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COMPUTER PROGRAM MANUAL

TRANSIENT MODEL OF HYDROGEN/OXYGEN REACTOR

by

E. J. SMITH and A. S. KESTEN

prepared for

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

FEBRUARY, 1971

CONTRACT NAS 3-13317

United Aircraft Research Laboratories

UNITED AIRCRAFT CORPORATION

EAST HARTFORD, CONNECTICUT 06108

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E. J. Smith and A. S. Kesten

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ABSTRACT

A machine computational program has been developed under NASA Contract NAS 3-13317 to calculate temperature and reactant concentrations as functions of time and axial position in typical catalyzed hydrogen-oxygen reaction chambers. The program is based upon a transient model of the reactor system which describes the behavior of reactors operated under conditions of continuous flow.

The computer program developed from this model is described in detail in this computer manual. The manual contains operating instructions for this program as well as descriptions of input and output formats, including all output messages.

FOREWORD

This work was performed by United Aircraft Research Laboratories for the National Aeronautics and Space Administration under Contract NAS 3-13317 initiated January 14, 1970.

Included among those who cooperated in performance of the work under NAS 3-13317 were Dr. A. S. Kesten, Program Manager, Dr. W. G. Burwell, Chief, Kinetics and Thermal Sciences Section, Mr. D. B. Smith, Project Analyst, and Mrs. E. J. Smith, Computer Analyst.

This work was conducted under program management of the NASA Lewis Research Center and the Technical Manager was Mr. P. N. Herr, NASA Lewis Research Center, Cleveland, Ohio.

Report K910962-13

Transient Model of Hydrogen/Oxygen Reactor

Contract NAS 3-13317

SUMMARY

The Research Laboratories of United Aircraft Corporation, under Contract NAS 3-13317 with the National Aeronautics and Space Administration, have performed an analytical study of the transient behavior of a hydrogen/oxygen catalytic ignition system. This study has included the development of a computer program which is used to calculate temperature and species concentration profiles as functions of time in typical reaction chamber configurations. This manual describes the computer program. A description of input and output for the transient program is included in the discussion together with examples for typical data cases. In addition, a short write-up of the subroutines contained in the deck is included.

INTRODUCTION

Under Contract NAS 3-13317, a comprehensive analytical program was formulated with the objectives of (1) developing a transient analysis of a continuous flow hydrogen-oxygen catalytic ignition system to permit the prediction of temperatures, pressures, and species concentrations as functions of time as well as axial position in typical reactor systems, (2) developing a computer program based on this analysis, and (3) performing calculations using this computer program to demonstrate the effects of various system parameters on the transient performance of the reactor, and thus to define ignition delay times. As part of the contract effort, attention has been directed toward preparing a manual describing to potential users the operation of the computer program. The manual includes a detailed discussion of the program.

DISCUSSION OF THE H_2/O_2 TRANSIENT COMPUTER PROGRAM

The equations representing the transient model of a H_2/O_2 catalytic reactor have been programmed for the UNIVAC 1108 digital computer using FORTRAN V.* This computer program is discussed below. Included in this discussion are input and output descriptions and a list and short description of the various routines in the program.

Input Description

The following is a description of the necessary input for the H_2/O_2 transient computer program. To complete each data case run with this program, a minimum of two separate runs must be made; a third type of run may also be necessary. The three types of runs are: (1) initial non-diffusion-controlled run (always necessary), (2) continuation of a non-diffusion-controlled run (sometimes needed), and (3) diffusion-controlled (concluding) run (always necessary). The non-diffusion-controlled runs (types 1 and 2) are based upon a very general reasonably complete model of the reactor system. It would be best to run this type of run all the time, but the large amount of computer time needed necessitates restricting its use to the lower temperature calculations and then switching to the much faster diffusion-controlled run which is accurate at the higher temperatures. Splitting each case up into two or more runs this way also allows for the use of fewer axial stations in the non-diffusion-controlled runs, which reduces computer time for these slower runs.

Initial Non-Diffusion-Controlled Run

This type of run is the first one made when running a transient H_2/O_2 case. A general input format is given in Table I. The coding of a sample data case is shown in Fig. 1, and a listing of the input data punch cards corresponding to this sample data case is shown in Fig. 2. Below is a detailed description of the input; the numbers correspond to the card numbers (first column) of Table I.

1. The first card contains the title of the data case plus two logical indicators, H2LEAD and DEBUG.

   Title: The title serves to give individual data case identification. It consists of any alpha numeric information desired and should be punched in card columns 1-78.

   H2LEAD: This is a logical unit which should indicate whether the catalyst in the reactor is preconditioned with hydrogen (hydrogen run through the reactor at its inlet concentration before the oxygen is turned on). If it <u>is</u> preconditioned, the letter "T" should

*Discussion of these equations and their derivation can be found in NASA Contract Report NASA CR-120799, "Final Report - Transient Model of Hydrogen/Oxygen Reactor", February, 1971.

appear in card column 79. If it is not, the letter "F" should be punched.

DEBUG: This logical unit indicates whether the detailed printing is desired. A large amount of print will be generated under this option. For example, a data case where NOFZ=16 and NPASS=5 (see description of these variables on card 2) will produce over 150 pages of detailed print. This printing will sometimes be necessary, however, since summary printing only gives the temperatures and concentrations at the end of every twenty time steps. To get the detailed print, the letter "T" should be punched in card column 80; if the letter "F" is punched, only the summary print will result.

2. The second card contains five variables, NOFZ, NPASS, INPERP, MODNO, PUNCH, and ITSTEP.

NOFZ: This is the number of axial positions (Z's) at which analysis will be made. These axial positions will be input on cards 6a, 6b, etc. The maximum number of Z's allowed by the program is 75. However, computer run time for the non-diffusion-controlled runs is affected drastically by the number of Z's. For these runs, it is best to use as few as possible (10-15 were used in test cases), especially for lower pressures. (Using 10 axial positions, one data case run at P=15 psia took over 30 minutes of computer time for the non-diffusion-controlled run. A comparable case run at P=300 psia took only four minutes.)

NPASS: This is the total number of time "passes" to be taken for this run. Each "pass" consists of "INPERP" time steps (see below), and during each pass, a constant time step size is used. For the non-diffusion-controlled runs, it is best to use NPASS=10 or less although the maximum number allowed by the program is 40. If the case completes the non-diffusion-controlled run before the 10 passes are through, the program will take care of itself (i.e., punch out the appropriate cards for the diffusion-controlled run (run type 3) and end). If more than 10 passes are needed (as in the low pressure cases) the program will punch out the cards for run type 2 (continuation of non-diffusion-controlled run) and end. For the two cases mentioned under the description of NOFZ, the low pressure case which took over 30 minutes to complete needed over 17 passes, whereas the high pressure case needed fewer than 2 passes which were completed in under 4 minutes.

If it is decided to input the time increments (see ITSTEP) NPASS must equal the number of input DELT's. However for non-diffusion-controlled runs, inputting the DELT's is not advised.

INPERP: This is the number of time increments per pass. The number used in the test cases was "20" which seemed to work out fairly well. Since summary plotting and printing is done only at the end of each pass, at times it might be desirable to use a smaller number for this variable.

MODNO: This number indicates which axial position values will be plotted on the summary printer-plots. If MODNO=1, every point will be plotted, if it equals 2, every-other point will be plotted, etc.

PUNCH: This variable indicates which of various read/write punch card options will be used. For an initial non-diffusion-controlled run, this variable should = 1. This indicates cards will be punched at the end of the run (either when NPASS is reached or when the non-diffusion-controlled part of the run is completed).

ITSTEP: This value indicates whether time steps will be input or calculated by the program. For non-diffusion-controlled runs, ITSTEP should equal 0 which indicates the program will calculate the time steps.

3. The third card contains the 8 values for G, TS, T(1), P(1), H(1), CIH2(1), CIO2(1) and CIHE(1).

G: This is the inlet (at Z=0) mass flow rate in lb/ft^2-sec. It must be greater than zero.

TS: This is the freezing temperature of water in deg R.

T(1): This is the inlet interstitial temperature in deg R.

P(1): This is the steady-state inlet chamber pressure in psia.

H(1): This is the inlet enthalpy in BTU/lb, (reference number, usually taken as 0).

CIH2(1): This is the inlet concentration of hydrogen in lb/ft^3.

CIO2(1): This is the inlet concentration of oxygen in lb/ft^3.

CIHE(1): This is the inlet concentration of helium in lb/ft^3.

4. The fourth card contains the 8 values, TI, PI, CH2I, CO2I, CH2OI, CHEI, PTI and SDTIME.

TI: This is the initial (at time = 0) interstitial temperature throughout the reactor in deg R.

PI: This is the initial chamber pressure throughout the reactor in psia.

CH2I: This is the initial concentration of hydrogen throughout the reactor in lb/ft^3.

CO2I: This is the initial concentration of oxygen throughout the reactor in lb/ft^3.

CH2OI: This is the initial concentration of water throughout the reactor in lb/ft^3.

CHEI: This is the initial concentration of helium throughout the reactor in lb/ft^3.

PTI: This is the initial catalyst bed temperature throughout the reactor in deg R.

SDTIME: This is the time in seconds at which the oxygen flow is shut off.

5. The fifth card contains the 8 values AW, CW, MW, DC, TA, HA, HA1 and HA2.

AW: This is the total surface area of the chamber plus nozzle walls in ft^2.

CW: This is the specific heat of the chamber walls in BTU/lb-deg R.

MW: This is the thermal mass of the chamber plus nozzle walls in lbs.

DC: This is the diameter of the reaction chamber in ft.

TA: This is the temperature of the surrounding atmosphere in deg R.

HA: This is the heat transfer coefficient for forced convection between the chamber and the surrounding atmosphere in BTU/ft^2-sec-deg R.

HA1: This is the heat transfer coefficient for natural convection between the chamber and the surrounding atmosphere in BTU/ft^2-sec-deg $R^{1.25}$.

HA2: This is the radiative heat transfer coefficient between the chamber and the surrounding atmosphere in BTU/ft^2-sec-deg R^4.

6. Card six should only be included for those cases where the catalyst is <u>not</u> preconditioned with hydrogen (H2LEAD = F on card 1). This card contains the 6 values PF, TSS, MBARSS, AC, VC and PREST.

PF: This is the feed pressure in psia.

TSS: This is steady-state bed exit temperature in deg R. This number can be obtained by running the H_2/O_2 steady-state computer program (see UARL Report H910721 . . . NASA CR-72567).

MBARSS: This is the steady-state bed exit average molecular weight. It can also be obtained from running the steady-state computer program.

AC: This is the cross-sectional area of the reaction chamber in ft^2.

VC: This is the volume of the reactor up to the nozzle throat exclusive of the volume occupied by catalyst particles in ft^3.

PREST: This is the pressure of the surrounding atmosphere in psia.

7. Cards 7a, 7b, etc. contain the axial station values (Z's) in feet at which calculations will be made. There should be NOFZ (see card 2) values of Z input at the rate of 8 per card. For most cases, it is recommended that more Z's be placed near the reactor inlet. The first Z must equal 0; the second Z must be very close to 0; the last Z equals the bed exit.

8. Cards 8a, 8b, etc. contain the input time increments (DELT's) in seconds. These cards should be included only if ITSTEP on card 2 equals 1. For non-diffusion-controlled runs, it is advisable to allow the program to calculate DELT's (ITSTEP=0).

Cards 9 through 11 contain AVSZ(I), the interpolation table used to obtain the catalyst particle radius at any point along the reactor bed. Subroutine UNBAR, an interpolation routine developed at UARL, is used to obtain an appropriate particle radius, A, for a given axial station along the bed. For this table, there should be a total of NZ (see third entry on card 9) values of Z and A.

9. Card 9 contains the four table descriptors needed by UNBAR. The first descriptor signifies the table number. For this program, it should equal 0.0. The second descriptor tells at what location in the array the table starts; the tables in this program are read in such that this number equals 1.0. The third descriptor is the number of independent variables in the table (in this case the number of Z's). This number is called NZ. The fourth descriptor for a univariate table such as this one should equal 0.0.

10. Cards 10a, 10b, etc. contain the monatonically increasing Z values in feet. Enough cards should be used to contain NZ values of Z at the rate of 10 per card. For example, if NZ=12, 12 values of Z should be input using two cards, with ten values on the first card and the two remaining values on the second card.

11. Cards 11a, 11b, etc. contain the A's (in feet) which correspond to the Z's listed on cards 10a, 10b, etc. Enough cards should be used to contain NZ values of A at the rate of 10 per card.

Cards 12 through 14 contain APVSZ(I), the interpolation table used to obtain the total external catalyst particle surface area per unit volume of bed (AP). These AP values are obtained as functions of Z using UNBAR as in the AVSZ table discussed above. For this table there should be a total of NZ values of Z and AP.

12. Card 12 contains the table descriptors and should be exactly the same as card 9.

13. Cards 13a, 13b, etc. contain the Z values and should be exactly the same as cards 10a, 10b, etc.

14. Cards 14a, 14b, etc. contain the AP values in ft^{-1} which correspond to the Z's listed in cards 13a, 13b, etc. Enough cards should be used to contain NZ values of AP at the rate of ten per card.

Cards 15 through 17 contain DELVSZ(I), the interpolation table used to obtain the interparticle void fraction (DELTA). These DELTA values are obtained as functions of Z using UNBAR as in the AVSZ table discussed above. For this table there should be a total of NZ values of Z and DELTA.

15. Card 15 contains the table descriptors and should be exactly the same as cards 9.

16. Cards 16a, 16b, etc. contain the Z values and should be exactly the same as cards 10a, 10b, etc.

17. Cards 17a, 17b, etc. contain the DELTA values which correspond to the Z's listed on cards 16a, 16b, etc. Enough cards should be used to contain NZ values of DELTA at the rate of 10 per card.

18. Card 18 contains the values CIH2(1) and CI02(1). These two values are the inlet concentrations of hydrogen and oxygen, respectively, after "shutdown" (that is, after the oxygen flow is turned off).

Continuation of a Non-Diffusion-Controlled Run

If the initial non-diffusion-controlled run completes the input NPASS number of passes without printing out "GO TO ALL DIFFUSION-CONTROLLED RUN", a continuation run will be necessary. Also if the continuation run ends without this printed message, a continuation of the continuation run should be made, etc. A general input format for this type of run is given in Table II. The listing of the punch cards for a continuation run is given in Figs. 3a - 3e. Below is a detailed description of the input; the numbers correspond to the card numbers (first column) of Table II.

1. The first card contains, again, the title H2LEAD and DEBUG. This card should be exactly the same for the continuation runs as it was for the initial non-diffusion-controlled run.

2. The second card again contains NOFZ, NPASS, INPERP, MODNO, PUNCH and ITSTEP.

   NOFZ: This value must be the same as it was for the initial run.

   NPASS: This is the number of time "passes" to be taken. It may be changed, but the maximum still equals 40.

   INPERP: This is the number of time increments per "pass". It may be changed.

   MODNO: This number indicates which axial position values will be plotted as before. It may be changed.

   PUNCH: This indicator specifies which read/write punch card option will be used. For continuation runs, it must equal 3. This indicates punch cards will be read in with the data case and also punched out at the end of the run.

