUBROUTINE CONDF(KK)
      COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
      COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
      COMMON/UNIT/ NRXR,NHX,NDIV,NMIX,NCDR,IRXR(2),RLNTH1,RLNTH2,
     1         IHX(5),ICDR(2),QCOND(2)
      COMMON/POINT/ ID(8)
      COMMON/MEP/ DUM(164),NC
C          SUBROUTINE COND SIMULATES A CONDENSOR UNIT.  GIVEN A
C          PARTICULAR STREAM AND THE DESIRED PERCENTAGE OF WATER
C          REMCVAL, CONDF WILL CALCULATE THE TEMPERATURE AND THE
C          WATER CONTENT OF BOTH STREAMS LEAVING THE UNIT.
C          THE WATER VAPOR PRESSURE IS DETERMINED FROM THE
C          ANTOINE EQUATION.
C
```

```
     6          DIMENSION T(25),YIEC(8),YILC1(8)
     6          LL = 1
     7          N = NC
    11          LOOP = 1
    12          TOL = 0.5
    13          IEC = IN(KK,1)
    20          ILC1 = NOUT(KK,1)
    24          ILC2 = NOUT(KK,2)
    31          DO 5 K = 1, NCDR
    33        5 IF(ICDR(K).EQ.IUNIT(KK)) LL=K
    44          CFRAC = CUMDAT(KK)
    47          PCOND = PRSTM(IEC)
    52          FTOL = FSTM(IEC,4) * CFRAC
          C          INITIALLY SET THE FLOW RATES OUT OF THE CONDENSOR*S TWO STMS
          C
    57          DO 10 I = 1, NC
    61          FSTM(ILC1,I) = FSTM(IEC,I)
    71       10 FSTM(ILC2,I) = 0.
          C
          C          CALCULATE THE FLOWRATE OF THE INERTS
   100          FINRT = TTFSTM(IEC) - FSTM(IEC,4)
          C          ASSUME AN INITIAL TEMPERATURE
          C
   110          T(LOOP) = 500.
   113       20 CONTINUE
          C          CALCULATE WATER VAPOR PRESSURE AT THE ASSUMED TEMPERATURE
          C          USING THE ANTOINE EQUATION (CONSTANTS TAKEN FROM PRS),IN PSIA
          C
   113          VPH2O = (EXP(18.3036 - 3816.44/(T(LOOP) - 46.13))) * 14.7/760.
          C          CALCULATE INERTS PRESSURE, IN PSIA
          C
   127          PINRT = PCOND - VPH2O
   131          IF (PINRT.LE.0.) GO TO 25
          C          CALCULATE LBMOLES OF STEAM CONDENSING
          C
   134          FVAP = FINRT * VPH2O / PINRT
   137          FCOND = FSTM(IEC,4) - FVAP
          C          CHECK FOR CONVERGENCE
          C
   145          DEL = FCOND - FTOL
   147          ADEL = ABS(DEL)
   153          IF (ADEL.LE.TOL) GO TO 30
          C          CALL FALSE POSITION ROUTINE TO CONVERGE TO A SOLUTION
          C
   157          CALL FALPOS (T(LOOP),DEL,LOOP,TNEW)
   164          LOOP = LOOP + 1
   166          T(LOOP) = TNEW
   171          IF (LOOP.EQ.26) GO TO 40
   175          GO TO 20
   176       25 CONTINUE
          C          USE THIS ROUTE IF THE VPH2O IS .GT. THE CONDENSOR PRESS.
          C
   176          T(LOOP) = T(LOOP) - 100.
   204          GO TO 20
   204       30 CONTINUE
   204          TKSTM(ILC1) = T(LOOP)
   211          TKSTM(ILC2) = T(LOOP)
   216          PRSTM(ILC1) = PCOND
   221          PRSTM(ILC2) = PCOND
   224          FSTM(ILC1,4) = FVAP
   231          FSTM(ILC2,4) = FCOND
   236          TTFSTM(ILC1) = 0.
   241          TTFSTM(ILC2) = 0.
   244          DO 35 I = 1, NC
   245          TTFSTM(ILC1) = TTFSTM(ILC1) + FSTM(ILC1,I)
   256          TTFSTM(ILC2) = TTFSTM(ILC2) + FSTM(ILC2,I)
   267       35 CONTINUE
          C
          C       CALCULATE THE MOLE FRACTION FOR THE STREAMS
   271          DO 45 I = 1, NC
   273          YIEC(I) = FSTM(IEC,I) / TTFSTM(IEC)
   304          YILC1(I) = FSTM(ILC1,I) / TTFSTM(ILC1)
   315       45 CONTINUE
          C
          C          CALCULATE HEAT DUTY OF CONDENSOR, QCOND, IN BTU/HR
   317          TRIEC = TKSTM(IEC) * 1.8
   323          CALL HGAS(ID,N,TRIEC,YIEC,CPIEC,HIEC)
```

```
      TRILC1 = TKSTM(ILC1) * 1.8
      CALL HGAS(ID,N,TRILC1,YILC1,CPILC1,HILC1)
      CALL HWATER(TKSTM(ILC2),HW)
      QCOND(LL) = (HIEC*TTFSTM(IEC)) - (HILC1*TTFSTM(ILC1))
     1     - (HW*TTFSTM(ILC2))
      RETURN
   40 WRITE (NO,100)
  100 FORMAT (/,10X,*COND IN TROUBLE*)
      RETURN
      END


       SUBROUTINE CONDQ(KK)
      COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
      COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
      COMMON/UNIT/ NRXR,NHX,NDIV,NMIX,NCDR,IRXR(2),RLNTH1,RLNTH2,
     1            IHX(5),ICDR(2),QCOND(2)
      COMMON/POINT/ ID(8)
      COMMON/MEP/ DUM(164),NC
      DIMENSION T(25),YIEC(8),YLC1(8),YLC2(8)
C
C          THIS SUBROUTINE SIMULATES A CONDENSER UNIT.  GIVEN
C          A PARTICULAR STREAM AND THE GIVEN HEAT DUTY,QCOND,
C          THE PERCENTAGE OF WATER REMOVAL AND THE EXIT
C          STREAM TEMPERATRUE IS CALCULATED.
C
      LOOP = 1
      TOL = 1000.
      IEC = IN(KK,1)
      ILC1 = NOUT(KK,1)
      ILC2 = NOUT(KK,2)
      DO 5 K = 1, NCDR
    5 IF (ICDR(K).EQ.IUNIT(KK)) LL=K
      QCOND(1) = DUMDAT(KK)
      PCOND = PRSTM(IEC)
      DO 10 I = 1, NC
      FSTM(ILC1,I) = FSTM(IEC,I)
      FSTM(ILC2,I) = 0.
      YIEC(I) = FSTM(IEC,I)/TTFSTM(IEC)
   10 CONTINUE
C
C          DETERMINE THE ENTHALPY OF THE ENTERING STREAM
      TRIEC = TKSTM(IEC) * 1.8
      CALL HGAS (ID,NC,TRIEC,YIEC,CPIEC,HIEC)
C          CALCULATE THE FLOWRATE OF THE INERTS
      FINRT = TTFSTM(IEC) - FSTM(IEC,4)
C
C          ASSUME AN INITIAL CONDENSOR TEMPERATURE, DEG K
      T(LOOP) = 400.
   20 CONTINUE
C
C          CALCULATE THE VAPOR PRESSURE OF WATER AT THE ASSUMED TEMPERAT
      TKSTM(ILC1) = T(LOOP)
      TKSTM(ILC2) = T(LOOP)
C          CALCULATE WATER VAPOR PRESSURE AT THE ASSUMED TEMPERATURE
C          USING THE ANTOINE EQUATION (CONSTANTS TAKEN FROM PRS),IN PSIA
      VPH2O = (EXP(18.3036 - 3816.44/(T(LOOP) - 46.13))) * 14.7/760.
      PPH2O = YIEC(4) * PRSTM(IEC)
C          CHECK IF THE VPH2O IS GREATER THAN THE PARTIAL PRESSURE
C          OF WATER, IF SO THEN NO CONDENSATION TAKES PLACE
C
      IF(PPH2O.LE.VPH2O) GO TO 70
      GO TO 22
   70 CONTINUE
C
C         FOR NO CONDENSATION TAKING PLACE
C
      DO 72 I = 1, NC
   72 YLC1(I) = YIEC(I)
      TRLC1 = TKSTM(ILC1) * 1.8
      CALL HGAS (ID,NC,TRLC1,YLC1,CPLC1,HLC1)
      DEL = HIEC*TTFSTM(IEC) - QCOND(1) - HLC1*TTFSTM(ILC1)
      GO TO 45
   22 CONTINUE
C
C          FOR CONDENSATION TAKING PLACE
```

```
C
C           CALCULATE INERTS PRESSURE, IN PSIA
      PINRT = PCOND - VPH2O
      IF (PINRT.LE.0.) GO TO 25
C           CALCULATE LBMOLES OF STEAM CONDENSING
C
      FSTM(ILC1,4) = FINRT * VPH2O / PINRT
      FSTM(ILC2,4) = FSTM(IEC,4) - FSTM(ILC1,4)
      IF (FSTM(ILC2,4).LT.0.) GO TO 26
C
C           CALCULATE THE MOLE FRACTION FOR LC1
      TTFSTM(ILC1) = 0.
      TTFSTM(ILC2) = 0.
      DO 30 I = 1, NC
      TTFSTM(ILC1) = TTFSTM(ILC1) + FSTM(ILC1,I)
      TTFSTM(ILC2) = TTFSTM(ILC2) + FSTM(ILC2,I)
   30 CONTINUE
      DO 40 I = 1, NC
      YLC1(I) = FSTM(ILC1,I)/TTFSTM(ILC1)
   40 CONTINUE
C           CALCULATE THE STREAM ENTHALPIES
C
      TRLC1 = TKSTM(ILC1) * 1.8
      CALL HGAS (ID,NC,TRLC1,YLC1,CPLC1,HLC1)
      CALL HWATER (TKSTM(ILC2),HLC2)
C
C           PERFORM THE ENERGY BALANCE
      DEL = (HIEC*TTFSTM(IEC)) - QCOND(1) - (HLC1*TTFSTM(ILC1)) -
     1     (HLC2*TTFSTM(ILC2))
   45 CONTINUE
C
C           CHECK FOR CONVERGENCE
      ADEL = ABS(DEL)
      IF (ADEL.LT.TOL) GO TO 50

      CALL FALPOS(T(LOOP),DEL,LOOP,TNEW)
      LOOP = LOOP + 1
      T(LOOP) = TNEW
      IF(LOOP.EQ.26) GO TO 60
      GO TO 20
   25 CONTINUE
      T(LOOP) = T(LOOP) - 75.
      GO TO 20
   26 CONTINUE
      T(LOOP) = T(LOOP) + 12.
      GO TO 20
   50 CONTINUE
      PRSTM(ILC1) = PCOND
      PRSTM(ILC2) = PCOND
      RETURN
   60 CONTINUE
      WRITE(6,100)
  100 FORMAT(/,10X,*CCND IN TROUBLE*)
      RETURN
      END


      SUBROUTINE HWATER(TEMPK,HW)
C
C
C           SUBROUTINE HWATER CALCULATES THE SPECIFIC ENTHALPY OF
C           LIQUID WATER IN UNITS OF BTU/LBMOLE.  THE BASIS IS H = 0 AT
C           TBASE = 255.6 K(460. R).  NOTE THAT THE TEMPERATURE T
C           IS IN DEGREES K.
C
      TBASE = 460./1.8
      CPAVE = (CP2(TEMPK) + CP2(TBASE))/2.
      HW = CPAVE*(TEMPK - TBASE) * 18.
      RETURN
      END
```

```
          FUNCTION CP2(TEMPK)
     C
     C
     C            FUNCTION CP2 CALCULATES THE HEAT CAPACITY OF LIQUID
     C            WATER IN BTU/LBL AS A FUNCTION OF TEMPERATURE.
     C            NOTE THAT THE TEMPERATURE IS IN DEGREES K.
     C
   6      CP2 = 1.8 + 0.13 * (TEMPK - 293.)/(508. - 293.)
  15      RETURN
  15      END


          SUBROUTINE FALPCS (T,DELTA,LOOP,TNEW)
     C
     C... THIS ROUTINE USES A BRACKETTING METHOD TO
     C... CONVERGE UPON THE DEPENDENT VALUE OF A FUNCTION
     C... WHEN IT CROSSES THE X-AXIS AT POINT A.
     C... LETTING     F = F(P)   ,
     C... AN INITIAL ESTIMATE OF THE ROOT (P1) IS
     C... USED TO ARRIVE AT ANOTHER ESTIMATE (P2)
     C... SUCH THAT F1 AND F2 ARE OF OPPOSITE SIGN.
     C... ADDITIONAL TRIAL VALUES (P(1)) ARE CALCULATED
     C... FROM THE EQUATICN
     C...     P(1) = P1 - ((P2-P1)/F2-F1)*F1
     C... AS THE PROCEDURE CONVERGES, THE VALUES
     C... FOR (P1,F1) OR (P2,F2) WILL BE REPLACED
     C... BY THE NEWLY GENERATED COORDINATES FOR
     C... A MORE ACCURATE ESTIMATE.
     C
     C
     C... INITIALIZE VALUES FOR 1ST RUN THROUGH THE ROUTINE
     C
  11      IF(LOOP.NE.1) GO TO 5
  13      TPOS = 0.
  14      TNEG = 0.
  15      DELTAP = 0.
  16      DELTAN = 0.
  17    5 CONTINUE
     C
     C... DETERMINE THE PLACEMENT OF THE PRESENT DEPENDENT VALUE,
     C... ON THE POSITIVE CR NEGATIVE SIDE OF X-AXIS
     C
  17      IF(DELTA.LT. 0.) GO TO 10
  21      TPOS = T
  22      DELTAP = DELTA
  23      GO TO 12
  24   10 CONTINUE
  24      TNEG = T
  25      DELTAN = DELTA
  26   12 CONTINUE
     C
     C... Q-- HAS THE DEPENDENT VARIABLE BRACKETTED ZERO
     C...        Y--CALCULATE PNEW VIA THE GIVEN EQ.
     C...         N--INCREMENT P FOR A NEW PNEW
     C
  26      IF((DELTAN.NE.0.).AND.(DELTAP.NE.0.)) GO TO 20
  36      IF(DELTAN.EQ.0.) GO TO 22
  40      TNEW = T - 100.
  42      RETURN
  42   22 CONTINUE
  42      TNEW = T + 100.
  44      RETURN
  44   20 CONTINUE
  44      TNEW = TNEG - ((TPOS-TNEG)/(DELTAP-DELTAN))*DELTAN
  54      RETURN
  55      END


          SUBROUTINE IDENT
     C...
     C...
     C... SUBROUTINE IDENT IDENTIFIES WHICH CHEM SPECIES FROM BLOCK DATA IS
     C... THE FIRST COMPONENT, WHICH IS THE SECONC, ETC FOR USE IN
     C... SUBSEQUENT CALCULATIONS.
```

```
          C...
          C...    ID = CODE NO. OF COMPOUND FROM THERMO DATA BANK
          C...    THIS CASE  4=CO  3=H2  13=CH4  12=H20  5=CO2  1=N2
          C...
     2            COMMON/POINT/ ID(8)
     2            ID(1) = 4
     5            ID(2) = 3
    10            ID(3) = 13
    13            ID(4) = 12
    16            ID(5) = 5
    21            ID(6) = 1
    24            RETURN
    24            END


                  SUBROUTINE STOICH
          C...
          C...
          C...    SUBROUTINE STOICH SETS THE STOICHIOMETRIC COEFFICIENTS FOR THE
          C...    CHEM REACTIONS ENCOUNTERED.
          C...
     2            COMMON/STOICH/ A(3,8), DELA(3)
          C...
          C...
          C...    A(J,I) = STOICHIOMETRIC COEFFICIENT FOR COMPONENT I IN REACTION J.
          C...
     2            A(1,1) = -1.
     7            A(1,2) = -3.
    14            A(1,3) =  1.
    21            A(1,4) =  1.
    25            A(1,5) =  0.
    32            A(1,6) = 0.
    36            A(2,1) = -1.
    43            A(2,2) =  1.
    47            A(2,3) =  0.
    53            A(2,4) = -1.
    60            A(2,5) =  1.
    65            A(2,6) = 0.
    72            RETURN
    72            END


                  SUBROUTINE HPREP
          C...
          C...
          C...    SUBROUTINE HPREP CALCULATES TEMPERATURE INDEPENDENT THERMODYNAMIC
          C...    CONSTANTS THAT ONLY NEED BE CALCULATED ONCE, BUT ARE USED
          C...    FREQUENTLY BY SUBSEQUENT TEMPERATURE DEPENDENT THERMODYNAMIC
          C...    CALCULATIONS.
          C...
     2            COMMON/MEP/ DUM(164),NC
     2            COMMON/POINT/ ID(8)
     2            COMMON/STOICH/ A(3,8), DELA(3)
     2            COMMON/HPASS/ HRX537(3),DELALF(3),DELBET(3),DELGT2(3),
                 1 DEGOV2(3),HI537(3),HO(3),GRX537(3),GI537(3),GO(3)
     2            COMMON /PDATA/ DUM22(990), GF537(45), HF537(45), HCOMB(45),
                 1              ALPHA(45), BETA(45), GAMT2(45), GAMOV2(45)
          C...
          C...
          C...    DELA   = DIFF IN STOICHIOMETRIC COEFFS
          C...    DELALF = DIFF IN ALPHAS IN CP GAS
          C...    DELBET = DIFF IN BETAS IN CP GAS
          C...    DELGT2 = DIFF IN GAMT2 IN CP GAS
          C...    GAMT2  = COEFF OF FORM  GAMMA*T*T
          C...    DEGOV2 = DIFF IN GAMOV2 IN CP GAS
          C...    GAMOV2 = COEFF OF FORM  GAMMA/T
          C...    HRX537 = HEAT OF REACTION AT 537 R
          C...    GRX537 = FREE ENERGY OF RX AT 537 R
          C...
     2            DO 12 J=1,2
     4            DELA(J) = 0.0
     6            DELALF(J) = 0.0
    11            DELBET(J) = 0.0
    14            DELGT2(J) = 0.0
    17            DEGOV2(J) = 0.0
```