   ITSTEP: As in the initial run, this indicates whether time increments will be input or internally calculated. Again, as in the initial run, it should equal 0 (internally calculated).

3-17. Cards 3 through 17 should be exactly the same as they were for the initial run.

   Cards 18-32 are obtained from the cards punched out at the end of an initial non-diffusion-controlled run or at the end of a previous continuation run if this is the 2nd or more continuation. These cards should only be included for continuation runs.

18. Cards 18a, 18b, etc. contain NOFZ values of Z(I) . . . (axial positions).

19. Cards 19a, 19b, etc. contain NOFZ values of PT(I). . . . (particle surface temperature at each axial station at end of previous run).

20. Cards 20a, 20b, etc. contain NOFZ values of T(I) . . . (interstitial temperature at each axial station at end of previous run).

21. Cards 21a, 21b, etc. contain NOFZ values of H(I) . . . (enthalpy at each axial station at end of previous run).

22. Cards 22a, 22b, etc. contain NOFZ values of P(I) . . . (chamber pressure at each axial station at end of previous run).

23. Cards 23a, 23b, etc. contain NOFZ values of CIH2(I) . . . (interstitial concentration of hydrogen at each axial station at end of previous run).

24. Cards 24a, 24b, etc. contain NOFZ values of CIO2(I) . . . (interstitial concentration of oxygen at each axial station at end of previous run).

25. Cards 25a, 25b, etc. contain NOFZ values of CIH2OV(I) . . . (interstitial concentration of water at each axial station at end of previous run).

26. Cards 26a, 26b, etc. contain NOFZ values of CIHE(I) . . . (interstitial concentration of helium at each axial station at end of previous run).

27. Cards 27a, 27b, etc. contain NOFZ values of PPT(I) . . . (particle surface temperature at each axial station one time increment previous to end of previous run).

28. Cards 28a, 28b, etc. contain NOFZ x NPP values of TPP(I, J). . . (temperature profile within catalyst particle at each axial station at end of previous run). NPP is the number of radial positions within the particle considered in the analysis (set at 30 in the program).

29. Cards 29a, 29b, etc. contain NOFZ x NPP values of CO2(I, J). . . (oxygen concentration profile within catalyst particle at each axial station at end of previous run).

30. Cards 30a, 30b, etc. contain NOFZ x NPP values of CH2(I, J) . . . (hydrogen concentration profile with catalyst particle at each axial station at end of previous run).

31. Cards 31a, 31b, etc. contain NOFZ values of MINT(I) . . . (diffusion-controlled indicator for each axial station at end of previous run).

32. Card 32 contains the values at the end of the previous run for TIME, TW, and DELTT.

TIME: is the cumulative reactor run time in seconds

TW: is the wall temperature in deg R

DELTT: is the time increment

33. Card 33 for the continuation run is exactly the same as card 18 of the initial non-diffusion-controlled run.

Diffusion-Controlled Run

This type of run is the last one to be made when running a transient H_2/O_2 case. When "GO TO ALL DIFFUSION-CONTROLLED RUN" is printed out at the end of an initial or continued non-diffusion-controlled run, this third type of run should follow. Compared to the first two types, this kind of run takes relatively little computer time. Depending on the number of axial stations being analyzed, a diffusion-controlled run, on the UARL UNIVAC 1108, took between three and five minutes for all cases run (between 20 and 40 Z's were used).

A general input format is given in Table III. A listing of the input data punch cards for a run of this type is shown in Fig. 4. Below is a detailed description of the input; the numbers correspond to the card numbers (first column) of Table III.

1. The first card again contains the title of the data case plus the logical indicators H2LEAD and DEBUG.

   Title: This should be the same as it was for the two previous run types.

   H2LEAD: This also should be the same as it was for the non-diffusion-controlled runs.

   DEBUG: This indicator should be set equal to "F" for the diffusion controlled runs; otherwise over 1000 pages of output may be produced. For the diffusion-controlled runs, the summary printing gives sufficient information.

2. The second card contains the five values of NOFZ, NPASS, INPERP, MODNO, PUNCH and ITSTEP.

   NOFZ: This is the number of axial positions (Z's) at which analysis will be made in the diffusion-controlled run. The maximum number allowed is 75. Since this type of run takes relatively little run time no matter how many Z's are used, it is advised to use the near the maximum (the test cases were run using 36 Z's).

NPASS: This is the total number of time "passes" to be taken for this run. For the diffusion-controlled runs, it is advised to input the time increments (see discussion of ITSTEP). If this is the case, NPASS must equal the number of time increments input on cards 8a, 8b, etc.; the maximum number allowed by the program is 40.

INPERP: This is the number of time increments per pass. It may change from previous run value.

MODNO: This number indicates which axial position values are to be summary plotted. It may be changed from previous run value.

PUNCH: This variable indicates which of various read/write punch card options will be used. For diffusion-controlled runs, this number must equal 4. This indicates a special set of data cards will be read in (see discussion of cards 18-25).

ITSTEP: This value indicates whether time steps will be input or calculated by the program (ITSTEP=1 means input . . . ITSTEP=0 means calculated). For diffusion-controlled runs, ITSTEP should equal 1 and the time increments (DELT's) should be input on cards 8a, 8b, etc. As the case approaches steady-state, larger DELT's might be desired (see sample input DELT's in Fig. 3). If ITSTEP is left equal to 0, all DELT's will be calculated equal to .001 sec for the diffusion-controlled runs.

3-6. Cards 3-6 should be exactly the same as they were for the non-diffusion-controlled runs.

7. Cards 7a, 7b, etc., contain the axial station values (Z's) in feet at which calculations will be made by the program. There should be NOFZ (see card 2) values of Z input at the rate of 8 per card. Note that this will be a different set of Z's than those used in the non-diffusion-controlled runs . . . there should be many more. However, as before, for most cases it is best to place more Z's near the reactor inlet. Also, the first Z must still equal 0, the second Z must be very close to 0, and the last Z must be at the bed exit.

8. Cards 8a, 8b, etc., contain the input time increments (DELT's) in seconds. These cards must be included if ITSTEP=1. It is recommended that these be input for diffusion-controlled runs.

9-17. Cards 9-17 should be exactly the same as they were for non-diffusion-controlled runs.

Cards 18-25 are obtained from the cards punched out at the end of the non-diffusion-controlled runs (when the message "GO TO ALL DIFFUSION-CONTROLLED RUN" is printed). These cards should only be included for diffusion-controlled runs.

18. Card 18 contains the number for NAXT. This value is the number of Z's used in the preceding non-diffusion-controlled runs.

19. Cards 19a, 19b, etc., contain ZT(I) . . . (the axial stations used in the non-diffusion-controlled runs). Enough cards are used to punch out NAXT values of ZT at the rate of 8 per card.

20. Cards 20a, 20b, etc., contain PTT(I) . . . (the particle surface temperature at each axial station at the end of the non-diffusion-controlled run). NAXT values of PTT are punched out.

21. Cards 21a, 21b, etc., contain CO2T(I) . . . (the oxygen concentration at each Z at the end of the non-diffusion-controlled run). NAXT values of CO2T are punched.

22. Cards 22a, 22b, etc., contain CH2T(I) . . . (the hydrogen concentration at each Z at the end of the non-diffusion-controlled run). NAXT values of CH2T are punched.

23. Cards 23a, 23b, etc., contain CH2OT(I) . . . (the water concentration at each Z at the end of the non-diffusion-controlled run). NAXT values of CH2OT are punched.

24. Cards 24a, 24b, etc., contain TTI(I) . . . (the interstitial temperature at each Z from the end of the non-diffusion-controlled run). NAXT values of TTI are punched.

25. Card 25 contains TIME and TW, the cumulative reactor run time in seconds and the wall temperature in deg R from the end of the non-diffusion-controlled run.

26. Card 26 of the diffusion-controlled run is exactly the same as card 18 of the initial non-diffusion-controlled run.

TABLE I

INPUT FORMAT

TRANSIENT H_2/O_2 COMPUTER PROGRAM: INITIAL NON-DIFFUSION-CONTROLLED RUN

CARD NO.	NO. OF CARDS	FORTRAN Ⅴ FORMAT	COLUMNS USED	SYMBOL OR DESCRIPTION	CORRESPONDING SYMBOL USED IN EQUATIONS	NOMENCLATURE
1	1	13A6, 2L1	1-78	Title	- -	
			79	H2LEAD	- -	Logical indicator
			80	DEBUG	- -	Logical indicator
2	1	6I4*	1-4	NOFZ	- -	Number of axial stations
			5-8	NPASS	- -	Number of "passes"
			9-12	INPERP	- -	Number of increments per "pass"
			13-16	MODNO	- -	Axial position plotting indicator
			17-20	PUNCH	- -	Punch card indicator
			21-24	ITSTEP	- -	Input time step indicator
3	1	8E10.5	1-10	G	G	Mass flow rate
			11-20	TS	- -	Freezing temperature of water
			21-30	T(1)	T_i	Inlet interstitial temperature
			31-40	P(1)	P	Steady-state inlet chamber pressure
			41-50	H(1)	h	Inlet enthalpy
			51-60	CIH2(1)	C_i^{H2}	Inlet concentration of hydrogen
			61-70	CIO2(1)	C_i^{O2}	Inlet concentration of oxygen
			71-80	CIHE(1)	C_i^{HE}	
4	1	8E10.5	1-10	TI	T_i	Initial interstitial temperature
			11-20	PI	P	Initial chamber pressure
			21-30	CH2I	C_i^{H2}	Initial concentration of hydrogen
			31-40	CO2I	C_i^{O2}	Initial concentration of oxygen

*right adjusted

TABLE I (Cont'd)

INPUT FORMAT

TRANSIENT H_2/O_2 COMPUTER PROGRAM: INITIAL NON-DIFFUSION-CONTROLLED RUN

CARD NO.	NO. OF CARDS	FORTRAN V FORMAT	COLUMNS USED	SYMBOL OR DESCRIPTION	CORRESPONDING SYMBOL USED IN EQUATIONS	NOMENCLATURE
4 (Cont'd)	1	8E10.5	41-50	CH2OI	$C_i^{H_2O}$	Initial concentration of water
			51-60	CHEI	C_i^{He}	Initial concentration of helium
			61-70	PTI	$(T_P)_s$	Initial catalyst bed temperature
			71-80	SDTIME	- -	Shutdown time
5	1	8E10.5	1-10	AW	A_W	Chamber wall total surface area
			11-20	CW	C_W	Chamber wall specific heat
			21-30	MW	m_W	Chamber wall thermal mass
			31-40	DC	dc	Reaction chamber diameter
			41-50	TA	T_a	Ambient temperature
			51-60	HA	h_a	Forced convection heat transfer coefficient
			61-70	HA1	h_a'	Natural convection heat transfer coefficient
			71-80	HA2	h_a''	Radiative heat transfer coefficient
6*	1	6E10.5	1-10	PF	P_F	Feed pressure
			11-20	TSS	T_i^{ss}	Steady-state exit interstitial temperature
			21-30	MBARSS	$\bar{M}^{ss}$	Steady-state exit average molecular weight
			31-40	AC	A_C	Cross-sectional area of reaction chamber
			41-50	VC	V_C	Volume of reactor minus catalyst volume
			51-60	PREST	- -	Ambient pressure
7a 7b etc.	**	8E10.5	1-10 11-20 ↓ 71-80	Z(I)	z	Axial station

*This card is included only if H2LEAD (Card 1) is equal to "F"

**Enough cards should be used to contain (NOFZ) values of z at the rate of 8 per card

TABLE I (Cont'd)

INPUT FORMAT

TRANSIENT H_2/O_2 COMPUTER PROGRAM: INITIAL NON-DIFFUSION-CONTROLLED RUN

CARD NO.	NO. OF CARDS	FORTRAN V FORMAT	COLUMNS USED	SYMBOL OR DESCRIPTION	CORRESPONDING SYMBOL USED IN EQUATIONS	NOMENCLATURE
8a* 8b etc.	**	8E10.5	1-10 11-20 ↓ 71-80	DELT(I)	Δt	Time increments
9	1	4E8.4	1-8 9-16 17-24 25-32	0. 1. NZ. 0.	- - - - - - - -	Table descriptor Table descriptor Table descriptor Table descriptor
10a 10b etc.	***	10E8.4	1-8 9-16 ↓ 73-80	Z(I)	z	Axial stations
11a 11b etc.	***	10E8.4	1-8 9-16 ↓ 73-80	A(I)	α	Catalyst particle radii
12	1	4E8.4	1-8 9-16 17-24 25-32	0. 1. NZ. 0.	- - - - - - - -	Table descriptors

*These cards are included only if ITSTEP (Card 2) is equal to "1"

**Enough cards should be used to contain (NPASS) values of Δt at the rate of 8 per card

***Enough cards should be used to contain (NZ) values of z, α, A_p, or δ at the rate of 10 per card

TABLE I (Cont'd)

INPUT FORMAT

TRANSIENT H_2/O_2 COMPUTER PROGRAM: INITIAL NON-DIFFUSION-CONTROLLED RUN

CARD NO.	NO. OF CARDS	FORTRAN V FORMAT	COLUMNS USED	SYMBOL OR DESCRIPTION	CORRESPONDING SYMBOL USED IN EQUATIONS	NOMENCLATURE
13a 13b etc.	*	10E8.4	1-8 9-16 ↓ 73-80	Z(I)	z	Axial stations
14a 14b etc.	*	10E8.4	1-8 9-16 ↓ 73-80	AP(I)	A_P	Total external catalyst particle surface areas per unit volume of bed
15	1	4E8.4	1-8 9-16 17-24 25-32	0. 1. NZ. 0.	- - - - - - - -	Table descriptors
16a 16b etc.	*	10E8.4	1-8 9-16 ↓ 73-80	Z(I)	z	Axial stations
17a 17b etc.	*	10E8.4	1-8 9-16 ↓ 73-80	DELTA(I)	δ	Interparticle void fractions

*Enough cards should be used to contain (NZ) values of z, α, A_P, or δ at the rate of 10 per card.

TABLE I (Cont'd)

INPUT FORMAT

TRANSIENT H_2/O_2 COMPUTER PROGRAM: INITIAL NON-DIFFUSION-CONTROLLED RUN

CARD NO.	NO. OF CARDS	FORTRAN V FORMAT	COLUMNS USED	SYMBOL OR DESCRIPTION	CORRESPONDING SYMBOL USED IN EQUATIONS	NOMENCLATURE
18	1	2E10.5	1-10	CIH2(1)	$c_i^{H_2}$	Inlet concentration of hydrogen after "shutdown"
			11-20	CIO2(1)	$c_i^{O_2}$	Inlet concentration of oxygen after "shutdown"

TABLE II

INPUT FORMAT

TRANSIENT H_2/O_2 COMPUTER PROGRAM: CONTINUATION OF NON-DIFFUSION-CONTROLLED RUN

CARD NO.	NO. OF CARDS	FORTRAN IV FORMAT	COLUMNS USED	SYMBOL OR DESCRIPTION	CORRESPONDING SYMBOL USED IN EQUATIONS	NOMENCLATURE
1-17	Cards 1-17 follow exactly the same <u>format</u> as cards 1-17 in Table I. Note, however, the differences in values on card 2 in the detailed discussion of continuation-run input.					
Cards 18-31 are cards punched out by the program at the end of an initial or previous continuation run.						
18a 18b etc.	*	8E10.5	1-10 11-20 ↓ 71-80	Z(I)	z	Axial stations
19a 19b etc.	*	8E10.5	"	PT(I)	$(T_p)_s$	Particle surface temperatures
20a 20b etc.	*	8E10.5	"	T(I)	T_i	Interstitial temperatures
21a 21b etc.	*	8E10.5	"	H(I)	h	Enthalpies

*Enough cards should be used to contain (NOFZ) values at the rate of 8 per card.