```
          HRX537(J) = 0.0
          GRX537(J) = 0.0
     12 CONTINUE
          DO 20 J=1,2
          DO 10 I=1,NC
          ACOEFF = A(J,I)
          IF ( ABS(ACOEFF).LT.0.001 ) GO TO 10
          NOC = ID(I)
          DELA(J) = DELA(J) + ACOEFF
          DELALF(J) = DELALF(J) + ACOEFF*ALPHA(NOC)
          DELBET(J) = DELBET(J) + ACOEFF*BETA(NOC)
          DELGT2(J) = DELGT2(J) + ACOEFF*GAMT2(NOC)
          DEGOV2(J) = DEGOV2(J) + ACOEFF*GAMOV2(NOC)
          HRX537(J) = HRX537(J) + ACOEFF*HF537(NOC)
          GRX537(J) = GRX537(J) + ACOEFF*GF537(NOC)
     10 CONTINUE
     20 CONTINUE
C...
C...
C...      HI537 = CONST USED IN CALC OF HEAT OF REACTION AT TEMP TK
C...      GI537 = FREE ENERGY SIMILAR TO HI537
C...      HO    = CONST DEFINED BY FOLLOWING EQATION IS USED IN CALCULATING
C...              HEAT OF REACTION AT TEMPERATURE TK
C...      GO    = FREE ENERGY SIMILAR TO HO
C...
          DO 14 J=1,2
          HI537(J) = DELALF(J)*537. + DELBET(J)/2.*537.*537. + DELGT2(J)/3.
        $ *537.*537.*537. - DEGOV2(J)/537.
          HO(J) = HRX537(J) - HI537(J)
          GI537(J) = HO(J)/537. - DELALF(J)*ALOG(537.) - DELBET(J)/2.*537. -
        $ DELGT2(J)/6.*537.*537. - DEGOV2(J)/2./537./537.
          GO(J) = GRX537(J)/537. - GI537(J)
     14 CONTINUE
          RETURN
          END


          SUBROUTINE HRXYCP (TK,HRXT,GOVT,KCHEM,CPAVG,Y,IP)
          REAL KCHEM(3)
          COMMON/PCINT/ ID(8)
          COMMON/MEP/ DUM(164),NC
          COMMON/HPASS/ HRX537(3),DELALF(3),DELBET(3),DELGT2(3),
        1 DEGOV2(3),HI537(3),HO(3),GRX537(3),GI537(3),GO(3)
           COMMON /PDATA/ DUM22(990), GF537(45), HF537(45), HCOMB(45),
        1                  ALPHA(45), BETA(45), GAMT2(45), GAMOV2(45)
          DIMENSION TK(41),HRXT(3),GOVT(3),Y(8)
C
CC...                                    HRXT = HEAT OF REACTION AT TK IN
CC...                                           CAL / G MOLE
CC...                                    GOVT = FREE ENERGY OF RX AT TK OVER T
          TT = TK(IP)*1.8
           DO 10 J=1,2
           HRXT(J) = HO(J) + DELALF(J)*TT + DELBET(J)/2.*TT*TT + DELGT2(J)
        *  /3.*TT*TT*TT - DEGOV2(J)/TT
           HRXT(J) = HRXT(J)/1.8
           GOVT(J) = GO(J) + HO(J)/TT - DELALF(J)*ALOG(TT) - DELBET(J)/2.*TT
        *  - DELGT2(J)/6.*TT*TT - DEGOV2(J)/2./TT/TT
           KCHEM(J) = EXP ( - GOVT(J)/1.987 )
     10 CONTINUE
CC...                                    CPAVG = HEAT CAPACITY OF ALL COMPOUND
CC...                                            IN THE REACTOR AT THE POINT OF
CC...                                            CALCULATION AT TEMP TT
CC...                                            IN CAL / G MOLE / DEG C
CC...
           CPAVG = 0.0
          DO 11 I = 1,NC
           NO = ID(I)
          CPAVG = CPAVG + Y(I)*( ALPHA(NO) + BETA(NO)*TT + GAMT2(NO)*TT*TT +
        *  GAMOV2(NO)/TT/TT)
     11 CONTINUE
           RETURN
           END
```

```
              SUBROUTINE RATE (TKK,P,Y,RATE1,RATE2,KCHEM,IP)
        C...
        C...
        C...  SUBROUTINE RATE CALCULATES THE RATE OF CHEMICAL REACTION FOR EACH
        C...  REACTION ENCOUNTERED.
        C...
        C...  1.  METHANATION REACTION      CO + 3H2 = CH4 + H2O
        C...  2.  SHIFT REACTION            CO + H2O = CO2 + H2
        C...
        C...  TK      TEMPERATURE IN K
        C...  Y(1)    MOLE FRACTION OF COMPONENT 1
        C...  P       PRESSURE IN PSIA
        C...  RATE1   RATE OF METHANATION REACTION IN LB MOLES/HR/CU FT CATALYST
        C...  RATE2   RATE OF SHIFT REACTION IN LB MOLES/HR/CU FT CATALYST
        C...
   12         COMMON/MEP/ DUM(164),NC
   12         DIMENSION TKK(41),Y(8)
   12         REAL KP, KCHEM(3)
   12         TK = TKK(IP)
        C...
        C...
        C...  THE PARTIAL PRESSURE OF EACH COMPONENT IS CALCULATED.
        C...
   15         PCO=Y(1)*P
   20         PH2=Y(2)*P
   23         PCH4=Y(3)*P
   26         PH2O=Y(4)*P
   31         PCO2=Y(5)*P
        C...
        C...
        C...  A CHECK IS MADE TO SEE IF ANY REACTANTS ARE COMPLETELY CONSUMED.
        C...
   34         IF (PCO.LE.0.0) GO TO 10
   37         IF (PH2.LE.0.0) GO TO 20
   42         IF (PH2O.LE.0.0) GO TO 30
        C...
        C...
        C...  IF NO REACTANTS ARE COMPLETELY CONSUMED, THE REACTION RATES
        C...  FOR BOTH REACTIONS ARE CALCULATED. NOTE THAT THE REACTIONS ARE
        C...  IRREVERSIBLE, EG. REACTION RATES CANNOT BE NEGATIVE.
        C...
   45         KP=KCHEM(1)/14.69/14.69
   52         A = PCH4*PH2O/PCO/PH2/PH2/PH2/KP
   57         RC1 = 79.4  * EXP(-3473/TK)
   65         RATE1 = RC1*PCO*SQRT(PH2)*(1.-A)/(1.+0.1*PH2+0.05*PCH4)
  111         IF (RATE1.LT.0.0) RATE1 = 0.0
  113         RATE2 = 0.
  114         IF (RATE2.LT.0.0) RATE2 = 0.0
  117         RETURN
        C...
        C...
        C...  IF CO IS COMPLETELY CONSUMED, THE REACTION RATES FOR BOTH
        C...  REACTIONS ARE SET EQUAL TO 0.
        C...
  120      10 RATE1 = 0.0
  121         RATE2 = 0.0
  122         RETURN
        C...
        C...
        C...  IF H2 IS COMPLETELY CONSUMED, THE METHANATION REACTION RATE IS
        C...  CONTROLLED BY THE SHIFT REACTION RATE.
        C...
  122      20 RC2=10250.*EXP(-3600.0/TK)/TK/TK
  132         RATE2=RC2*(PCO*PH2O-PCO2*PH2/KCHEM(2))
  145         IF(RATE2.LT.0.0) RATE2=0.0
  150         RATE1 = RATE2/3.
  152         RETURN
        C...
        C...
        C...  IF H2O IS COMPLETELY CONSUMED, THE SHIFT REACTION RATE IS
        C...  CONTROLLED BY THE METHANATION REACTION RATE.
        C...
  152      30 A=PCH4*PH2O/PH2/PH2/SQRT(PH2)/KP
  161         RC1=0.0025030*EXP(2940./TK)
  167         RATE1=RC1*(PCO*SQRT(PH2)-A)/(1.+0.1*PH2+0.05*PCH4)
  213         IF (RATE1.LT.0.0) RATE1 = 0.0
```

```
 215        RATE2 = RATE1
 216        RETURN
 217        END


            SUBROUTINE HGAS (ID,NC,T,Y,CPIGM,H)
  11        DIMENSION ID(8), Y(8)
  11        TBASE = 460.
      C...
      C...
      C...  SUBROUTINE HGAS CALCULATES THE SPECIFIC ENTHALPY OF A GAS
      C...  STREAM IN UNITS OF BTU/LB-MOLE.  THE BASIS FOR ALL CALCULATIONS
      C...  IS THAT ALL COMPONENTS HAVE H = 0 AT TBASE = 460 R.  IT SHOULD BE
      C...  NOTED THAT HGAS IS ONLY VALID IF NO REACTIONS OCCUR AND IF THE
      C...  HEAT OF MIXING OF THE GAS COMPONENTS IS ZERO.  NOTE ALSO THAT THE
      C...  TEMPERATURE T IS IN DEGREES R.
      C...
  12        CALL CPMEAN (ID,NC,T,TBASE,Y,CPIGM)
  15        H = CPIGM*(T-TBASE)
  24        RETURN
  24        END


            SUBROUTINE XADJ (X,IPTS,RELIN,P,IP)
      C...
      C...
      C...  SUBROUTINE XADJ CHECKS TO SEE IF ANY REACTANT IS COMPLETELY
      C...  CONSUMED AT ANY POINT IN A REACTOR.  IF ONE OR MORE OF THE
      C...  REACTANTS IS COMPLETELY CONSUMED, THE FRACTIONAL CONVERSIONS
      C...  OF CO BY EACH REACTION IS ADJUSTED SO THAT NEGATIVE FLOWRATES
      C...  ARE ELIMINATED.
      C...
  11        DIMENSION X(41,2), RELIN(8)
  11        X1 = X(IP,1)
  16        X2 = X(IP,2)
      C...
      C...
      C...  AT ANY POINT IN A REACTOR, ALL REACTANTS ARE CHECKED TO SEE IF
      C...  ANY ARE COMPLETELY CONSUMED.  A FLAG VARIABLE (IFLAG) IS
      C...  USED TO KEEP TRACK OF WHICH REACTANTS ARE CONSUMED.
      C...
      C...       IFLAG = 0      NO REACTANTS ARE CONSUMED.
      C...       IFLAG = 1      H2 IS COMPLETELY CONSUMED.
      C...       IFLAG = 2      H2O IS COMPLETELY CONSUMED.
      C...       IFLAG = 3      H2 AND H2O ARE COMPLETELY CONSUMED.
      C...       IFLAG = 10     CO IS COMPLETELY CONSUMED.
      C...       IFLAG = 11     CO AND H2 ARE COMPLETELY CONSUMED.
      C...       IFLAG = 12     CO AND H2O ARE COMPLETELY CONSUMED.
      C...       IFLAG = 13     CO, H2, AND H2O ARE COMPLETELY CONSUMED.
      C...
  22        IFLAG = 0
      C...
      C...
      C...  A CHECK IS MADE TO SEE IF CO IS COMPLETELY CONSUMED.  IF CO IS
      C...  COMPLETELY CONSUMED, IFLAG IS SET EQUAL TO 10 AND THE REACTOR
      C...  FRACTIONAL CONVERSIONS ARE ADJUSTED.
      C...
  23        SUMX = X1 + X2
  25        IF (SUMX.LT.1.) GO TO 21
  30        IFLAG = 10
  32        X1 = X1/SUMX
  34        X2 = X2/SUMX
      C...
      C...
      C...  A CHECK IS MADE TO SEE IF H2 AND H2O ARE COMPLETELY CONSUMED.
      C...  IF EITHER REACTANT IS CONSUMED, IFLAG IS SET EQUAL TO THE CORRECT
      C...  VALUE.
      C...
  35     21 RX2 = (RELIN(2) + X2)/3. - 1.0E-8
  44        WRX2 = RELIN(4) + X1 - 1.0E-8
  51        IF (X1.GE.RX2) IFLAG = IFLAG + 1
  55        IF (X2.GE.WRX2) IFLAG = IFLAG + 2
      C...
      C
      C       REACTION PROCEEDS IN ONLY ONE DIRECTION,
```

```
         C        PREVENT NUMERICAL DROP IN CO CONVERSION BY CALCULATION FROM
         C           FROM ONE GRID POINT TO ANOTHER.
         C
  62             IF (IP.EQ.1) GO TO 52
  64             IPM1 = IP - 1
  66             IF(X(IP,1).LT.X(IPM1,1)) X1 = X(IPM1,1)
 102          52 CONTINUE
         C...
         C...    A SERIES OF IF STATEMENTS CHECKS THE VALUE OF IFLAG, AND
         C...    TRANSFERS THE PROGRAM TO THE PROPER STATEMENTS THAT WILL
         C...    CORRECTLY ADJUST THE REACTION FRACTIONAL CONVERSIONS.
         C...
 102             IF (IFLAG.EQ.0) GO TO 40
 104             IF (IFLAG.EQ.10) GO TO 40
 107             IF (IFLAG.EQ.1) GO TO 22
 112             IF (IFLAG.EQ.2) GO TO 23
 115             IF (IFLAG.EQ.11) GO TO 24
 120             IF (IFLAG.EQ.12) GO TO 25
 123             IF (IFLAG.EQ.3)  GO TO 26
 126             GO TO 27
         C...
         C...
         C...    H2 IS COMPLETELY CONSUMED.  THE FRACTIONAL CONVERSION OF CO BY
         C...    THE METHANATION REACTION IS ADJUSTED.
         C...
 127          22 X1 = RX2
 131             GO TO 40
         C...
         C...
         C...    H2O IS COMPLETELY CONSUMED.  THE FRACTIONAL CONVERSION OF CO BY
         C...    THE SHIFT REACTION IS ADJUSTED.
         C...
 131          23 X2 = WRX2
 133             GO TO 40
         C...
         C...
         C...    CO AND H2 ARE COMPLETELY CONSUMED.  BOTH FRACTIONAL CONVERSIONS
         C...    OF CO ARE ADJUSTED.
         C...
 133          24 X1 = (1. + RELIN(2))/4.
 141             X2 = (3. - RELIN(2))/4.
 145             WRX2 = RELIN(4) + X1
 151             IF (X2.GT.WRX2) GO TO 26
 154             GO TO 40
         C...
         C...
         C...    CO AND H2O ARE COMPLETELY CONSUMED.  BOTH FRACTIONAL CONVERSIONS
         C...    ARE ADJUSTED.
         C...
 155          25 X1 = (1. - RELIN(4))/2.
 163             X2 = (1. + RELIN(4))/2.
 167             RX2 = (RELIN(2) + X2)/3.
 175             IF (X1.GT.RX2) GO TO 26
 200             GO TO 40
         C...
         C...
         C...    H2 AND H2O ARE COMPLETELY CONSUMED.  BOTH FRACTIONAL CONVERSIONS
         C...    OF CO ARE ADJUSTED.
         C...
 201          26 X1 = (RELIN(2) + RELIN(4))/2.
 211             X2 = (RELIN(2) + 3.*RELIN(4))/2.
 222             GO TO 40
         C...
         C...
         C...    CO, H2, AND H2O ARE COMPLETELY CONSUMED.  BOTH FRACTIONAL
         C...    CONVERSIONS OF CO ARE ADJUSTED.
         C...
 222          27 X1 = (1. + RELIN(2))/4.
 230             X2 = (3. - RELIN(2))/4.
 234             WRX2 = RELIN(4) + X1
 240             IF (X2.LT.WRX2) GO TO 40
 243             X1 = (1. - RELIN(4))/2.
 251             X2 = (1. + RELIN(4))/2.
 255             RX2 = (RELIN(2) + X2)/3.
 263             IF (X1.LT.RX2) GO TO 40
 266             X1 = (RELIN(2) + RELIN(4))/2.
 276             X2 = (RELIN(2) + 3.*RELIN(4))/2.
```

```
307      40  X(IP,1) = X1
314          X(IP,2) = X2
320          RETURN
321          END


             SUBROUTINE YSFLCH(IP,TK,P,X,TOTMIN,TOTMOL,FIN,TKOUT,PSIAOT,
            1 FTOTOT,FOUT,Y)
      C...
      C...
      C...   SUBROUTINE YSFLOW CALCULATES MOLE FRACTION AND THE OUTLET VECTOR
      C...   OF TEMP., PRESS, AND FLOW OF EACH SPECIES IN MOLES PER HR.  VECTOR
      C...   IS CALCULATED AT EACH PT. IN REACTOR AND OVERWRITTEN SUCH THAT
      C...   ONLY OUTLET IS AVAILABLE FOR SUBSEQUENT USE.
      C...
      C...
17           COMMON/MEP/ DUM(164),NC
17           COMMON/STOICH/ A(3,8), DELA(3)
17           COMMON/HPASS/ HRX537(3),DELALF(3),DELBET(3),DELGT2(3),
            1 DEGOV2(3),HI537(3),HO(3),GRX537(3),GI537(3),GO(3)
17           COMMON/STORL/ DUM2(284),RATE1(41),DUM3(50),YCOMP(41,8)
17           DIMENSION TK(41),X(41,2),FIN(8),FOUT(8),Y(8)
      C...
      C...
      C...   THE TEMPERATURE, PRESSURE, AND FLOWRATES AT THE ADVANCING POINT
      C...   IN THE REACTOR ARE STORED AS TKOUT, PSIAOT, AND FOUT.  AT THE
      C...   REACTOR OUTLET, THE OUTPUT VECTOR IS FILLED.
      C...
17           TKOUT = TK(IP)
22           PSIAOT = P
23           X11 = X(IP,1)
30           X22 = X(IP,2)
      C...
      C...
      C...   TOTAL MOLES AT ANY POINT BASED ON UNITY FOR
      C...   LIMITING REACTANT IS CALCULATED.
      C...
34           TOTMOL = TOTMIN    + DELA(1)*X11+ DELA(2)*X22
      C...
      C...
      C...   TOTAL MOLAR FLOW AT ANY POINT IS CALCULATED.
      C...
44           FTOTOT = 0.
45           DO 12 I = 1, NC
47           FOUT(I) = FIN(I) + FIN(1)*( A(1,I)*X11+ A(2,I)*X22)
75           FTOTOT = FOUT(I) + FTOTOT
102      12  CONTINUE
105          DO 10 I = 1, NC
106          Y(I) = FOUT(I)/FTOTOT
115          IF(Y(I).LT.0.) Y(I)=0.
      C
      C      STORE FOR PRINT OUT
      C
124          YCOMP(IP,I) = Y(I)
134      10  CONTINUE
137          RETURN
137          END