TABLE II (Cont'd)

INPUT FORMAT

TRANSIENT H_2/O_2 COMPUTER PROGRAM: CONTINUATION OF NON-DIFFUSION-CONTROLLED RUN

CARD NO.	NO. OF CARDS	FORTRAN V FORMAT	COLUMNS USED	SYMBOL OR DESCRIPTION	CORRESPONDING SYMBOL USED IN EQUATIONS	NOMENCLATURE
22a 22b etc.	*	8E10.5	1-10 11-20 ↓ 71-80	P(I)	P	Chamber pressures
23a 23b etc.	*	8E10.5	"	CIH2(I)	$c_i^{H_2}$	Interstitial hydrogen concentrations
24a 24b etc.	*	8E10.5	"	CIO2(I)	$c_i^{O_2}$	Interstitial oxygen concentrations
25a 25b etc.	*	8E10.5	"	CIH2OV(I)	$c_i^{H_2O^V}$	Interstitial water concentration
26a 26b etc.	*	8E10.5	"	CIHE(I)	c_i^{He}	Interstitial helium concentration
27a 27b etc.	*	8E10.5	"	PPT(I)	$(T_p)_s$	Particle surface temperatures at previous time

*Enough cards should be used to contain (NOFZ) values at the rate of 8 per card.

TABLE II (Cont'd)

INPUT FORMAT

TRANSIENT H_2/O_2 COMPUTER PROGRAM: CONTINUATION OF NON-DIFFUSION-CONTROLLED RUN

CARD NO.	NO. OF CARDS	FORTRAN IV FORMAT	COLUMNS USED	SYMBOL OR DESCRIPTION	CORRESPONDING SYMBOL USED IN EQUATIONS	NOMENCLATURE
28a 28b etc.	**	8E10.5	1-10 11-20 ↓ 71-80	TPP(I,J)	$T(x,t)$	Particle temperatures
29a 29b etc.	**	8E10.5	"	CO2(I,J)	$\rho_{O_2}(x,t)$	Particle oxygen concentration
30a 30b etc.	**	8E10.5	"	CH2(I,J)	$\rho_{H_2}(x,t)$	Particle hydrogen concentration
31a 31b etc.	*	40I2***	1-2 3-4 ↓ 79-80	MINT(I)	- -	Diffusion-controlled indicators
32	1	3E10.5	1-10 11-20 21-30	TIME TW DELTT	t T_W Δt	Cumulative time Wall temperature Time increment
33	1	2E10.5	1-10 11-20	CIH2(1) CIO2(1)	$c_i^{H_2}$ $c_i^{O_2}$	Inlet concentration of hydrogen after "shutdown" Inlet concentration of oxygen after "shutdown"

*Enough cards should be used to contain (NOFZ) values at the rate of 8 per card.

**Enough cards should be used to contain (NOFZ x NPP) values at the rate of 8 per card (NPP values for first Z, then NPP values for second Z . . . etc. . . to NPP values for (NOFZ) Z).

***Right adjusted.

TABLE III

INPUT FORMAT

TRANSIENT H_2/O_2 COMPUTER PROGRAM: DIFFUSION-CONTROLLED RUN

CARD NO.	NO. OF CARDS	FORTRAN Ⅴ FORMAT	COLUMNS USED	SYMBOL OR DESCRIPTION	CORRESPONDING SYMBOL USED IN EQUATIONS	NOMENCLATURE
1-17	Cards 1-17 follow exactly the same format as cards 1-17 in Table I. Note, however, the differences in values on cards 1, 2, 7 and 8 in the detailed discussion of diffusion-controlled input.					
Cards 18-25 are cards punched out by the program at the end of the final non-diffusion-controlled run.						
18	1	I2*	1-2	NAXT	- -	Number of Z's in non-d.c. runs
19	**	8E10.5	1-10 11-20 ↓ 71-80	ZT(I)	z	Axial stations in non-d.c. runs
20a 20b etc.	**	8E10.5	"	PTT(I)	$(T_p)_s$	Particle surface temperatures at end of non-d.c. runs
21a 21b etc.	**	8E10.5	"	CO2T(I)	$c_i^{O_2}$	Interstitial concentrations of oxygen at end of non-d.c. runs
22a 22b etc.	**	8E10.5	"	CH2T(I)	$c_i^{H_2}$	Interstitial concentrations of hydrogen at end of non-d.c. runs

*Right adjusted.

**Enough cards should be used to contain (NAXT) values at the rate of 8 per card

TABLE III (Cont'd)

INPUT FORMAT

TRANSIENT H_2/O_2 COMPUTER PROGRAM: DIFFUSION-CONTROLLED RUN

CARD NO.	NO. OF CARDS	FORTRAN V FORMAT	COLUMNS USED	SYMBOL OR DESCRIPTION	CORRESPONDING SYMBOL USED IN EQUATIONS	NOMENCLATURE
23a. 23b etc.	*	8E10.5	1-10 11-20 ↓ 71-80	CH2OT(I)	$c_i^{H_2O}$	Interstitial concentrations of water at end of non-d.c. runs
24a 24b etc.	*	8E10.5	"	TTI(I)	T_i	Interstitial temperatures at end of non-d.c. runs
25	1	2E10.5	1-10 11-20	TIME TW	t T_W	Cumulative time at end of non-d.c. runs Wall temperature at end of non-d.c. runs
26	1	2E10.5	1-10 11-20	CIH2(1) CIO2(1)	$c_i^{H_2}$ $c_i^{O_2}$	Inlet concentration of hydrogen after "shutdown" Inlet concentration of oxygen after "shutdown"

*Enough cards should be used to contain (NAXT) values at the rate of 8 per card.

CODING OF A SAMPLE DATA CASE

TRANSIENT H2/O2 COMPUTER PROGRAM: Initial Non-Diffusion-Controlled Run

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Columns 1–80

CARD NO.								
1	** TRANSIENT H2/O2 CASE 13 ** (P=300 * G=1.05 * TF=360 * O/F=1 * 25-30 MSH)TT							
2	11	10	20	1	1	0		
3	1.05	492.	360.	300.	0.	.1472	.1472	0.
4	360.	300.	.1472	0.	0.	0.	360.	0.5
5	.0047	0.12	.0066	.0358	360.	0.	.00011	0.
7a	0.	.00001	.001	.002	.004	.006	.008	.010
7b	.012	.015	.020					
9	0.	1.	4.	0.				
10	0.	.01	.03	.05				
11	.001	.001	.001	.001				
12	0.	1.	4.	0.				
13	0.	.01	.03	.05				
14	2100.	2100.	2100.	2100.				
15	0.	1.	4.	0.				
16	0.	.01	.03	.05				
17	.41	.41	.41	.41				
18	.2944	0.						

FIG. 1

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LISTING OF INPUT DATA PUNCH CARDS: Sample Input

TRANSIENT H_2/O_2 COMPUTER PROGRAM

(Initial Non–Diffusion–Controlled Run)

```
                                                                                              Card No.
** TRANSIENT H2/O2 CASE 13 **   (P=300 * G=1.05 * TF=360 * O/F=1 * 25-30 MSH)TT                  1
 11  10   20   1   1   0                                                                          2
 1.05       492.       360.       300.       0.        .1472      .1472      0.                   3
 360.       300.       .1472      0.         0.        0.         360.       0.5                  4
 .0047      0.12       .0066      .0358      360.      0.         .00011     0.                   5
 0.         .00001     .001       .002       .004      .006       .008       .010                 7a
 .012       .015       .020                                                                       7b
 0.         1.         4.         0.                                                              9
 0.         .01        .03        .05                                                             10
 .001       .001       .001       .001                                                            11
 0.         1.         4.         0.                                                              12
 0.         .01        .03        .05                                                             13
 2100.      2100.      2100.      2100.                                                           14
 0.         1.         4.         0.                                                              15
 0.         .01        .03        .05                                                             16
 .41        .41        .41        .41                                                             17
 .2944      0.                                                                                    18
```


FIG. 2

LISTING OF INPUT DATA PUNCH CARDS: Sample Input

TRANSIENT H_2/O_2 COMPUTER PROGRAM (Continuation of Non–Diffusion–Controlled Run)

K910962-13

```
                                                                                                  Card No.
** TRANSIENT H2/O2 CASE 13 **   (P=300 * G=1.05 * TF=360 * O/F=1 * 25-30 MSH)TT                  1
 11  10  20   1   5   0                                                                            2
 1.05      492.       360.       300.       0.         .1472      .1472      0.                    3
 360.      300.       .1472      0.         0.         0.         360.       0.5                   4
 .0047     0.12       .0066      .0358      360.       0.         .00011     0.                    5
 0.        .00001     .001       .002       .004       .006       .008       .010                  7a
 .012      .015       .020                                                                         7b
 0.        1.         4.         0.                                                                9
 0.        .01        .03        .05                                                               10
 .001      .001       .001       .001                                                              11
 0.        1.         4.         0.                                                                12
 0.        .01        .03        .05                                                               13
 2100.     2100.      2100.      2100.                                                             14
 0.        1.         4.         0.                                                                15
 0.        .01        .03        .05                                                               16
 .41       .41        .41        .41                                                               17
.00000    .10000-04  .10000-02  .20000-02  .40000-02  .60000-02  .80000-02  .10000-01              18a
.12000-01 .15000-01  .20000-01                                                                     18b
.43575+03 .43575+03  .45520+03  .47044+03  .48000+03  .47417+03  .46072+03  .44732+03              19a
.43539+03 .41906+03  .39722+03                                                                     19b
.36026+03 .38809+03  .41217+03  .44521+03  .45768+03  .45661+03  .44953+03  .44040+03              20a
.42447+03 .40009+03                                                                                20b
.45379-00 .48473+02  .91102+02  .15125+03  .17444+03  .17235+03  .15794+03  .13892+03              21a
.10525+03 .52982+02                                                                                21b
.30000+03 .30000+03  .30000+03  .30000+03  .29999+03  .29999+03  .29999+03  .29999+03              22a
.29998+03 .29998+03                                                                                22b
.14710-00 .13630-00  .12837-00  .11852+00  .11599+00  .11677+00  .11892+00  .12155+00              23a
.12618-00 .13376-00                                                                                23b
.14703-00 .12992-00  .11576+00  .10306+00  .88582-01  .80914-01  .76944-01  .75017-01              24a
.74098-01 .73103-01                                                                                24b
.00000    .00000     .00000     .00000     .00000     .00000     .00000     .00000                 25a
.00000    .00000                                                                                   25b
.00000    .00000     .00000     .00000     .00000     .00000     .00000     .00000                 26a
.00000    .00000                                                                                   26b
.00000    .42134+03  .43569+03  .44666+03  .45616+03  .45292+03  .44431+03  .43466+03              27a
.42554+03 .41223+03  .39352+03                                                                     27b
.00000    .00000     .00000     .00000     .00000     .00000     .00000     .00000                 28a
.00000    .00000     .00000     .00000     .00000     .00000     .00000     .00000                 28b
.00000    .00000     .00000     .00000     .00000     .00000     .00000     .00000                 28c
```

FIG. 3a

LISTING OF INPUT DATA PUNCH CARDS (Cont.)

								Card No.
.00000	.00000	.00000	.00000	.00000	.00000	.40805+03	.40819+03	28d
.40855+03	.40911+03	.40992+03	.41098+03	.41230+03	.41391+03	.41581+03	.41805+03	28e
.42064+03	.42361+03	.42700+03	.43085+03	.43518+03	.44004+03	.44545+03	.45145+03	28f
.45805+03	.46525+03	.47301+03	.48122+03	.48968+03	.49798+03	.50539+03	.51047+03	28g
.51044+03	.50194+03	.48435+03	.43575+03	.40609+03	.40620+03	.40655+03	.40705+03	28h
.40781+03	.40879+03	.41001+03	.41150+03	.41326+03	.41533+03	.41773+03	.42048+03	28i
.42363+03	.42720+03	.43124+03	.43577+03	.44083+03	.44648+03	.45271+03	.45958+03	28j
.46704+03	.47506+03	.48353+03	.49217+03	.50054+03	.50756+03	.51101+03	.50773+03	28k
.49607+03	.45520+03	.40415+03	.40424+03	.40457+03	.40503+03	.40574+03	.40664+03	28l
.40777+03	.40916+03	.41078+03	.41271+03	.41492+03	.41747+03	.42039+03	.42370+03	28m
.42744+03	.43165+03	.43637+03	.44164+03	.44748+03	.45395+03	.46103+03	.46872+03	28n
.47696+03	.48559+03	.49432+03	.50241+03	.50809+03	.50869+03	.50216+03	.47044+03	28o
.39994+03	.40004+03	.40033+03	.40072+03	.40133+03	.40209+03	.40305+03	.40423+03	28p
.40561+03	.40723+03	.40911+03	.41125+03	.41371+03	.41649+03	.41963+03	.42316+03	28q
.42712+03	.43155+03	.43647+03	.44193+03	.44795+03	.45453+03	.46168+03	.46932+03	28r
.47733+03	.48528+03	.49221+03	.49649+03	.49648+03	.48203+03	.39592+03	.39607+03	28s
.39631+03	.39665+03	.39716+03	.39782+03	.39864+03	.39963+03	.40080+03	.40217+03	28t
.40375+03	.40556+03	.40761+03	.40993+03	.41254+03	.41547+03	.41873+03	.42238+03	28u
.42641+03	.43087+03	.43578+03	.44114+03	.44696+03	.45318+03	.45973+03	.46634+03	28v
.47248+03	.47722+03	.47948+03	.47417+03	.39219+03	.39238+03	.39258+03	.39287+03	28w
.39331+03	.39387+03	.39457+03	.39542+03	.39642+03	.39758+03	.39891+03	.40043+03	28x
.40215+03	.40409+03	.40626+03	.40868+03	.41136+03	.41434+03	.41762+03	.42123+03	28y
.42516+03	.42944+03	.43404+03	.43894+03	.44405+03	.44925+03	.45423+03	.45851+03	28z
.46143+03	.46072+03	.38881+03	.38901+03	.38918+03	.38944+03	.38981+03	.39030+03	28aa
.39090+03	.39163+03	.39248+03	.39347+03	.39460+03	.39589+03	.39734+03	.39897+03	28bb
.40078+03	.40280+03	.40502+03	.40747+03	.41015+03	.41308+03	.41626+03	.41968+03	28cc
.42334+03	.42720+03	.43122+03	.43531+03	.43932+03	.44301+03	.44595+03	.44732+03	28dd
.38580+03	.38600+03	.38614+03	.38636+03	.38669+03	.38711+03	.38763+03	.38826+03	28ee
.38899+03	.38985+03	.39082+03	.39192+03	.39316+03	.39454+03	.39607+03	.39776+03	28ff
.39962+03	.40166+03	.40388+03	.40629+03	.40888+03	.41166+03	.41462+03	.41772+03	28gg
.42094+03	.42420+03	.42745+03	.43057+03	.43326+03	.43539+03	.38154+03	.38172+03	28hh
.38184+03	.38202+03	.38228+03	.38262+03	.38304+03	.38354+03	.38412+03	.38480+03	28ii
.38557+03	.38643+03	.38740+03	.38847+03	.38966+03	.39096+03	.39237+03	.39391+03	28jj
.39557+03	.39736+03	.39926+03	.40128+03	.40341+03	.40562+03	.40789+03	.41019+03	28kk
.41250+03	.41480+03	.41691+03	.41906+03	.37525+03	.37540+03	.37547+03	.37560+03	28ll
.37578+03	.37601+03	.37629+03	.37663+03	.37702+03	.37747+03	.37799+03	.37856+03	28mm
.37919+03	.37989+03	.38065+03	.38148+03	.38238+03	.38334+03	.38436+03	.38544+03	28nn
.38658+03	.38776+03	.38898+03	.39022+03	.39147+03	.39271+03	.39392+03	.39511+03	28oo
.39618+03	.39722+03							28pp

FIG. 3b

LISTING OF INPUT DATA PUNCH CARDS (Cont.)

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								Card No.
.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	29a
.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	29b
.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	29c
.00000	.00000	.00000	.00000	.00000	.00000	.95972-02	.95618-02	29d
.95392-02	.94819-02	.93789-02	.92345-02	.90633-02	.88778-02	.86808-02	.84691-02	29e
.82431-02	.80131-02	.77951-02	.76036-02	.74497-02	.73468-02	.73186-02	.74024-02	29f
.76468-02	.81119-02	.88809-02	.10082-01	.11921-01	.14712-01	.18932-01	.25276-01	29g
.34662-01	.47984-01	.65471-01	.11025+00	.12618-01	.12573-01	.12536-01	.12461-01	29h
.12340-01	.12177-01	.11982-01	.11765-01	.11527-01	.11268-01	.10989-01	.10698-01	29i
.10408-01	.10132-01	.98811-02	.96673-02	.95121-02	.94474-02	.95155-02	.97691-02	29j
.10280-01	.11156-01	.12561-01	.14748-01	.18091-01	.23146-01	.30693-01	.41636-01	29k
.56584-01	.97675-01	.15770-01	.15718-01	.15669-01	.15581-01	.15451-01	.15282-01	29l
.15078-01	.14845-01	.14585-01	.14300-01	.13993-01	.13670-01	.13340-01	.13015-01	29m
.12705-01	.12423-01	.12189-01	.12031-01	.11984-01	.12097-01	.12433-01	.13084-01	29n
.14187-01	.15946-01	.18667-01	.22802-01	.29006-01	.38104-01	.50854-01	.87845-01	29o
.22816-01	.22757-01	.22704-01	.22618-01	.22503-01	.22358-01	.22183-01	.21978-01	29p
.21745-01	.21488-01	.21212-01	.20920-01	.20617-01	.20310-01	.20011-01	.19732-01	29q
.19490-01	.19307-01	.19210-01	.19241-01	.19455-01	.19925-01	.20759-01	.22108-01	29r
.24189-01	.27318-01	.31938-01	.38630-01	.48038-01	.76389-01	.28929-01	.28873-01	29s
.28838-01	.28782-01	.28708-01	.28616-01	.28505-01	.28375-01	.28228-01	.28067-01	29t
.27897-01	.27721-01	.27542-01	.27367-01	.27205-01	.27067-01	.26969-01	.26927-01	29u
.26968-01	.27123-01	.27441-01	.27983-01	.28833-01	.30111-01	.31979-01	.34662-01	29v
.38464-01	.43771-01	.51024-01	.72497-01	.33806-01	.33756-01	.33741-01	.33719-01	29w
.33692-01	.33659-01	.33620-01	.33575-01	.33528-01	.33479-01	.33433-01	.33393-01	29x
.33362-01	.33347-01	.33356-01	.33398-01	.33485-01	.33634-01	.33866-01	.34208-01	29y
.34698-01	.35386-01	.36340-01	.37647-01	.39428-01	.41841-01	.45089-01	.49428-01	29z
.55153-01	.71597-01	.37485-01	.37442-01	.37446-01	.37455-01	.37470-01	.37491-01	29aa
.37518-01	.37552-01	.37595-01	.37649-01	.37716-01	.37801-01	.37906-01	.38037-01	29bb
.38200-01	.38405-01	.38661-01	.38982-01	.39384-01	.39892-01	.40534-01	.41350-01	29cc
.42391-01	.43724-01	.45438-01	.47644-01	.50484-01	.54133-01	.58797-01	.71775-01	29dd
.40118-01	.40081-01	.40102-01	.40138-01	.40189-01	.40257-01	.40341-01	.40442-01	29ee
.40563-01	.40704-01	.40868-01	.41059-01	.41279-01	.41533-01	.41826-01	.42166-01	29ff
.42561-01	.43023-01	.43565-01	.44206-01	.44968-01	.45884-01	.46993-01	.48347-01	29gg
.50011-01	.52070-01	.54624-01	.57798-01	.61738-01	.72349-01	.42484-01	.42458-01	29hh
.42501-01	.42575-01	.42679-01	.42813-01	.42978-01	.43176-01	.43406-01	.43670-01	29ii
.43971-01	.44311-01	.44692-01	.45118-01	.45592-01	.46120-01	.46709-01	.47365-01	29jj
.48099-01	.48922-01	.49852-01	.50909-01	.52118-01	.53514-01	.55139-01	.57045-01	29kk
.59297-01	.61971-01	.65158-01	.73348-01	.41568-01	.41558-01	.41632-01	.41757-01	29ll
.41931-01	.42156-01	.42431-01	.42758-01	.43137-01	.43569-01	.44054-01	.44595-01	29mm
.45192-01	.45849-01	.46566-01	.47347-01	.48194-01	.49113-01	.50107-01	.51182-01	29nn
.52347-01	.53611-01	.54986-01	.56489-01	.58140-01	.59964-01	.61989-01	.64251-01	29oo
.66790-01	.72823-01							29pp

FIG. 3c

LISTING OF INPUT DATA PUNCH CARDS (Cont.)

								Card No.
.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	30a
.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	30b
.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	30c
.00000	.00000	.00000	.00000	.00000	.00000	.13658-00	.13657-00	30d
.13658-00	.13658-00	.13658-00	.13659-00	.13660-00	.13661-00	.13662-00	.13664-00	30e
.13666-00	.13668-00	.13670-00	.13673-00	.13677-00	.13681-00	.13686-00	.13692-00	30f
.13700-00	.13709-00	.13720-00	.13734-00	.13753-00	.13778-00	.13812-00	.13860-00	30g
.13926-00	.14017-00	.14133-00	.14424-00	.13233-00	.13233-00	.13232-00	.13230-00	30h
.13229-00	.13226-00	.13224-00	.13221-00	.13217-00	.13213-00	.13209-00	.13204-00	30i
.13198-00	.13193-00	.13187-00	.13180-00	.13174-00	.13168-00	.13162-00	.13157-00	30j
.13153-00	.13150-00	.13151-00	.13157-00	.13170-00	.13193-00	.13232-00	.13292-00	30k
.13375-00	.13610-00	.12923-00	.12922-00	.12920-00	.12918-00	.12914-00	.12910-00	30l
.12905-00	.12899-00	.12892-00	.12884-00	.12875-00	.12865-00	.12853-00	.12841-00	30m
.12828-00	.12815-00	.12800-00	.12785-00	.12769-00	.12754-00	.12739-00	.12725-00	30n
.12713-00	.12705-00	.12703-00	.12709-00	.12727-00	.12764-00	.12822-00	.13008-00	30o
.12554-00	.12553-00	.12550-00	.12546-00	.12541-00	.12534-00	.12526-00	.12516-00	30p
.12504-00	.12491+00	.12477+00	.12460+00	.12442+00	.12422+00	.12400+00	.12377+00	30q
.12353+00	.12327+00	.12300+00	.12272+00	.12243+00	.12215+00	.12188+00	.12164+00	30r
.12143+00	.12129+00	.12123+00	.12130+00	.12154+00	.12260+00	.12472+00	.12470+00	30s
.12468+00	.12464+00	.12458+00	.12450+00	.12441+00	.12431+00	.12418+00	.12404+00	30t
.12388+00	.12370+00	.12350+00	.12329+00	.12306+00	.12281+00	.12254+00	.12226+00	30u
.12197+00	.12166+00	.12135+00	.12104+00	.12074+00	.12046+00	.12020+00	.11999+00	30v
.11985+00	.11981+00	.11988+00	.12047+00	.12541-00	.12540-00	.12538-00	.12534-00	30w
.12528-00	.12521-00	.12512-00	.12502-00	.12490+00	.12477+00	.12461+00	.12445+00	30x
.12426+00	.12406+00	.12383+00	.12360+00	.12335+00	.12308+00	.12281+00	.12252+00	30y
.12223+00	.12193+00	.12165+00	.12137+00	.12112+00	.12091+00	.12075+00	.12065+00	30z
.12065+00	.12097+00	.12686-00	.12685-00	.12682-00	.12679-00	.12674-00	.12667-00	30aa
.12660-00	.12650-00	.12639-00	.12627-00	.12613-00	.12598-00	.12581-00	.12563-00	30bb
.12543-00	.12522-00	.12499+00	.12475+00	.12451+00	.12425+00	.12399+00	.12373+00	30cc
.12347+00	.12322+00	.12300+00	.12280+00	.12264+00	.12253+00	.12249+00	.12266+00	30dd
.12863-00	.12862-00	.12860-00	.12857-00	.12852-00	.12846-00	.12839-00	.12831-00	30ee
.12821-00	.12810-00	.12798-00	.12785-00	.12770-00	.12753-00	.12736-00	.12717-00	30ff
.12697-00	.12676-00	.12655-00	.12632-00	.12609-00	.12587-00	.12564-00	.12543-00	30gg
.12523-00	.12505-00	.12490+00	.12480+00	.12474+00	.12483+00	.13190-00	.13189-00	30hh
.13187-00	.13185-00	.13181-00	.13176-00	.13171-00	.13164-00	.13156-00	.13147-00	30ii
.13137-00	.13126-00	.13114-00	.13101-00	.13087-00	.13073-00	.13057-00	.13040-00	30jj
.13023-00	.13005-00	.12987-00	.12969-00	.12952-00	.12935-00	.12919-00	.12905-00	30kk
.12893-00	.12884-00	.12878-00	.12881-00	.13780-00	.13779-00	.13778-00	.13776-00	30ll
.13774-00	.13770-00	.13766-00	.13762-00	.13756-00	.13750-00	.13743-00	.13736-00	30mm

FIG. 3d

K910962-13

LISTING OF INPUT DATA PUNCH CARDS (Cont.)

								Card No.
.13727-00	.13718-00	.13709-00	.13699-00	.13688-00	.13677-00	.13665-00	.13653-00	30nn
.13641-00	.13629-00	.13617-00	.13605-00	.13594-00	.13585-00	.13576-00	.13569-00	30oo
.13565-00	.13563-00							30pp
1 1 1 1 1	1 1 1 1 1 1							31
.29000-01	.36046+03	.10000-02						32
.2944	0.							33

FIG. 3e

LISTING OF INPUT DATA PUNCH CARDS: Sample Input

TRANSIENT H_2/O_2 COMPUTER PROGRAM (All Diffusion–Controlled Run)

```
                                                                                Card No.
** TRANSIENT H2/O2 CASE 12 **   (P=300 * G=2.10 * TF=360 * O/F=1 * 14-18 MSH)TF     1
 24  20  20   1   4   1                                                             2
 2.10      492.      360.      300.      0.        .1472     .1472     0.          3
 360.      300.      .1472     0.        0.        0.        360.      2.0         4
 .0047     0.12      .0066     .0358     360.      0.        .00011    0.          5
 0.        .0002     .0004     .0006     .0008     .0010     .0012     .0015       7a
 .0020     .0025     .0030     .0040     .0050     .0060     .0070     .0080       7b
 .0090     .0100     .0110     .0120     .0140     .0160     .0180     .0200       7c
 .001      .001      .001      .002      .002      .002      .005      .005        8a
 .005      .005      .010      .010      .020      .020      .020      .020        8b
 .050      .050      .050      .10                                                 8c
 0.        1.        4.        0.                                                  9
 0.        .01       .03       .05                                                 10
 .0016     .0016     .0016     .0016                                               11
 0.        1.        4.        0.                                                  12
 0.        .01       .03       .05                                                 13
 1300.     1300.     1300.     1300.                                               14
 0.        1.        4.        0.                                                  15
 0.        .01       .03       .05                                                 16
 .41       .41       .41       .41                                                 17
10                                                                                 18
.00000    .10000-02 .20000-02 .40000-02 .60000-02 .80000-02 .10000-01 .12000-01   19a
.15000-01 .20000-01                                                                19b
.49425+03 .49425+03 .49579+03 .50970+03 .52166+03 .51481+03 .51263+03 .51010+03   20a
.50783+03 .49804+03                                                                20b
.14720-00 .12909-00 .11385+00 .88390-01 .69297-01 .55351-01 .44606-01 .36167-01   21a
.26540-01 .16162-01                                                                21b
.14720-00 .13956-00 .13330-00 .12282+00 .11501+00 .11013+00 .10683+00 .10460+00   22a
.10247+00 .10149+00                                                                22b
.00000    .13505-01 .25079-01 .44412-01 .58977-01 .70682-01 .80296-01 .88311-01   23a
.97996-01 .11017+00                                                                23b
.36000+03 .37705+03 .39226+03 .42021+03 .44399+03 .45987+03 .47091+03 .47834+03   24a
.48514+03 .48626+03                                                                24b
.31000-01 .36067+03                                                                25
 .2944     0.                                                                      26
```

FIG. 4

Output Description

Output from the H_2/O_2 transient program consists of both printout and punch cards. The printing is basically the same for all of the three types of runs discussed under the input description; however, the form of the punch card output varies.

Printout

There are two different types of printed output from this program: (1) summary printing (when input indicator DEBUG=F), and (2) detailed printing (when DEBUG=T). The detailed form yields a considerable amount of printed output since everything produced by the summary output is printed out as well as a full station-by-station and time-by-time account of reactor calculations. This can yield over 2000 lines of printing per pass. The detailed printing should be used only when the summary form doesn't give enough detailed information (as for example, at the very beginning of an initial non-diffusion-controlled run for fast reacting cases), where the summary printing for only every twentieth time step may not allow enough information for plotting. An abridged sample of the detailed output from a transient H_2/O_2 run is shown in Figs. 5a through 5t. The output shown in the top of Fig. 5a and in Figs. 5e - 5t is what would have been produced if the summary printing alone had been requested. A description of the printed output produced for both the detailed and summary forms follows, along with the name of the routine from which it is printed.