             SUBROUTINE CPMEAN(ID,NC,THI,TLO,Y,CPIGM)
      C...
      C...
      C...   THIS SUBROUTINE CALCULATES THE INTEGRATED MEAN IDEAL GAS HEAT
      C...   CAPACITY BETWEEN TWO TEMPERATURES THI AND TLO.
      C...       INPUT
      C...          ID     ARRAY WHICH HOLDS THE IDENTIFICATION NUMBERS OF THE
      C...                 SPECIES OF INTEREST.  FOR EXAMPLE, FOR THE ORDER
      C...                 CARBON MONOXIDE, HYDROGEN, METHANE, WATER, CARBON
      C...                 DIOXIDE
      C...                        ID (1) = 4
      C...                        ID (2) = 3
      C...                        ID (3) = 13
      C...                        ID (4) = 12
      C...                        ID (5) = 5
      C...          NC     NUMBER OF COMPONENTS IN GAS
```

```
C...        THI   HIGH TEMPERATURE OF INTEREST IN R.
C...        TLC   LOW TEMPERATURE OF INTEREST IN R.
C...        Y     MOLE FRACTION ARRAY IN THE SAME ORDER AS THE SPECIES
C...              HAVE BEEN SET UP IN THE ID ARRAY.
C...     OUTPUT
C...        CPMEAN INTEGRATED MEAN IDEAL GAS HEAT CAPACITY IN
C...              BTU/LB MOLE R  OR CAL/G MOLE K
C...
      COMMON /PDATA/ DUM22(990), GF537(45), HF537(45), HCOMB(45),
     1               ALPHA(45), BETA(45), GAMT2(45), GAMOV2(45)
      DIMENSION ID(8), Y(8)
C...
      AMIX   = 0.0
      BMIX   = 0.0
      GT2MIX = 0.0
      GOVMIX = 0.0
      DO 1 I=1,NC
      J = ID(I)
      AMIX   = AMIX   + Y(I) *  ALPHA(J)
      BMIX   = BMIX   + Y(I) *   BETA(J)
      GT2MIX = GT2MIX + Y(I) *  GAMT2(J)
      GOVMIX = GOVMIX + Y(I) * GAMOV2(J)
    1 CONTINUE
      CPIGM = AMIX + 0.5*BMIX*(THI + TLO) + GT2MIX/3.*
     1 (THI*THI + THI*TLO + TLO*TLO) + GOVMIX/THI/TLO
      RETURN
      END


      SUBROUTINE CPIGAS(ID,NC,T,Y,CPIG)
C...
C...
C...  THIS SUBROUTINE CALCULATES THE IDEAL GAS HEAT CAPACITY AS A
C...  FUNCTION OF TEMPERATURE.
C...     INPUT
C...        ID     ARRAY WHICH HOLDS THE IDENTIFICATION NUMBERS OF THE
C...               SPECIES OF INTEREST.  FOR EXAMPLE, FOR THE ORDER
C...               CARBON MONOXIDE, HYDROGEN, METHANE, WATER, CARBON
C...               DIOXIDE
C...                     ID(1) =  4
C...                     ID(2) =  3
C...                     ID(3) = 13
C...                     ID(4) = 12
C...                     ID(5) =  5
C...        NC     NUMBER OF ELEMENTS IN THE ID ARRAY.
C...        T      TEMPERATURE OF INTEREST IN R.
C...        Y      MOLE FRACTION ARRAY IN THE SAME ORDER AS THE SPECIES
C...               HAVE BEEN SET UP IN THE ID ARRAY.
C...     OUTPUT
C...        CPIG   IDEAL GAS HEAT CAPACITY IN BTU/LB MOLE F OR CAL/GMOLEK
C...
      COMMON /PDATA/ DUM22(990), GF537(45), HF537(45), HCOMB(45),
     1               ALPHA(45), BETA(45), GAMT2(45), GAMOV2(45)
      DIMENSION ID(8), Y(8)
      CPIG = 0.
      DO 1 I=1,NC
      J=ID(I)
      CP=ALPHA(J)+BETA(J)*T+GAMT2(J)*T*T+GAMOV2(J)/(T*T)
      CPIG=CPIG+Y(I)*CP
    1 CONTINUE
      RETURN
      END


      SUBROUTINE TCALC (ID,NC,Y,T1,T2,H1,H2,T,H)
C...
C...
C...  SUBROUTINE TCALC CALCULATES THE TEMPERATURE OF A GAS STREAM
C...  GIVEN ITS SPECIFIC ENTHALPY.  IT IS USED WHEN TWO GAS STREAMS
C...  ARE COMBINED TO GIVE A NEW GAS STREAM.  AN INTERVAL HALVING
C...  ITERATION METHOD IS USED TO CONVERGE TO THE CORRECT TEMPERATURE.
C...
C...
C...  INPUT
C...     ID       ARRAY WHICH HOLDS THE IDENTIFICATION NUMBERS
```

```
      C...              FOR THE COMPONENTS OF INTEREST.  FOR EXAMPLE,
      C...              FOR THE ORDER CO, H2, CH4, H2O, AND CO2
      C...                      ID(1) =  4
      C...                      ID(2) =  3
      C...                      ID(3) = 13
      C...                      ID(4) = 12
      C...                      ID(5) =  5
      C...     NC       NUMBER OF COMPONENTS IN GAS
      C...     Y        MOLE FRACTION ARRAY IN THE SAME ORDER AS THE
      C...              COMPONENTS HAVE BEEN SET UP IN THE ID ARRAY
      C...     T1,T2    INITIAL GUESSES OF TEMPERATURE IN R
      C...     H1,H2    SPECIFIC ENTHALPIES OF GAS AT GUESSED TEMPERATURES
      C...              T1 AND T2 IN UNITS OF BTU/LB-MOLE
      C...     H        SPECIFIC ENTHALPY OF COMBINED GAS STREAM IN BTU/LB-MOLE
      C...  OUTPUT
      C...     T        CALCULATED TEMPERATURE OF COMBINED GAS STREAM IN R.
      C...
            DIMENSION ID(8), Y(8)
      C...
      C...
      C...  AN INITIAL GUESS OF TEMPERATURE (TEST) IS CALCULATED BY
      C...  LINEAR INTERPOLATION BETWEEN THE GIVEN TEMPERATURES (T1 AND T2)
      C...  AND SPECIFIC ENTHALPIES (H1 AND H2).
      C...
            IF (H2.NE.H1) GO TO 1
            TEST = T1
            GO TO 2
          1 TEST = (H-H1)*(T2-T1)/(H2-H1) + T1
      C...
      C...
      C...  THE SPECIFIC ENTHALPY OF THE GAS STREAM AT THE GUESSED
      C...  TEMPERATURE IS CALCULATED AND COMPARED TO THE ACTUAL VALUE.  IF
      C...  THEY AGREE WITHIN 0.10 PERCENT, THE TEMPERATURE IS CONSIDERED
      C...  CORRECT.  IF THEY DO NOT AGREE WITHIN 0.10 PERCENT, THE GUESSED
      C...  TEMPERATURE IS CHANGED USING AN INTERVAL HALVING ITERATION METHOD.
      C...
          2 LOOP = 0
            FLAGM = -1.
            FLAGP = -1.
            DT = 10.
         50 LOOP = LOOP + 1
            IF (LOOP.GT.200) GO TO 101
            CALL HGAS (ID,NC,TEST,Y,CPIGM,HCALC)
            PCERR = ABS((HCALC-H)/H*100.)
            IF (PCERR.LT.0.1) GO TO 100
            IF (HCALC-H) 10,10,20
         10 IF (FLAGP.LT.0.) GO TO 11
            DT = DT/2.
         11 TEST = TEST + DT
            FLAGM = 1.
            GO TO 50
         20 IF (FLAGM.LT.0.) GO TO 21
            DT = DT/2.
         21 TEST = TEST - DT
            FLAGP = 1.
            GO TO 50
        100 T = TEST
            RETURN
      C...
      C...
      C...  IF AN EXCESSIVE NUMBER OF LOOPS IS TRIED, AN ERROR MESSAGE IS
      C...  PRINTED AND THE PROGRAM STOPS.
      C...
        101 PRINT 150
        150 FORMAT (10X,21HENDLESS LOOP IN TCALC)
            STOP
            END