Detailed Form

F874:

A listing of the program input including the data case title (see top of Fig. 5a). The extra punch card input for the continuation and all diffusion-controlled runs is not printed.

The following message which concludes each run (see Fig. 5t):

```
******* OPERATIONS COMPLETE ********
TOTAL EXECUTION TIME = XX.XX MINUTES
```

Subroutine MCALC:

The following message which is printed when the non-diffusion-controlled phase of a data case is completed (see Fig. 5t):

```
**********************************
GO-TO-ALL-DIFFUSION-CONTROLLED RUN
      TIME = XX.XX SECONDS
**********************************
```

Subroutine DEBUG3:

1. A complete list of the following values for each axial station and every time increment of each pass (see Figs. 5b - 5d):

a. interstitial concentrations of hydrogen in lb/ft^3
b. interstitial concentrations of oxygen in lb/ft^3
c. interstitial concentrations of water in its solid phase in lb/ft^3
d. interstitial concentrations of water in its liquid phase in lb/ft^3
e. interstitial concentrations of water in its vapor phase in lb/ft^3
f. interstitial concentrations of helium in lb/ft^3
g. interstitial temperatures in deg R
*h. particle surface temperatures
i. enthalpies in BTU/lb
j. interstitial pressures in psia
k. corresponding axial positions in ft.

2. The cumulative time (sec) and wall temperature (deg R) at the end of every time step. (See Figs. 5b - 5d).

Subroutine PRPLOT:

Printer plots of the following values vs. axial position (in feet), corresponding to the last time step of each pass. Each plot summarizes the last five passes or whatever passes remain. (See Figs. 5e - 5k).

a. interstitial temperatures (deg R)
*b. particle surface temperatures (deg R)
c. chamber pressures (psia)
d. hydrogen mole-fractions
e. oxygen mole-fractions
f. water mole-fractions
g. helium mole-fractions.

Subroutine OUTPUT:

Summary printing of the seven variables mentioned under subroutine PRPLOT vs. axial position (ft) at the end of every pass. This printing is produced after every tenth pass and/or at the end of the last pass. (See Figs. 5ℓ - 5r).

Subroutine TMPRNT:

Summary printing of wall temperature (deg R) and interface location (axial position) in feet of water change-of-phase) vs. time (values printed correspond to the end of each pass). (See Fig. 5s). Also, if H2LEAD=F, pressure in psia and mass flow rate in lb/ft^2-sec vs. time are printed. This printing is done after every tenth pass and/or at the end of the last pass.

---

*Irregularities in the values for particle surface temperature, caused by water change-of-phase, may be exaggerated in some cases due to use of too few axial positions.

Summary Form

Everything printed under the detailed printing described above is also produced for the summary form except those things printed from subroutine DEBUG3.

Punch Cards

Two different types of punch card output can be produced by this program. For the all diffusion-controlled runs, no punch cards will be produced at all. For both of the two types of non-diffusion-controlled runs (initial and continuation) the two possible types of punch card output are described below.

Continuation Cards

These cards are described in detail under the input discussion section (cards 18-32 under "continuation run"). They will be produced when PUNCH=1 or 3 and when a run completes NPASS number of passes without reaching the all diffusion-controlled phase.

Diffusion-Controlled Cards

These cards are described in detail under the input discussion of all diffusion-controlled runs (cards 18-25). They will be produced whenever the non-diffusion-controlled phase of a data case is completed.

LISTING OF OUTPUT FOR SAMPLE DATA CASE

K910962-13

***** PROGRAM INPUT *****

TRANSIENT ANALYSIS OF H2/02 CATALYTIC REACTOR
** TRANSIFNT H2/02 CASE 13 ** (P=300 * G=1.05 * TF=360 * 0/F=1 * 25-30 MSH)

NOFZ	NPASS	INPERP	DEBUG	MODNO	PUNCH
11	10	20	T	1	1

G	TS	MH2	MO2	MH20	MHE	D0H2	D002	D0H20	KP	ALPHA
.10500+01	.49200+03	.20200+01	.32000+02	.18020+02	.40030+01	.16760-02	.75720-03	.63550-03	.40000-04	.16000+14

ALPHAK	GAMMA
.31740+08	.50000+04

AW	CW	MW	DC	TA	HA	HA1	HA2
.47000-02	.12000+00	.66000-02	.35800-01	.36000+03	.00000	.11000-03	.00000

INITIAL TEMPERATURES, PRESSURES, AND CONCENTRATIONS

T	P	CIH2	CI02	CIH20	CIHE	TPS
.36000+03	.30000+03	.14720-00	.00000	.00000	.00000	.36000+03

INLET TEMPERATURE, PRESSURE, ENTHALPY, AND CONCENTRATIONS

T	P	H	CIH2	CI02	CIHE
.36000+03	.30000+03	.00000	.14720-00	.14720-00	.00000

INPUT AXIAL STATIONS

35 .00000 .10000-04 .10000-02 .20000-02 .40000-02 .60000-02 .80000-02 .10000-01 .12000-01 .15000-01 .20000-01

A, AP, DELTA VS Z TABLES

			.00000	.10000+01	.40000+01	.00000
.00000	.10000-01	.30000-01	.50000-01			
.10000-02	.10000-02	.10000-02	.10000-02			

			.00000	.10000+01	.40000+01	.00000
.00000	.10000-01	.30000-01	.50000-01			
.21000+04	.21000+04	.21000+04	.21000+04			

			.00000	.10000+01	.40000+01	.00000
.00000	.10000-01	.30000-01	.50000-01			
.41000-00	.41000-00	.41000-00	.41000-00			

INTERSTITIAL CONCENTRATIONS OF H2

.14720-00 .14722-00 .14898-00 .15034-00 .15229-00 .15357-00 .15444-00 .15507-00 .15553-00 .15604-00
.15658-00

INTERSTITIAL CONCENTRATIONS OF O2

.14720-00 .14689-00 .11922+00 .97876-01 .67544-01 .48046-01 .34870-01 .25661-01 .19071-01 .12376-01
.61781-02

INTERSTITIAL CONCENTRATIONS OF H20(S)

FIG. 5a

K910962-13

.00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000
.00000

INTERSTITIAL CONCENTRATIONS OF H2O(L)

.00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000
.00000

INTERSTITIAL CONCENTRATIONS OF H2O(V)

.00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000
.00000

INTERSTITIAL CONCENTRATIONS OF HE

.00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000
.00000

INTERSTITIAL TEMPERATURES

.36000+03 .36000+03 .36000+03 .36000+03 .36000+03 .36000+03 .36000+03 .36000+03 .36000+03 .36000+03
.36000+03

PARTICLE SURFACE TEMPERATURES

.36000+03 .36000+03 .36000+03 .36000+03 .36000+03 .36000+03 .36000+03 .36000+03 .36000+03 .36000+03
.36000+03

ENTHALPIES

.00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000
.00000

INTERSTITIAL PRESSURES

.30000+03 .30000+03 .30000+03 .30000+03 .30000+03 .29999+03 .29999+03 .29999+03 .29999+03 .29998+03
.29998+03

AXIAL POSITIONS

.00000 .10000-04 .10000-02 .20000-02 .40000-02 .60000-02 .80000-02 .10000-01 .12000-01 .15000-01
.20000-01

TIME = .20000-02 WALL TEMP = .36000+03

INTERSTITIAL CONCENTRATIONS OF H2

.14720-00 .14720-00 .14756-00 .14814-00 .14964-00 .15098-00 .15209-00 .15298-00 .15370-00 .15453-00
.15543-00

INTERSTITIAL CONCENTRATIONS OF O2

.14720-00 .14716-00 .13882-00 .12832-00 .10386+00 .82945-01 .65949-01 .52380-01 .41606-01 .29094-01
.15674-01

INTERSTITIAL CONCENTRATIONS OF H2O(S)

.00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000
.00000

INTERSTITIAL CONCENTRATIONS OF H2O(L)

.00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000
.00000

INTERSTITIAL CONCENTRATIONS OF H2O(V)

.00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000
.00000

INTERSTITIAL CONCENTRATIONS OF HE

.00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000
.00000

FIG. 5b

K910962-13

INTERSTITIAL TEMPERATURES

.36000+03	.36001+03	.36038+03	.36059+03	.36069+03	.36064+03	.36055+03	.36046+03	.36038+03	.36027+03
.36015+03									

PARTICLE SURFACE TEMPERATURES

.36159+03	.36159+03	.36133+03	.36113+03	.36083+03	.36062+03	.36048+03	.36037+03	.36029+03	.36021+03
.36012+03									

ENTHALPIES

.00000	.92068-02	.65744-00	.10206+01	.12052+01	.11143+01	.92575-00	.71480-00	.51278-00	.23538-00
.00000									

INTERSTITIAL PRESSURES

.30000+03	.30000+03	.30000+03	.30000+03	.30000+03	.29999+03	.29999+03	.29999+03	.29999+03	.29999+03
.29998+03									

AXIAL POSITIONS

.00000	.10000-04	.10000-02	.20000-02	.40000-02	.60000-02	.80000-02	.10000-01	.12000-01	.15000-01
.20000-01									

TIME = .40000-02 WALL TEMP = .36000+03

FIG. 5C.

K910962-13

INTERSTITIAL CONCENTRATIONS OF H2

.14720-00	.14574-00	.48469-01	.37510-01	.28211-01	.29236-01	.32801-01	.37604-01	.42859-01	.51447-01	.65301-01

INTERSTITIAL CONCENTRATIONS OF O2

.14720-00	.14549-00	.25569-01	.14985-01	.56506-02	.35308-02	.24959-02	.18540-02	.13951-02	.97574-03	.68054-03

INTERSTITIAL CONCENTRATIONS OF H2O(S)

.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000

INTERSTITIAL CONCENTRATIONS OF H2O(L)

.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000

INTERSTITIAL CONCENTRATIONS OF H2O(V)

.00000	.32600-03	.29557-01	.29075-01	.29144-01	.33216-01	.39165-01	.46204-01	.53591-01	.65236-01	.67235-01

INTERSTITIAL CONCENTRATIONS OF HE

.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000

INTERSTITIAL TEMPERATURES

.36000+03	.36353+03	.74477+03	.92759+03	.11766+04	.11279+04	.99467+03	.85695+03	.74387+03	.60733+03	.46241+03

PARTICLE SURFACE TEMPERATURES

.11596+04	.11596+04	.14381+04	.12711+04	.13648+04	.11413+04	.95012+03	.79626+03	.68695+03	.57105+03	.45104+03

ENTHALPIES

.00000	.60869+01	.66409+03	.10224+04	.14719+04	.13838+04	.11442+04	.89827+03	.69743+03	.45599+03	.20488+03

INTERSTITIAL PRESSURES

.30000+03	.30000+03	.30000+03	.29999+03	.29998+03	.29997+03	.29995+03	.29994+03	.29993+03	.29992+03	.29991+03

AXIAL POSITIONS

.00000	.10000-04	.10000-02	.20000-02	.40000-02	.60000-02	.80000-02	.10000-01	.12000-01	.15000-01	.20000-01