            SUBROUTINE PRINT(NI,NO)
      C...
      C...
      C...  SUBROUTINE PRINT WRITES TO LOGICAL UNIT NUMBER NO THE CURRENT
      C...  VALUES OF TEMPERATURES AND FLOWRATES THAT ARE PRINTED.
      C...
      C...
```

```
      6            COMMON /T/ T,NFIN,NRUN
      6            COMMON/Y/ TK(41,2)
      6            COMMON/F/ DTK(41,2)
      6            COMMON/INDAT/ NUNITS,NSTMS,IORD(15)
      6            COMMON/STMDAT/ FSTM(25,8),TTFSTM(25),TKSTM(25),PRSTM(25)
      6            COMMON/PROCESS/ IUNIT(15),KT(15),IN(15,3),NOUT(15,2),DUMDAT(15)
      6            COMMON/UNIT/ NRXR,NHX,NDIV,NMIX,NCDR,IRXR(2),RLNTH(2),
                  1           IHX(5),ICDR(2),QCOND(2)
      6            COMMON/MEP/ X1(41,2),X2(41,2),NC,NFLAG,NFLAG1,NPTS,ND,L(41)
      6             COMMON/OOFEED/ TKFDOD,PRFDOD,FDOD(8),TTFDOD
      6            COMMON/PRT/ Q(16),RATE1(41,2),RATE2(41,2),YCOMP(41,8,2)
      6            COMMON/STOICH/ A(3,8), DELA(3)
      6            COMMON/HPASS/ HRX537(3),DELALF(3),DELBET(3),DELGT2(3),
                  1 DEGOV2(3),HI537(3),HO(3),GRX537(3),GI537(3),GO(3)
      6            COMMON/POINT/ IC(8)
      6            REAL L
             C
             C
             C             WRITE INFORMATION SUBMITTED TO SIMULATION
             C
             C
      6            WRITE(NO,50)
     12            WRITE(NO,700) (Q(I), I = 1, 16)
     25        700 FORMAT(20X,8A10,/,20X,8A10,///)
     25            WRITE(NO,200) T
     33            IF (NFLAG.NE.0) GO TO 12
     36            WRITE(NO,4)
     42          4 FORMAT(//,10X,37HINITIAL CONDITIONS FOR REACTOR SYSTEM)
     42         12 CONTINUE
     42            WRITE(NO,710)
     46        710 FORMAT (10X,29HPROCESS FLOWSHEET INFORMATION,//,15X,
                  1*KEY-UNIT TYPE(KT),1=RXR1, 2=HXQ, 3=DIV, 4=MIX, 5=CDRF, 6=RXR2, 7=
                  2HXT, 8=CDRQ*,//,
                  2    36X,6HSTM IN,13X,7HSTM OUT,/,10X,7HUNIT NO,5X,4HTYPE,5X,
                  3    2H 1,5X,2H 2,5X,2H 3,7X,2H 1,5X,2H 2,5X,10HUNIT INFOR,
                  4    5X,10HRXR LENGTH,/)
     46            GO TO (8,7,9,9,7,8,7,7),JKT
     63            JR = 0
***NPW*************************
     64            DO 10 J = 1, NUNITS
     66            JJ = IUNIT(J)
     71            JKT = KT(J)
     74            GO TO (8,7,9,9,7,8),JKT
    105          9 CONTINUE
    105            WRITE(NO,720) (IUNIT(J),KT(J),(IN(J,I),I=1,3),(NOUT(J,I),I=1,2),
                  1    DUMDAT(JJ))
    144        720 FORMAT(12X,I2,9X,I2,6X,I2,5X,I2,5X,I2,7X,I2,5X,I2,5X,F10.5)
    144            GO TO 10
    146          8 CONTINUE
    146            JR = JR + 1
    150            WRITE(NO,718) (IUNIT(J),KT(J),(IN(J,I),I=1,3),(NOUT(J,I),I=1,2),
                  1    DUMDAT(JJ),RLNTH(JR))
    212        718 FORMAT(12X,I2,9X,I2,6X,I2,5X,I2,5X,I2,7X,I2,5X,I2,2(5X,F10.5))
    212            GO TO 10
    214          7 CONTINUE
    214            WRITE(NO,719) (IUNIT(J),KT(J),(IN(J,I),I=1,3),(NOUT(J,I),I=1,2),
                  1                   DUMDAT(JJ))
    253        719 FORMAT (12X,I2,9X,I2,6X,I2,5X,I2,5X,I2,7X,I2,5X,I2,5X,E12.4)
    253         10 CONTINUE
             C
             C             PRINT INPUT INFORMATION
             C
    257            WRITE(NO,722)
    263        722 FORMAT(//,10X,23HFEED STREAM INFORMATION,//,7X,6HSTREAM,6X,2HTK,
                  18X,4HPSIA,20X,21HFLOWRATES(LBMOLES/HR),/,40X,3HCO ,7X,3HH2 ,7X,
                  2    3HCH4,7X,3HH2O,7X,3HCO2,7X,3HN2 ,7X,5HTOTAL,/)
    263            WRITE(NO,724)  TKFDOD,PRFDOD,(FDOD(I),I=1,NC),TTFDOD
    304        724 FORMAT (7X,*INITIAL*,4X,F7.1,3X,F6.1,2X,7F10.2)
    304            NFD = 1
    306            WRITE(NO,725)  TKSTM(NFD),PRSTM(NFD),(FSTM(NFD,I),I=1,NC),
                  1               TTFSTM(NFD)
    335        725 FORMAT (7X,*NEW*,8X,F7.1,3X,F6.1,2X,7F10.2)
    335            WRITE(NO,728) (IORD(I),I=1,NUNITS)
    351        728 FORMAT(//,10X,28HUNIT ORDERING OF CALCULATION,3X,15I5)
    351            WRITE(NO,732)
    355        732 FORMAT(1H1)
    355            WRITE(NO,730)
    361        730 FORMAT(10X,*FLOW STREAM INFORMATION FOR DYNAMIC SIMULATION*,
```

```
         1    //,7X,6HSTREAM,6X,2HTK,8X,
         1    4HPSIA,20X,21HFLOWRATES(LBMOLES/HR),/,40X,3HCO  ,7X,3HH2  ,7X,
         2    3HCH4,7X,3HH2O,7X,3HCO2,7X,3HN2  ,3X,5HTOTAL)
              DO 30 J = 1, NSTMS
              WRITE(NO,740) (J,TKSTM(J),PRSTM(J),(FSTM(J,I),I=1,NC),TTFSTM(J))
      740 FORMAT(6X,I2,9X,F7.1,3X,F6.1,2X,7F10.2)
       30 CONTINUE
              DO 32 II = 1 , NRXR
              WRITE(NO,742) II
      742 FORMAT(//,10X,11HREACTOR NO.,I3)
              WRITE(NO,310)
              WRITE(NO,312) (L(I),TK(I,II),X1(I,II),X2(I,II),RATE1(I,II),
         1        YCOMP(I,1,II),I = 1, NPTS)
       32 CONTINUE
              NFLAG = NFLAG + 1
              OUTPUT,QCOND(1)
              RETURN
C...
C...
C...     FORMAT CARDS ARE LISTED.
C...
       50 FORMAT (1H1)
      200 FORMAT ( /,7X,4HTIME,E12.4,5H  HRS,/)
      310 FORMAT(7X,7HREACTOR,5X,8HTEMP (K),3X,27HFRACTIONAL CONVERSION OF C
         1O,8X,5HRATE1,7X,3HYCO,/,7X,6HLENGTH,24X,4HMETH,5X,5HSHIFT)
      312 FORMAT(7X,F6.2,3X,F10.2,5X,2F10.4,8X,E13.4,5X,F7.5)
              END

NP*******WARNING:  NO PATH TO THIS STATEMENT
         64


              SUBROUTINE DSS014(XL,XU,N,U,UX,V)
C...
C...
C...     SUBROUTINE DSS014 IS AN APPLICATION OF SECOND-ORDER DIRECTIONAL
C...     DIFFERENCING IN THE NUMERICAL METHOD OF LINES.  IT IS INTENDED
C...     SPECIFICALLY FOR THE ANALYSIS OF CONVECTIVE SYSTEMS MODELLED BY
C...     FIRST-ORDER HYPERBOLIC PARTIAL DIFFERENTIAL EQUATIONS AS DIS-
C...     CUSSED IN SUBROUTINE DSS012.  THE COEFFICIENTS OF THE FINITE
C...     DIFFERENCE APPROXIMATIONS USED HEREIN ARE TAKEN FROM BICKLEY, W.
C...     G., FORMULAE FOR NUMERICAL DIFFERENTIATION, THE MATHEMATICAL
C...     GAZETTE, PP. 19-27, 1941, N = 2, M = 1, P = 0, 1, 2.
C...
              DIMENSION U(N),UX(N)
C...
C...
C...     COMPUTE THE COMMON FACTOR FOR EACH FINITE DIFFERENCE APPROXIMATION
C...     CONTAINING THE SPATIAL INCREMENT, THEN SELECT THE FINITE DIFFER-
C...     ENCE APPROXIMATION DEPENDING ON THE SIGN OF V (SIXTH ARGUMENT).
C...
              DX=(XU-XL)/FLOAT(N-1)
              R2FDX=1./(2.*DX)
              IF(V.LT.0.)GO TO 10
C...
C...
C...        (1)  FINITE DIFFERENCE APPROXIMATION FOR POSITIVE V
C...
              UX(1)=R2FDX*
         1(        -3.     *U(   1)     +4.     *U(   2)      -1.     *U(   3))
              UX(2)=R2FDX*
         1(        -1.     *U(   1)     +0.     *U(   2)      +1.     *U(   3))
              DO 1 I=3,N
              UX(I)=R2FDX*
         1(         1.     *U(I-2)     -4.     *U(I-1)      +3.     *U(   I))
        1     CONTINUE
              RETURN
C...
C...
C...        (2)  FINITE DIFFERENCE APPROXIMATION FOR NEGATIVE V
C...
       10     NM2=N-2
              DO 2 I=1,NM2
              UX(I)=R2FDX*
         1(        -3.     *U(   I)     +4.     *U(I+1)      -1.     *U(I+2))
        2     CONTINUE
```