TIME = .75000-01 WALL TEMP = .37495+03

FIG.5d

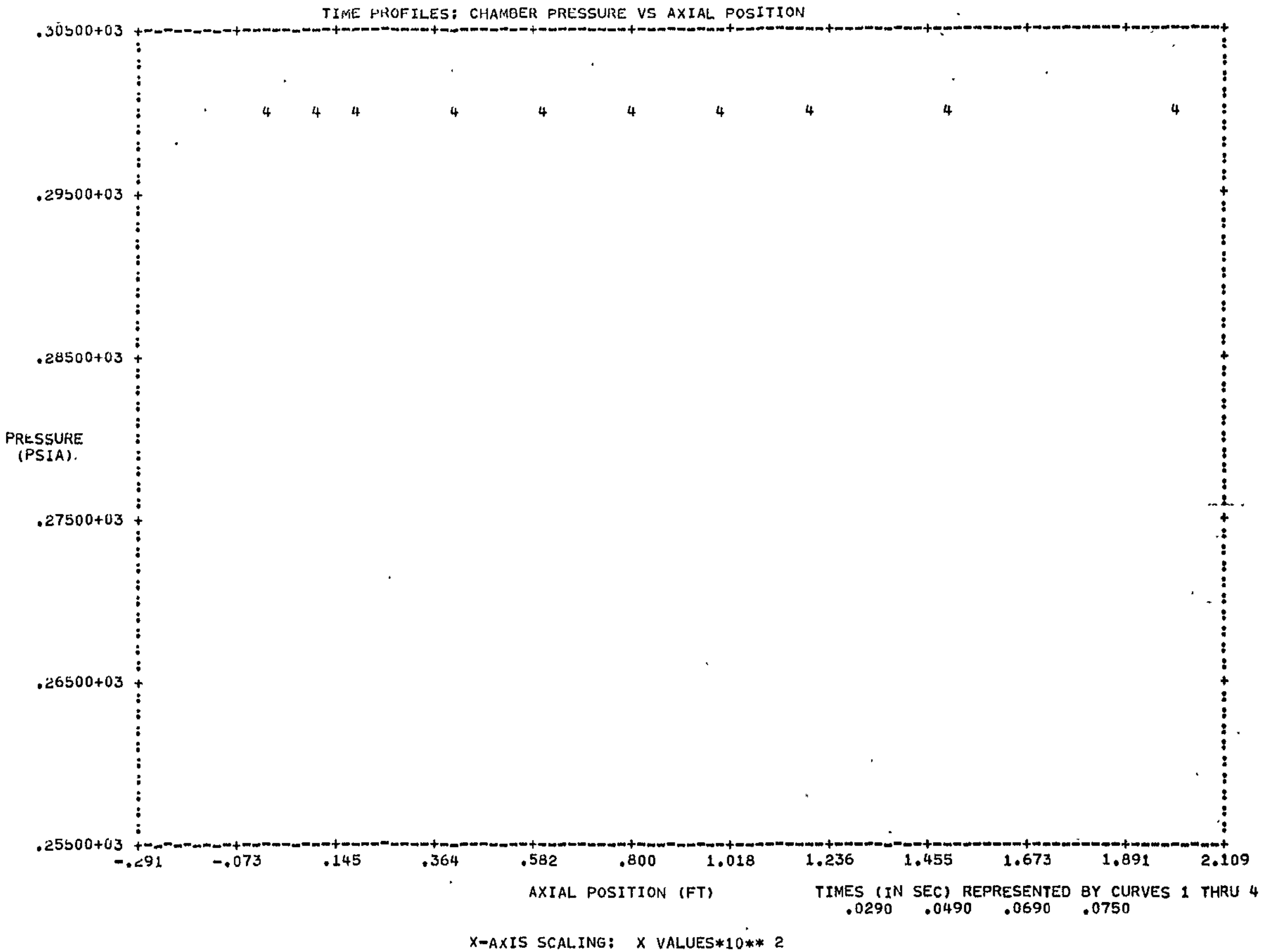

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FIG. 5e

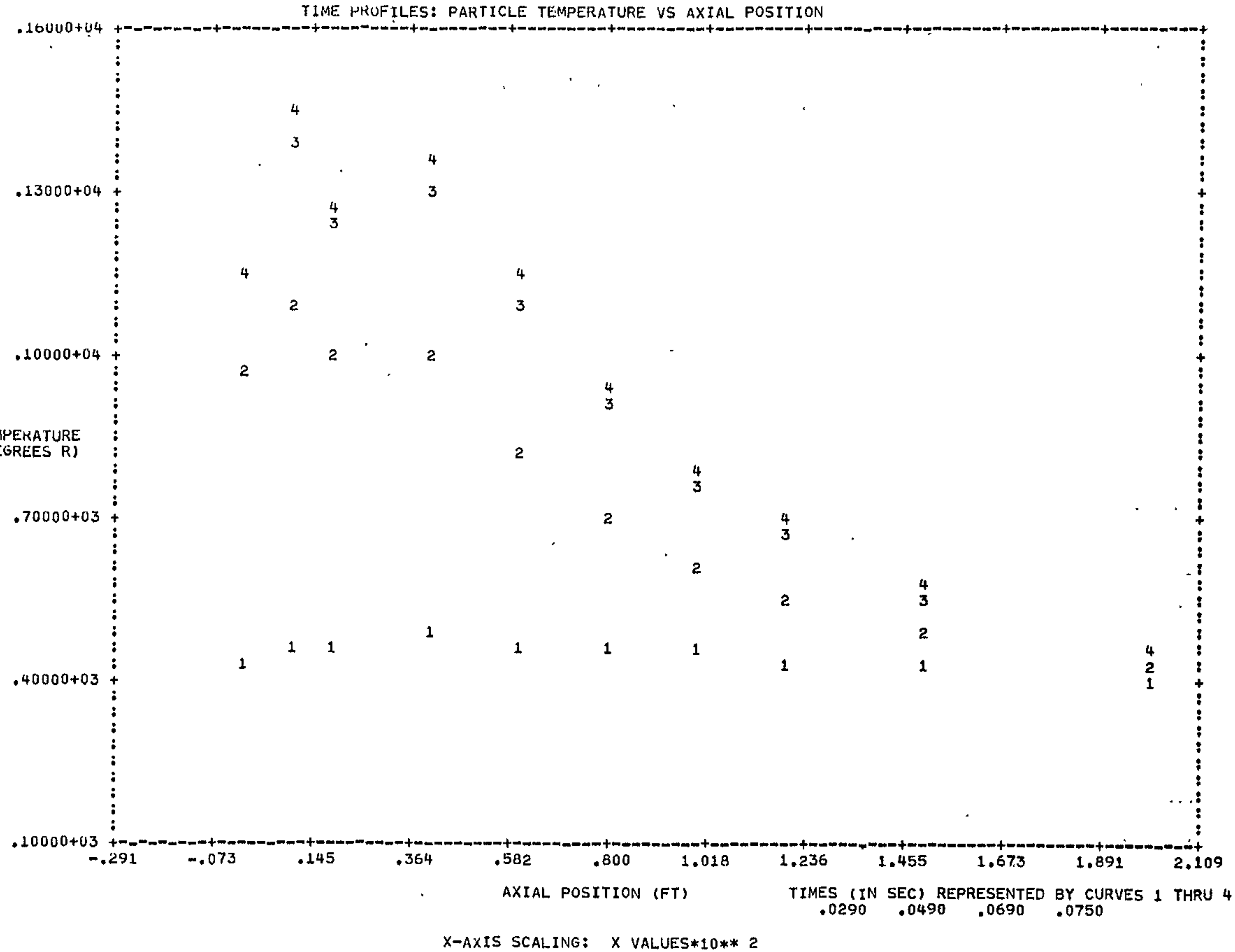
TIME PROFILES: PARTICLE TEMPERATURE VS AXIAL POSITION
.16000+04
.13000+04
.10000+04
.70000+03
.40000+03
.10000+03
TEMPERATURE
(DEGREES R)
-.291
-.073
.145
.364
.582
.800
1.018
1.236
1.455
1.673
1.891
2.109
AXIAL POSITION (FT)
TIMES (IN SEC) REPRESENTED BY CURVES 1 THRU 4
.0290 .0490 .0690 .0750
X-AXIS SCALING: X VALUES*10** 2

FIG. 5f

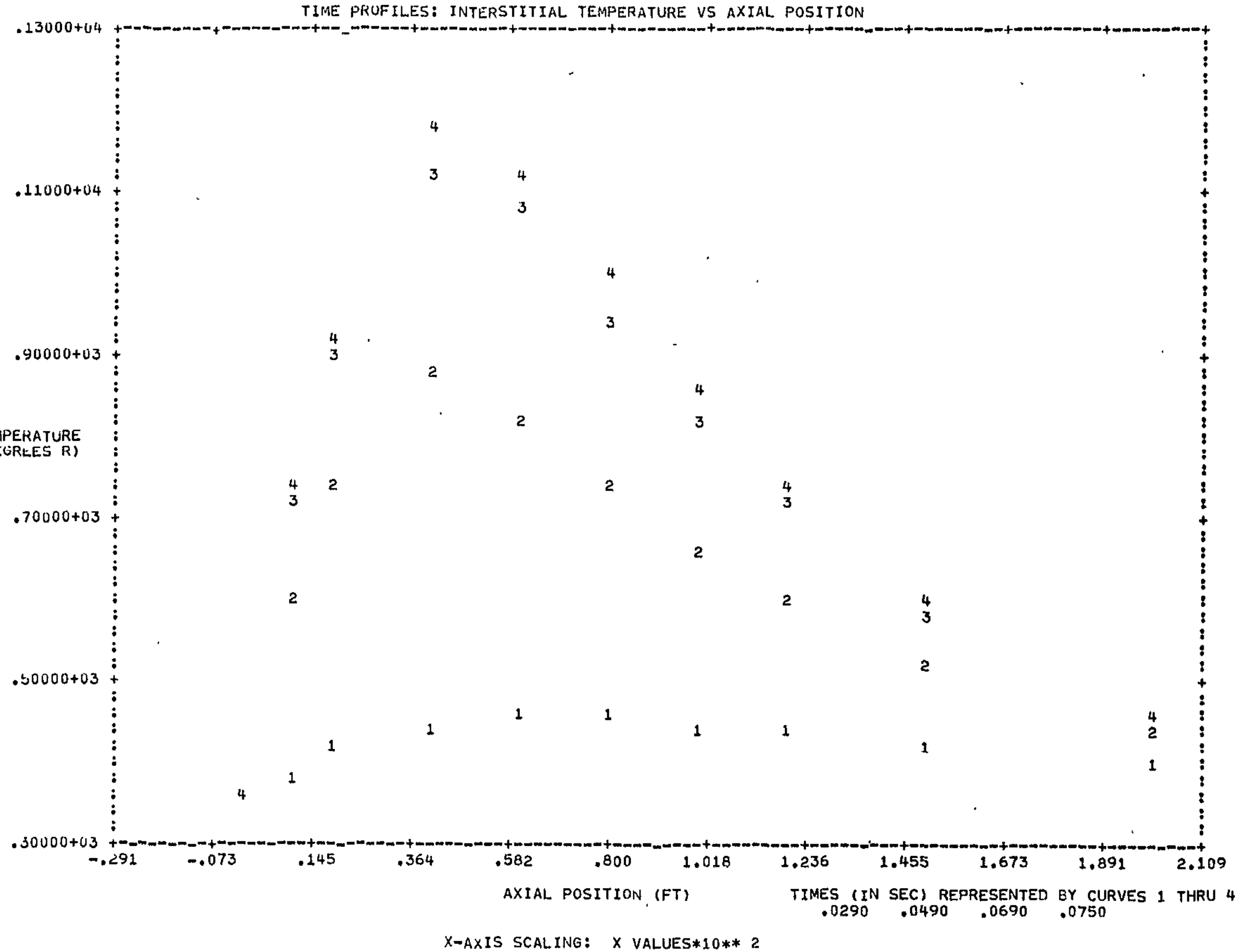

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FIG. 5g

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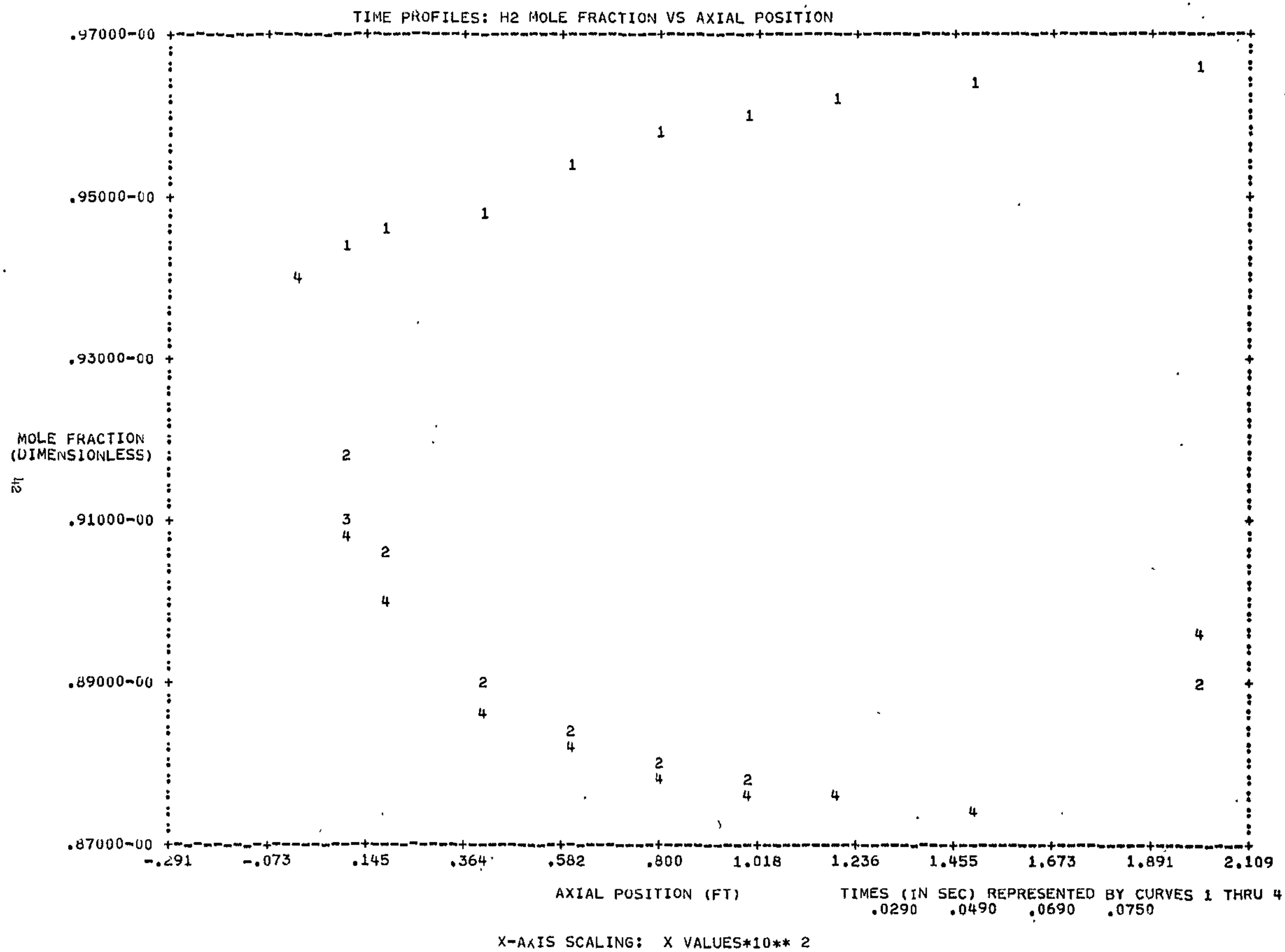