```
153        UX(N-1)=R2FDX*
           1(      -1.    *U(N-2)     +0.    *U(N-1)     +1.    *U(  N))
176        UX(N)=R2FDX*
           1(      1.     *U(N-2)     -4.    *U(N-1)     +3.    *U(  N))
220        RETURN
221        END
```

```
      SUBROUTINE D3L(K,X,U,UX)
C...
C...  D3L = NUMERICAL DIFFERENTIATOR BASED ON THE 3-POINT LAGRANGE
C...        -                                      -         -
C...        POLYNOMIAL
C...
C...  D3L IS THE CORE DIFFERENTIATION ROUTINE BASED ON THE THREE-
C...  POINT LAGRANGE POLYNOMIAL.  IT CONSISTS OF THREE SECTIONS
C...  FOR UPWIND, CENTERED AND DOWNWIND APPROXIMATIONS OF THE
C...  DERIVATIVE.
C...
C...  THE THREE-POINT LAGRANGE INTERPOLATION POLYNOMIAL IS
C...
C...          (X  - X2)(X  - X3)
C...  U(X) = .................. U(X1)
C...          (X1 - X2)(X1 - X3)
C...
C...          (X  - X1)(X  - X3)
C...       + .................. U(X2)                               (1)
C...          (X2 - X1)(X1 - X3)
C...
C...          (X  - X1)(X  - X2)
C...       + .................. U(X3)
C...          (X3 - X1)(X3 - X2)
C...
C...  EQUATION (1) CAN BE DIFFERENTIATED WITH RESPECT TO X TO OBTAIN
C...  THE DERIVATIVE UX(X).  THIS DERIVATIVE CAN THEN BE EVALUATED
C...  AT X = X1, X2 AND X3 TO OBTAIN DOWNWIND, CENTERED AND UPWIND
C...  NUMERICAL APPROXIMATIONS OF THE DERIVATIVE.  NOTE THAT THIS
C...  PROCEDURE APPLIES TO A NONUNIFORM GRID SINCE X1, X2 AND X3
C...  ARE ARBITRARILY SELECTED BY THE USER.
C...
C...  ARGUMENT LIST
C...
C...     K          INTEGER INDEX TO SELECT THE TYPE OF DERIVATIVE
C...                APPROXIMATION.  1 = DOWNWIND, 2 = CENTERED, 3 =
C...                UPWIND (INPUT)
C...
C...     X          ONE-DIMENSIONAL ARRAY CONTAINING THE THREE VALUES
C...                OF THE INDEPENDENT VARIABLE (INPUT)
C...
C...     U          ONE-DIMENSIONAL ARRAY CONTAINING THE THREE VALUES
C...                OF THE DEPENDENT VARIABLE (INPUT)
C...
C...     UX         NUMERICAL DERIVATIVE OF U WITH RESPECT TO X AT
C...                GRID POINT K (OUTPUT)
C...
      DIMENSION X(3),U(3)
C...
C...  SELECT THE DERIVATIVE APPROXIMATION
      GO TO (1,2,3),K
C...
C...  ******************************************************************
C...
C...  COMPUTE UX(X1) USING THE DERIVATIVE OF EQUATION (1) WITH X = X1
C...
1     SUM=0.
C...
C...  COMPUTE THE U(X1), U(X2) AND U(X3) TERMS IN THE DERIVATIVE OF
C...  EQUATION (1) BY DO LOOP 18, STARTING WITH THE DENOMINATOR OF
C...  EACH TERM
      DO 18 I=1,3
      TERM=U(I)
```

```
      DO 11 J=1,3
      IF(J.EQ.I)GO TO 11
      TERM=TERM/(X(I)-X(J))
11    CONTINUE
      IF(I.EQ.1)GO TO 13
C...
C...  COMPLETE THE U(X2) AND U(X3) TERMS IN THE DERIVATIVE OF EQUATION
C...  (1) BY DO LOOP 12
      DO 12 J=1,3
      IF(J.EQ.1)GO TO 12
      IF(J.EQ.I)GO TO 12
      TERM=(X(1)-X(J))*TERM
12    CONTINUE
      GO TO 17
C...
C...  COMPLETE THE U(X1) TERM IN THE DERIVATIVE OF EQUATION (1) BY DO
C...  LOOP 15
13    SUM1=0.
      DO 15 JSUM=1,3
      IF(JSUM.EQ.1)GO TO 15
      TERM1=1.
      DO 14 J=1,3
      IF(J.EQ.1)GO TO 14
      IF(J.EQ.JSUM)GO TO 14
      TERM1=TERM1*(X(1)-X(J))
14    CONTINUE
      SUM1=SUM1+TERM1
15    CONTINUE
      TERM=SUM1*TERM
17    SUM=SUM+TERM
C...
C...  COMPUTE THE NEXT TERM IN THE DERIVATIVE OF EQUATION (1)
18    CONTINUE
C...
C...  ALL OF THE TERMS IN THE DERIVATIVE OF EQUATION (1) HAVE BEEN
C...  COMPUTED.  RETURN TO THE CALLING PROGRAM WITH THE NUMERICAL
C...  DERIVATIVE UX
      UX=SUM
      RETURN
C...
C...  ******************************************************************
C...
C...  COMPUTE UX(X1) USING THE DERIVATIVE OF EQUATION (1) WITH X = X1
C...
2     SUM=0.
C...
C...  COMPUTE THE U(X1), U(X2) AND U(X3) TERMS IN THE DERIVATIVE OF
C...  EQUATION (1) BY DC LOOP 18, STARTING WITH THE DENOMINATOR OF
C...  EACH TERM
      DO 28 I=1,3
      TERM=U(I)
      DO 21 J=1,3
      IF(J.EQ.I)GO TO 21
      TERM=TERM/(X(I)-X(J))
21    CONTINUE
      IF(I.EQ.2)GO TO 23
C...
C...  COMPLETE THE U(X2) AND U(X3) TERMS IN THE DERIVATIVE OF EQUATION
C...  (1) BY DO LOOP 12
      DO 22 J=1,3
      IF(J.EQ.2)GO TO 22
      IF(J.EQ.I)GO TO 22
      TERM=(X(2)-X(J))*TERM
22    CONTINUE
      GO TO 27
C...
```

```
C...  COMPLETE THE U(X1) TERM IN THE DERIVATIVE OF EQUATION (1) BY DO
C...  LOOP 15
23    SUM2=0.
      DO 25 JSUM=1,3
      IF(JSUM.EQ.2)GO TC 25
      TERM2=1.
      DO 24 J=1,3
      IF(J.EQ.2)GO TO 24
      IF(J.EQ.JSUM)GO TO 24
      TERM2=TERM2*(X(2)-X(J))
24    CONTINUE
      SUM2=SUM2+TERM2
25    CONTINUE
      TERM=SUM2*TERM
27    SUM=SUM+TERM
C...
C...  COMPUTE THE NEXT TERM IN THE DERIVATIVE OF EQUATION (1)
28    CONTINUE
C...
C...  ALL OF THE TERMS IN THE CERIVATIVE OF EQUATION (1) HAVE BEEN
C...  COMPUTED.  RETURN TO THE CALLING PROGRAM WITH THE NUMERICAL
C...  DERIVATIVE UX
      UX=SUM
      RETURN
C...
C...  ***************************************************************
C...
C...  COMPUTE UX(X1) USING THE DERIVATIVE OF EQUATION (1) WITH X = X1
C...
3     SUM=0.
C...
C...  COMPUTE THE U(X1), U(X2) AND U(X3) TERMS IN THE DERIVATIVE OF
C...  EQUATION (1) BY DO LOOP 18, STARTING WITH THE DENOMINATOR OF
C...  EACH TERM
      DO 38 I=1,3
      TERM=U(I)
      DO 31 J=1,3
      IF(J.EQ.I)GO TO 31
      TERM=TERM/(X(I)-X(J))
31    CONTINUE
      IF(I.EQ.3)GO TO 33
C...
C...  COMPLETE THE U(X2) AND U(X3) TERMS IN THE DERIVATIVE OF EQUATION
C...  (1) BY DO LOOP 12
      DO 32 J=1,3
      IF(J.EQ.3)GO TO 32
      IF(J.EQ.I)GO TO 32
      TERM=(X(3)-X(J))*TERM
32    CONTINUE
      GO TO 37
33    SUM3=0.
      DO 35 JSUM=1,3
      IF(JSUM.EQ.3)GO TO 35
      TERM3=1.
      DO 34 J=1,3
      IF(J.EQ.3)GO TO 34
      IF(J.EQ.JSUM)GO TO 34
      TERM3=TERM3*(X(3)-X(J))
34    CONTINUE
      SUM3=SUM3+TERM3
35    CONTINUE
      TERM=SUM3*TERM
37    SUM=SUM+TERM
C...
C...  COMPUTE THE NEXT TERM IN THE DERIVATIVE OF EQUATION (1)
38    CONTINUE
```