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FIG. 5h

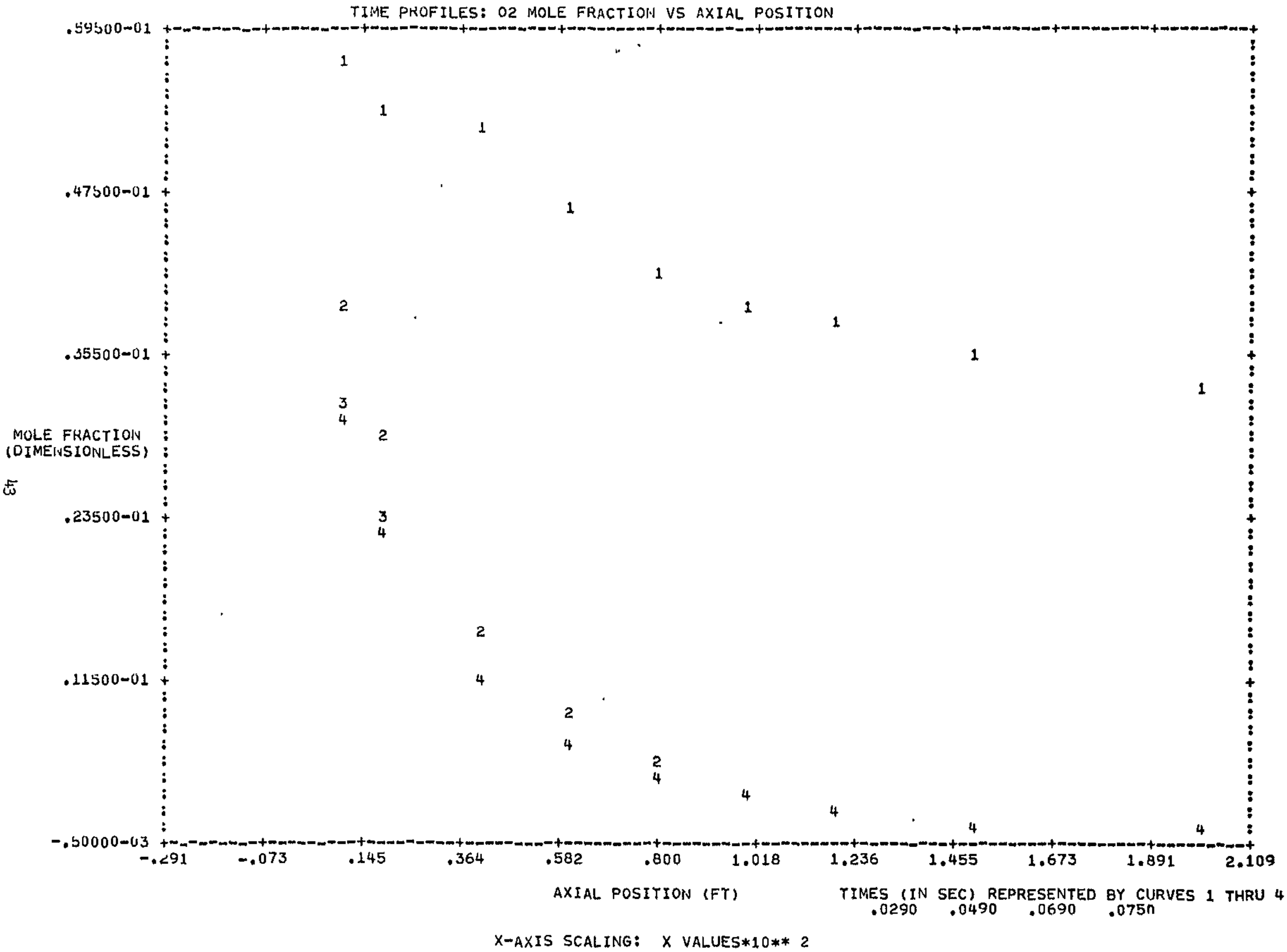

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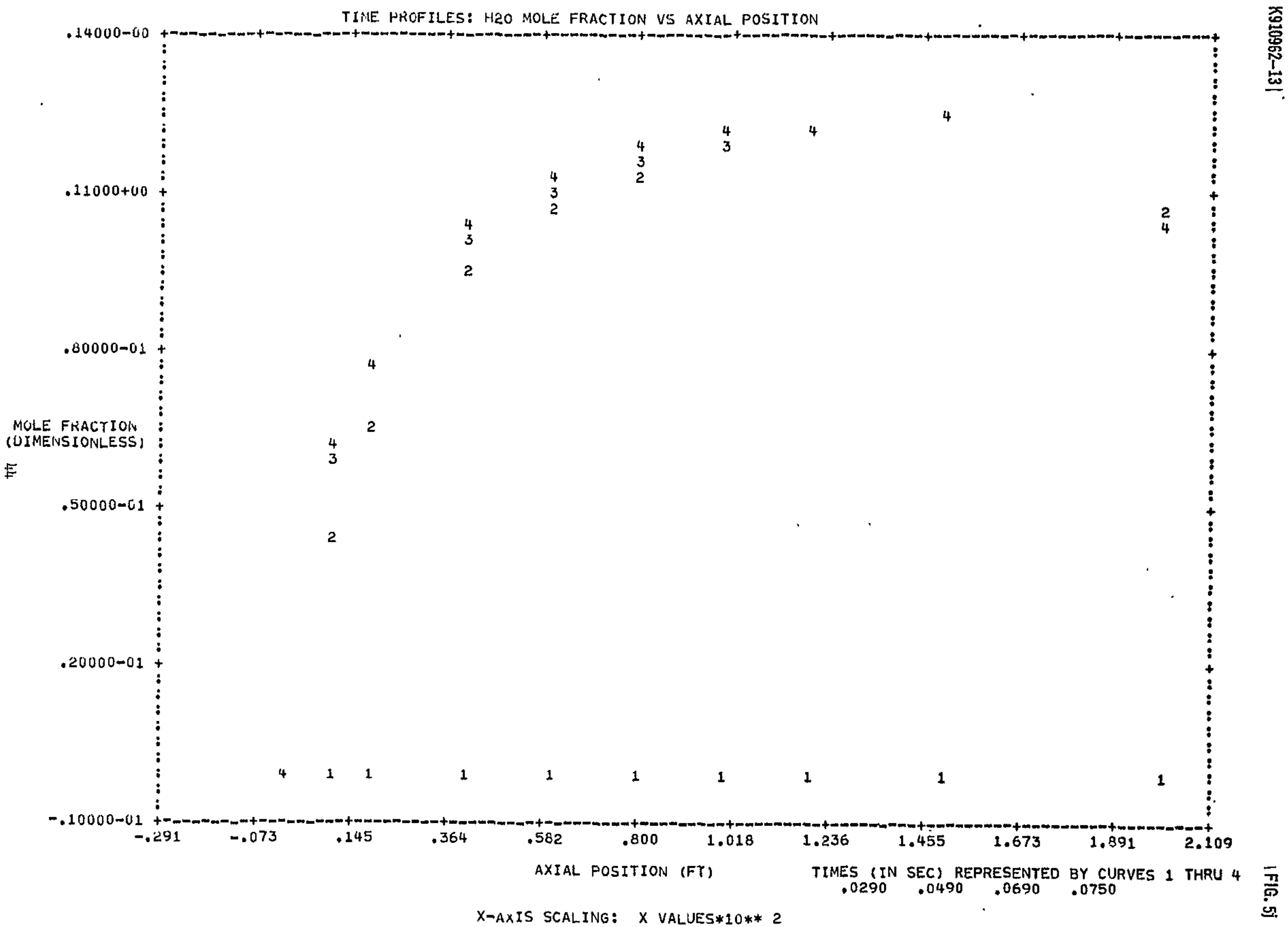
FIG. 5I



TIME PROFILES: H2O MOLE FRACTION VS AXIAL POSITION
.14000-00
.11000+00
.80000-01
.50000-01
.20000-01
-.10000-01
MOLE FRACTION
(DIMENSIONLESS)
-.291
-.073
.145
.364
.582
.800
1.018
1.236
1.455
1.673
1.891
2.109
AXIAL POSITION (FT)
TIMES (IN SEC) REPRESENTED BY CURVES 1 THRU 4
.0290 .0490 .0690 .0750
X-AXIS SCALING: X VALUES*10** 2
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FIG. 5

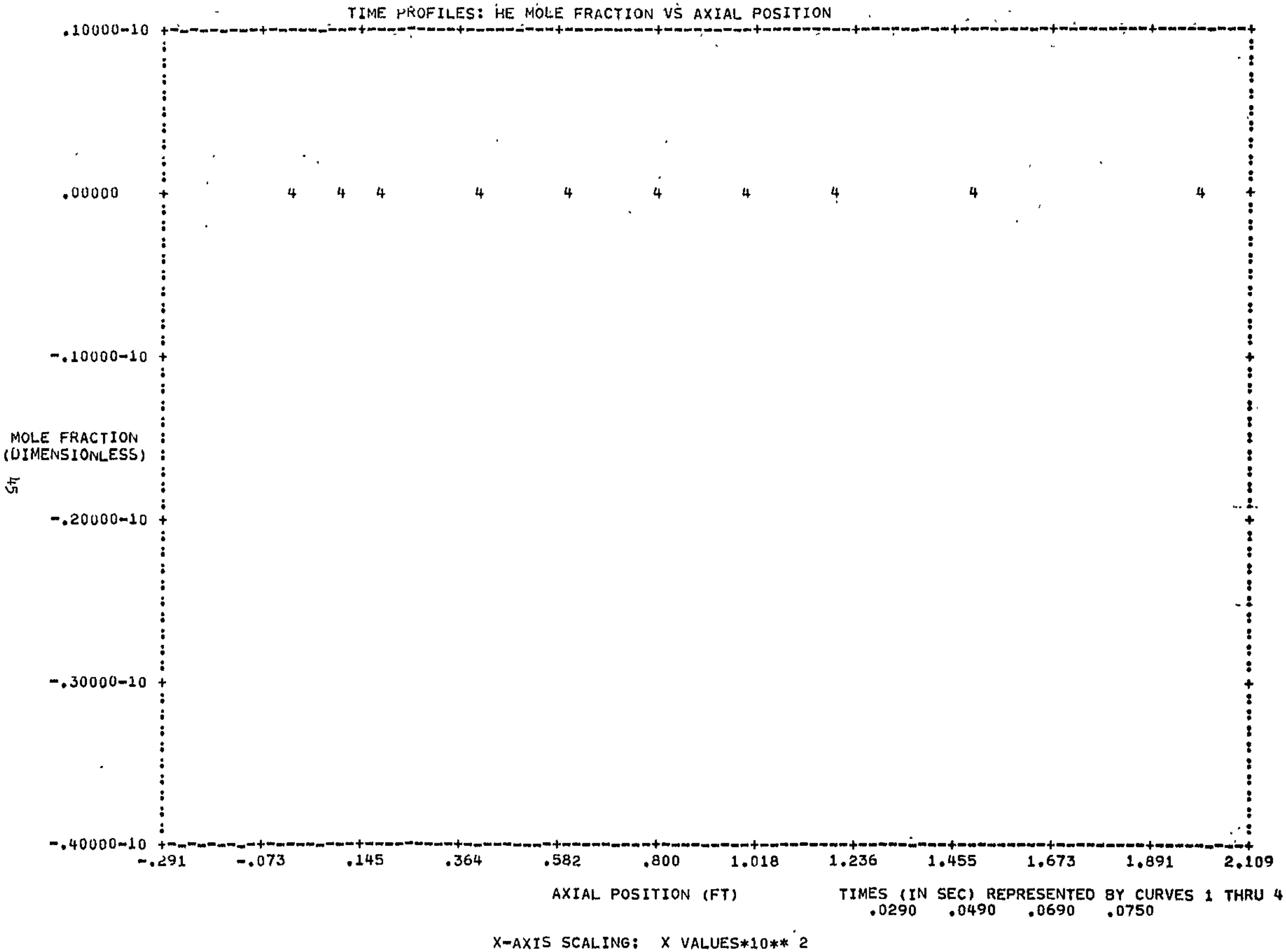

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FIG. 5K

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TIME PROFILES OF INTERSTITIAL TEMPERATURE VS AXIAL POSITION

AXIAL POSITION (FT)	*	TEMPERATURE (DEGREES R) .0290 SEC	.0490 SEC	.0690 SEC	.0750 SEC						
.0000	*	.36000+03	.36000+03	.36000+03	.36000+03	.00000	.00000	.00000	.00000	.00000	.00000
.1000-04	*	.36026+03	.36257+03	.36342+03	.36353+03	.00000	.00000	.00000	.00000	.00000	.00000
.1000-02	*	.38809+03	.60845+03	.72352+03	.74477+03	.00000	.00000	.00000	.00000	.00000	.00000
.2000-02	*	.41217+03	.74391+03	.90246+03	.92759+03	.00000	.00000	.00000	.00000	.00000	.00000
.4000-02	*	.44521+03	.87814+03	.11287+04	.11766+04	.00000	.00000	.00000	.00000	.00000	.00000
.6000-02	*	.45768+03	.82655+03	.10729+04	.11279+04	.00000	.00000	.00000	.00000	.00000	.00000
.8000-02	*	.45061+03	.73519+03	.94292+03	.99467+03	.00000	.00000	.00000	.00000	.00000	.00000
.1000-01	*	.44953+03	.65285+03	.81355+03	.85695+03	.00000	.00000	.00000	.00000	.00000	.00000
.1200-01	*	.44040+03	.59176+03	.71008+03	.74387+03	.00000	.00000	.00000	.00000	.00000	.00000
.1500-01	*	.42447+03	.51446+03	.58606+03	.60733+03	.00000	.00000	.00000	.00000	.00000	.00000
.2000-01	*	.40009+03	.43799+03	.45632+03	.46241+03	.00000	.00000	.00000	.00000	.00000	.00000

FIG. 52

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TIME PROFILES OF PARTICLE TEMPERATURE VS AXIAL POSITION

TEMPERATURE (DEGREES R)

AXIAL POSITION (FT)	*	.0290 SEC	.0490 SEC	.0690 SEC	.0750 SEC						
.0000	*	.43575+03	.97026+03	.11390+04	.11596+04	.00000	.00000	.00000	.00000	.00000	.00000
.1000-04	*	.43575+03	.97026+03	.11390+04	.11596+04	.00000	.00000	.00000	.00000	.00000	.00000
.1000-02	*	.45520+03	.10798+04	.13824+04	.14381+04	.00000	.00000	.00000	.00000	.00000	.00000
.2000-02	*	.47044+03	.10119+04	.12411+04	.12711+04	.00000	.00000	.00000	.00000	.00000	.00000
.4000-02	*	.48000+03	.10011+04	.13028+04	.13648+04	.00000	.00000	.00000	.00000	.00000	.00000
.6000-02	*	.47417+03	.81849+03	.10789+04	.11413+04	.00000	.00000	.00000	.00000	.00000	.00000
.8000-02	*	.46072+03	.69309+03	.89575+03	.95012+03	.00000	.00000	.00000	.00000	.00000	.00000
.1000-01	*	.44732+03	.60826+03	.75381+03	.79626+03	.00000	.00000	.00000	.00000	.00000	.00000
.1200-01	*	.43539+03	.55712+03	.65608+03	.68695+03	.00000	.00000	.00000	.00000	.00000	.00000
.1500-01	*	.41906+03	.49171+03	.55219+03	.57105+03	.00000	.00000	.00000	.00000	.00000	.00000
.2000-01	*	.39722+03	.43226+03	.44603+03	.45104+03	.00000	.00000	.00000	.00000	.00000	.00000

FIG. 5m

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TIME PROFILES OF CHAMBER PRESSURE VS AXIAL POSITION

AXIAL POSITION (FT)	PRESSURE (PSIA) .0290 SEC	.0490 SEC	.0690 SEC	.0750 SEC						
.0000	.30000+03	.30000+03	.30000+03	.30000+03	.00000	.00000	.00000	.00000	.00000	.00000
.1000-04	.30000+03	.30000+03	.30000+03	.30000+03	.00000	.00000	.00000	.00000	.00000	.00000
.1000-02	.30000+03	.30000+03	.30000+03	.30000+03	.00000	.00000	.00000	.00000	.00000	.00000
.2000-02	.30000+03	.30000+03	.29999+03	.29999+03	.00000	.00000	.00000	.00000	.00000	.00000
.4000-02	.30000+03	.29999+03	.29998+03	.29998+03	.00000	.00000	.00000	.00000	.00000	.00000
.6000-02	.29999+03	.29998+03	.29997+03	.29997+03	.00000	.00000	.00000	.00000	.00000	.00000
.8000-02	.29999+03	.29998+03	.29996+03	.29995+03	.00000	.00000	.00000	.00000	.00000	.00000
.1000-01	.29999+03	.29997+03	.29995+03	.29994+03	.00000	.00000	.00000	.00000	.00000	.00000
.1200-01	.29999+03	.29997+03	.29994+03	.29993+03	.00000	.00000	.00000	.00000	.00000	.00000
.1500-01	.29998+03	.29996+03	.29993+03	.29992+03	.00000	.00000	.00000	.00000	.00000	.00000
.2000-01	.29998+03	.29995+03	.29992+03	.29991+03	.00000	.00000	.00000	.00000	.00000	.00000

FIG. 5n

TIME PROFILES OF H2 MOLE FRACTION VS AXIAL POSITION

H2 MOLE FRACTION (DIMENSIONLESS)

AXIAL POSITION (FT)	*	.0290 SEC	.0490 SEC	.0690 SEC	.0750 SEC						
.0000	*	.94062-00	.94062-00	.94062-00	.94062-00	.00000	.00000	.00000	.00000	.00000	.00000
.1000-04	*	.94065-00	.94050-00	.94050-00	.94050-00	.00000	.00000	.00000	.00000	.00000	.00000
.1000-02	*	.94324-00	.91756-00	.90955-00	.90772-00	.00000	.00000	.00000	.00000	.00000	.00000
.2000-02	*	.94614-00	.90642-00	.90048-00	.89919-00	.00000	.00000	.00000	.00000	.00000	.00000
.4000-02	*	.94796-00	.89075-00	.88696-00	.88617-00	.00000	.00000	.00000	.00000	.00000	.00000
.6000-02	*	.95401-00	.88380-00	.88156-00	.88107-00	.00000	.00000	.00000	.00000	.00000	.00000
.8000-02	*	.95609-00	.87984-00	.87854-00	.87823-00	.00000	.00000	.00000	.00000	.00000	.00000
.1000-01	*	.96076-00	.87746-00	.87673-00	.87654-00	.00000	.00000	.00000	.00000	.00000	.00000
.1200-01	*	.96250-00	.87598-00	.87560-00	.87549-00	.00000	.00000	.00000	.00000	.00000	.00000
.1500-01	*	.96425-00	.87478-00	.87468-00	.87463-00	.00000	.00000	.00000	.00000	.00000	.00000
.2000-01	*	.96065-00	.89093-00	.89514-00	.89600-00	.00000	.00000	.00000	.00000	.00000	.00000