```
C...
C...  ALL OF THE TERMS IN THE DERIVATIVE OF EQUATION (1) HAVE BEEN
C...  COMPUTED.  RETURN TO THE CALLING PROGRAM WITH THE NUMERICAL
C...  DERIVATIVE UX
      UX=SUM
      RETURN
      END
      SUBROUTINE PDL32(N,X,U,UX)
C...
C...  PDL32 = POLYNOMIAL DIFFERENTIATOR BASED ON LAGRANGE 3-POINT
C...          -          -                   -        -
C...          POLYNOMIAL, DERIVATIVE AT POINT 2
C...                                          -
C...
C...  SUBROUTINE PDL32 PERFORMS A NUMERICAL DIFFERENTIATION OF DATA
C...  BY APPROXIMATING THE DATA WITH A SECOND-ORDER (THREE-POINT)
C...  LAGRANGE INTERPOLATION POLYNOMIAL.  THE POLYNOMIAL IS DIFFER-
C...  TIATED ANALYTICALLY TO OBTAIN THE DERIVATIVE, WHICH CAN THEN
C...  BE EVALUATED NUMERICALLY AT ANY OF THE THREE POINTS AS SELECTED
C...  BY THE USER.
C...
C...  PDL32 IN TURN CALLS THE THREE-POINT CORE DIFFERENTIATOR D3L
C...  TO COMPUTE THE NUMERICAL DERIVATIVE.  PDL32 CALLS D3L SO
C...  THAT THE DERIVATIVE IS EVALUATED AT THE SECOND (MIDDLE) POINT
C...  AND THEREFORE GIVES A THREE-POINT CENTERED APPROXIMATION OF
C...  THE DERIVATIVE.
C...
C...  ARGUMENT LIST
C...
C...     N          TOTAL NUMBER OF DATA PAIRS (INPUT)
C...
C...     X          ONE-DIMENSIONAL ARRAY CONTAINING THE INDEPENDENT
C...                VARIABLE (INPUT)
C...
C...     U          ONE-DIMENSIONAL ARRAY CONTAINING THE DEPENDENT
C...                VARIABLE (INPUT)
C...
C...     UX         ONE-DIMENSIONAL ARRAY CONTAINING THE DERIVATIVE
C...                OF THE DEPENDENT VARIABLE, U, WITH RESPECT TO THE
C...                INDEPENDENT VARIABLE, X (OUTPUT)
C...
      DIMENSION X(N),U(N),UX(N)
      DIMENSION X3(3),U3(3)
C...
C...  PUT THE FIRST THREE DATA PAIRS IN WORK ARRAYS X3 AND U3, I.E.,
C...  (X(1),U(1)), (X(2),U(2)), (X(3),U(3))
      DO 10 K=1,3
      X3(K)=X(K)
      U3(K)=U(K)
10    CONTINUE
C...
C...  CALL CORE DIFFERENTIATOR D3L TO COMPUTE A THREE-POINT DOWNWIND
C...  APPROXIMATION OF THE DERIVATIVE AT THE FIRST POINT
      CALL D3L(1,X3,U3,UX(1))
C...
C...  STORE SUCCESSIVE SETS OF THREE DATA PAIRS IN WORK ARRAYS X3 AND
C...  U3 FOR THE CALCULATION OF A THREE-POINT CENTERED APPROXIMATION
C...  OF THE DERIVATIVE AT POINTS I = 2 TO N-1
      NM1=N-1
      DO 30 I=2,NM1
      DO 20 K=1,3
      X3(K)=X(I-2+K)
      U3(K)=U(I-2+K)
20    CONTINUE
C...
C...  CALL CORE DIFFERENTIATOR D3L TO COMPUTE A THREE-POINT CENTERED
```

```
C...  APPROXIMATION OF THE DERIVATIVE AT POINTS I = 2 TO N-1
      CALL D3L(2,X3,U3,UX(I))
30    CONTINUE
C...
C...  PUT THE LAST THREE DATA PAIRS IN WORK ARRAYS X3 AND U3, I.E.,
C...  (X(N-2),U(N-2)), (X(N-1),U(N-1)), (X(N),U(N))
      DO 40 K=1,3
      X3(K)=X(N-3+K)
      U3(K)=U(N-3+K)
40    CONTINUE
C...
C...  CALL CORE DIFFERENTIATOR D3L TO COMPUTE A THREE-POINT UPWIND
C...  APPROXIMATION OF THE DERIVATIVE AT THE LAST POINT
      CALL D3L(3,X3,U3,UX(N))
      RETURN
      END
      SUBROUTINE PDL33(N,X,U,UX)
C...
C...  PDL33 = POLYNOMIAL DIFFERENTAITOR BASED ON LAGRANGE 3-POINT
C...           -             -                 -        -
C...
C...          POLYNOMIAL, DERIVATIVE AT POINT 3
C...                                          -
C...
C...
C...  SUBROUTINE PDL33 PERFORMS A NUMERICAL DIFFERENTIATION OF DATA
C...  BY APPROXIMATING THE DATA WITH A SECOND-ORDER (THREE-POINT)
C...  LAGRANGE INTERPOLATION POLYNOMIAL.  THE POLYNOMIAL IS DIFFER-
C...  TIATED ANALYTICALLY TO OBTAIN THE DERIVATIVE, WHICH CAN THEN
C...  BE EVALUATED NUMERICALLY AT ANY OF THE THREE POINTS AS SELECTED
C...  BY THE USER.
C...
C...  PDL33 IN TURN CALLS THE THREE-POINT CORE DIFFERENTIATOR D3L
C...  TO COMPUTE THE NUMERICAL DERIVATIVE.  PDL33 CALLS D3L SO
C...  THAT THE DERIVATIVE IS EVALUATED AT THE THIRD (RIGHT-MOST)
C...  POINT AND THEREFORE GIVES A THREE-POINT UPWIND APPROXIMATION
C...  OF THE DERIVATIVE.
C...
C...  ARGUMENT LIST
C...
C...     N          TOTAL NUMBER OF DATA PAIRS (INPUT)
C...
C...     X          ONE-DIMENSIONAL ARRAY CONTAINING THE INDEPENDENT
C...                VARIABLE (INPUT)
C...
C...     U          ONE-DIMENSIONAL ARRAY CONTAINING THE DEPENDENT
C...                VARIABLE (INPUT)
C...
C...     UX         ONE-DIMENSIONAL ARRAY CONTAINING THE DERIVATIVE
C...                OF THE DEPENDENT VARIABLE, U, WITH RESPECT TO THE
C...                INDEPENDENT VARIABLE, X (OUTPUT)
C...
      DIMENSION X(N),U(N),UX(N)
      DIMENSION X3(3),U3(3)
C...
C...  PUT THE FIRST THREE DATA PAIRS IN WORK ARRAYS X3 AND U3, I.E.,
C...  (X(1),U(1)), (X(2),U(2)), (X(3),U(3))
      DO 10 K=1,3
      X3(K)=X(K)
      U3(K)=U(K)
10    CONTINUE
C...
C...  CALL CORE DIFFERENTIATOR D3L TO COMPUTE A THREE-POINT DOWNWIND
C...  APPROXIMATION OF THE DERIVATIVE AT THE FIRST POINT
      CALL D3L(1,X3,U3,UX(1))
```



```
C...
C...  CALL CORE DIFFERENTIATOR D3L TO COMPUTE A THREE-POINT CENTERED
C...  APPROXIMATION OF THE DERIVATIVE AT THE SECOND POINT
```

```
      CALL D3L(2,X3,U3,UX(2))
C...
C...  STORE SUCCESSIVE SETS OF THREE DATA PAIRS IN WORK ARRAYS X3 AND
C...  U3 FOR THE CALCULATION OF A THREE-POINT UPWIND APPROXIMATION
C...  OF THE DERIVATIVE AT POINTS I = 3 TO I = N
      DO 30 I=3,N
      DO 20 K=1,3
      X3(K)=X(I-3+K)
      U3(K)=U(I-3+K)
20    CONTINUE
C...
C...  CALL CORE DIFFERENTIATOR D3L TO COMPUTE A THREE-POINT UPWIND
C...  APPROXIMATION OF THE DERIVATIVE AT POINTS I = 3 TO I = N
      CALL D3L(3,X3,U3,UX(I))
30    CONTINUE
      RETURN
      END
```