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FIG. 50

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TIME PROFILES OF O2 MOLE FRACTION VS AXIAL POSITION

O2 MOLE FRACTION (DIMENSIONLESS)

AXIAL POSITION (FT)	*	.0290 SEC	.0490 SEC	.0690 SEC	.0750 SEC						
.0000	*	.59377-01	.59377-01	.59377-01	.59377-01	.00000	.00000	.00000	.00000	.00000	.00000
.1000-04	*	.59350-01	.59263-01	.59266-01	.59266-01	.00000	.00000	.00000	.00000	.00000	.00000
.1000-02	*	.56757-01	.38946-01	.31847-01	.30228-01	.00000	.00000	.00000	.00000	.00000	.00000
.2000-02	*	.53860-01	.29086-01	.23815-01	.22676-01	.00000	.00000	.00000	.00000	.00000	.00000
.4000-02	*	.52036-01	.15279-01	.11909-01	.11205-01	.00000	.00000	.00000	.00000	.00000	.00000
.6000-02	*	.45991-01	.91678-02	.71535-02	.67170-02	.00000	.00000	.00000	.00000	.00000	.00000
.8000-02	*	.41907-01	.56854-02	.44932-02	.42184-02	.00000	.00000	.00000	.00000	.00000	.00000
.1000-01	*	.39241-01	.35891-02	.29001-02	.27280-02	.00000	.00000	.00000	.00000	.00000	.00000
.1200-01	*	.37497-01	.22823-02	.19053-02	.17989-02	.00000	.00000	.00000	.00000	.00000	.00000
.1500-01	*	.35745-01	.12365-02	.10983-02	.10471-02	.00000	.00000	.00000	.00000	.00000	.00000
.2000-01	*	.33350-01	.77516-03	.62783-03	.58944-03	.00000	.00000	.00000	.00000	.00000	.00000

FIG. 5p

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TIME PROFILES OF H2O MOLE FRACTION VS AXIAL POSITION

H2O MOLE FRACTION (DIMENSIONLESS)

AXIAL POSITION (FT)	.0290 SEC	.0490 SEC	.0690 SEC	.0750 SEC						
.0000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
.1000-04	.00000	.24157-03	.23631-03	.23582-03	.00000	.00000	.00000	.00000	.00000	.00000
.1000-02	.00000	.43493-01	.58605-01	.62051-01	.00000	.00000	.00000	.00000	.00000	.00000
.2000-02	.00000	.64489-01	.75707-01	.78131-01	.00000	.00000	.00000	.00000	.00000	.00000
.4000-02	.00000	.93976-01	.10113+00	.10262+00	.00000	.00000	.00000	.00000	.00000	.00000
.6000-02	.00000	.10703+00	.11129+00	.11221+00	.00000	.00000	.00000	.00000	.00000	.00000
.8000-02	.00000	.11447+00	.11697+00	.11755+00	.00000	.00000	.00000	.00000	.00000	.00000
.1000-01	.00000	.11895+00	.12037+00	.12073+00	.00000	.00000	.00000	.00000	.00000	.00000
.1200-01	.00000	.12174+00	.12250+00	.12271+00	.00000	.00000	.00000	.00000	.00000	.00000
.1500-01	.00000	.12398+00	.12422+00	.12432+00	.00000	.00000	.00000	.00000	.00000	.00000
.2000-01	.00000	.10830+00	.10423+00	.10341+00	.00000	.00000	.00000	.00000	.00000	.00000

FIG. 5q

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TIME PROFILES OF HE MOLE FRACTION VS AXIAL POSITION

HE MOLE FRACTION (DIMENSIONLESS)

AXIAL POSITION (FT)	.0290 SEC	.0490 SEC	.0690 SEC	.0750 SEC						
.0000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
.1000-04	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
.1000-02	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
.2000-02	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
.4000-02	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
.6000-02	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
.8000-02	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
.1000-01	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
.1200-01	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
.1500-01	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
.2000-01	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000

FIG. 5r

WALL TEMPERATURE, INTERFACE VARIATIONS VS TIME

TIME (SEC)	*	WALL TEMP (DEGREES R)	SOLID/SOLID-LIQUID (FT)	SOLID-LIQUID/LIQUID (FT)	LIQUID/LIQUID-VAPOR (FT)	LIQUID-VAPOR/VAPOR (FT)
	*					
.0290	*	.36046+03	.20000-01	.20000-01	.20000-01	.20000-01
.0490	*	.36428+03	.20000-01	.20000-01	.20000-01	.20000-01
.0690	*	.37203+03	.20000-01	.20000-01	.20000-01	.20000-01
.0750	*	.37495+03	.20000-01	.20000-01	.20000-01	.20000-01

FIG. 5s

K910962-13

```
*************************************
* GO TO ALL DIFFUSION-CONTROLLED RUN *
*          TIME = .7500-01 SEC       *
*************************************


****** OPERATIONS COMPLETE ******
TOTAL EXECUTION TIME:  4.0 MINUTES
```


FIG. 5t

Description of Routines

The following is a list and brief description of all the routines in the H_2/O_2 transient computer program:

F874: This routine handles the reading and writing of the standard deck input. Subroutine MCALC is called from it.

MCALC: This routine handles the main body of reactor calculations. Most of the other subroutines are called from it.

DERIV: This subroutine calculates the values of the derivative expressions.

PCALCT: This subroutine does the non-diffusion-controlled catalyst particle analysis.

PCALCS: This subroutine does the diffusion-controlled catalyst particle analysis.

GREEN: This subroutine finds the values of the Green's functions used in calculations in subroutine PCALCT.

ROOT: This subroutine finds the roots of the characteristic equation $x \cdot \cot(x)+C=0$. using a modified method of successive substitutions. These roots are used to find the Green's functions in subroutine GREEN.

INSERT: This subroutine inserts the interface axial positions (positions where water changes phase) into the original Z array.

DELETE: This subroutine deletes the inserted interface axial positions at the end of each time step.

OVSTEP: This subroutine makes appropriate adjustments to temperature, pressure, concentrations, etc., when axial positioning has overstepped the interface boundaries.

FMAX: This routine is used to find the maximum value of elements in an array.

FMIN: This routine is used to find the minimum value of elements in an array.

RDPNCH: This subroutine handles the punching and reading of the extra input needed by the continuation and all diffusion-controlled runs.

OUTPUT: This routine prints the temperature, pressure, and mole-fraction profiles in summary form.

SETUP: This subroutine is used to setup the arrays needed for the printer plots in subroutine PRPLOT.

PRPLOT: This subroutine is used to develop and print the printer plots of temperatures, mole-fractions, etc. vs. axial position at various times.

TMPRNT: This subroutine handles the printing of wall and interface position values vs. time. For non-hydrogen-lead cases, it also handles printing of the mass flow rate and pressure vs. time.

DEBUG3: This subroutine handles the detailed printing which is produced only when input logical indicator DEBUG=T.

UNBAR: This subroutine will do linear quadratic or cubic interpolation between tabulated points. Interpolation may be either univariate or bivariate.

TABLES: This subroutine contains tables of heat of reaction, species viscosities, species specific heats, vapor pressure, heat of condensation, and species thermal conductivities.

APPENDIX I

LISTING OF COMPUTER PROGRAM

```
      LOGICAL DEBUG,H2LEAD
      INTEGER TITLE(13),PUNCH
      REAL  KAPPA,KP,KCH2,KCO2,KCH20,MH2,MO2,MH20,MHE,MW,MU,MBAR,MBARSS
      PARAMETER NAX=70, NTI=40
      PARAMETER NPP=30, NRTS=200
      COMMON /CB1/ TPP(NPP,NAX),CO2(NPP,NAX),CH2(NPP,NAX),CH20(NPP,NAX),
     X       T(NAX),P(NAX),PT(NAX),H(NAX),CIH2(NAX),CIO2(NAX),CIH20(NAX),
     X       CIH20S(NAX),CIH20L(NAX),CIH20V(NAX),CIHE(NAX),DELT(NTI),
     X       PPT(NAX)
      COMMON /CB2/ Z(NAX),ZSSL(NTI),ZSLL(NTI),ZLLV(NTI),ZLVV(NTI)
      COMMON /CB3/ ALPHA,GAMMA,KAPPA,HC,KP,A,DELTT,KCH2,KCO2,KCH20,TCH2,
     X       TCO2,TCH20,PCH2,PCO2,PCH20,MH2,MO2,MH20,MHE,HR,HA,HA1,HA2,
     X       AW,CW,MW,DC,TA,D0H2,D0O2,D0H20,ALPHAK,AP,DELTA,G,MU,HS,HL,
     X       HV,TW,RHOM,WH2,WO2,WH20S,WH20L,WH20V,WHE,CFBAR,MBAR,CICP1,
     X       CICP2,CICP3,RHO,RHOV,DELHC,TITPS,DTDZ,DHDZ,TS,TL,DPDZ,DC1DZ,
     X       DC2DZ,DC3SDZ,DC3LDZ,DC3VDZ,DC4DZ,RHOP,CP,DELTP,DPTPS,SDTIME,
     X       PF,TSS,AC,VC,PREST,GSS,MBARSS
      COMMON /CB4/ NOFZ,NPASS,NAXIAL,INPERP,MODPC,MODNO,PUNCH,ITSTEP,
     X       JDP,ISHUT,IHOT
      COMMON /TABLES/ AVSZ(40),APVSZ(40),DELVSZ(40),HRVST(36),TC1(22),
     X       TC2(20),TC3V(20),TC4(18),MU1VST(34),MU2VST(34),MU3VST(32),
     X       MU4VST(34),CF1VST(34),CF2VST(34),CF3VST(34),CF3SVT(20),
     X       CF4VST(20),VPVST(60),TVSVP(48),DHCVST(24)
      DATA  ALPHA,ALPHAK,GAMMA,KP,MH2,MO2,MH20,MHE,PCH2,PCO2,PCH20 /
     X       .160 E+14, .3174 E+8, .50 E+4, .40 E-4, 2.02, 32.0, 18.02,
     X       4.003, 188.16, 730.59, 3200.2 /
      DATA  TCH2,TCO2,TCH20,D0H2,D0O2,D0H20,RHOP,CP /
     X       59.94, 277.92, 1164.6, .1676 E-2, .7572 E-3, .6355 E-3,
     X       124.9, .177 /
      KAPPA = KP/(RHOP*CP)
6     CALL TMINS (TSTART)
      READ (5,1,END=99) TITLE,H2LEAD,DEBUG
1     FORMAT (13A6,2L1)
      READ (5,3) NOFZ,NPASS,INPERP,MODNO,PUNCH,ITSTEP
3     FORMAT (20I4)
      READ (5,2) G,TS,T(1),P(1),H(1),CIH2(1),CIO2(1),CIHE(1)
2     FORMAT (8E10.5)
      READ (5,2) TI,PI,CH2I,CO2I,CH20I,CHEI,PTI,SDTIME
      READ (5,2) AW,CW,MW,DC,TA,HA,HA1,HA2
      NAXIAL = NOFZ
      IF (PUNCH.EQ.4) NAXIAL=NOFZ+4
      IF (H2LEAD) GO TO 101
      GSS = G
      READ (5,102) PF,TSS,MBARSS,AC,VC,PREST
102   FORMAT (6E10.5)
101   READ (5,2) (Z(I),I=1,NOFZ)
      IF (ITSTEP.EQ.0) GO TO 7
      READ (5,2) (DELT(I),I=1,NPASS)
7     WRITE (6,10) TITLE
10    FORMAT ('1' 53X '***** PROGRAM INPUT *****' ///
     X       43X 'TRANSIENT ANALYSIS OF H2/O2 CATALYTIC REACTOR' /
     X       30X  14A6 )
      WRITE (6,17) NOFZ,NPASS,INPERP,DEBUG,MODNO,PUNCH
17    FORMAT ('0' // 37X 'NOFZ' 6X 'NPASS' 5X 'INPERP' 5X 'DEBUG' 7X
     X       'MODNO' 6X 'PUNCH' / 37X, I3, 9X, I2, 8X, I2, 9X, L2, 9X,
     X       I2, 10X, I1)
      WRITE (6,12) G,TS,MH2,MO2,MH20,MHE,D0H2,D0O2,D0H20,KP,ALPHA
12    FORMAT ('0'12X 'G' 10X 'TS' 8X 'MH2' 8X 'MO2' 8X 'MH20' 7X 'MHE'
```

```
     X       8X 'DOH2' 7X 'DOO2' 6X 'DOH2O' 8X 'KP' 7X 'ALPHA' /
     X       6X, 11E11.5 )
      WRITE (6,13) ALPHAK,GAMMA
13    FORMAT ('0' 9X 'ALPHAK' 6X 'GAMMA' / 6X, 11E11.5)
      WRITE (6,5) AW,CW,MW,DC,TA,HA,HA1,HA2
5     FORMAT ('0' 27X 'AW' 9X 'CW' 9X 'MW' 9X 'DC' 9X 'TA' 9X 'HA' 8X
     X       'HA1' 8X 'HA2' / 22X, 8E11.5/ )
      WRITE (6,19) TI,PI,CH2I,CO2I,CH2OI,CHEI,PTI
19    FORMAT ('0' 40X 'INITIAL TEMPERATURES, PRESSURES, AND CONCENTRATIO
     XNS' / 33X 'T' 10X 'P' 8X 'CIH2' 8X 'CIO2' 6X 'CIH2O' 7X 'CIHE'
     X       8X 'TPS' / 28X, 7E11.5 /)
      WRITE (6,14) T(1),P(1),H(1),CIH2(1),CIO2(1),CIHE(1)
14    FORMAT ('0'  37X 'INLET TEMPERATURE, PRESSURE, ENTHALPY, AND CONCE
     XNTRATIONS' / 39X 'T' 10X 'P' 10X 'H' 9X 'CIH2' 7X 'CIO2' 7X 'CIHE'
     X       / 33X, 6E11.5  / )
      WRITE (6,16) (Z(I),I=1,NOFZ)
16    FORMAT ('0'  56X 'INPUT AXIAL STATIONS' / (12E11.5) )
      IF (ITSTEP.EQ.0) GO TO 8
      WRITE (6,18) (DELT(I),I=1,NPASS)
18    FORMAT ('0'  51X 'TIME INCREMENTS FOR EACH PASS' / (12E11.5) )
8     IF (H2LEAD) GO TO 104
      WRITE (6,103) PF,TSS,MBARSS,AC,VC
103   FORMAT ('0' 54X 'VALUES USED TO CALCULATE DPDT' / 39X 'PF' 12X
     X          'TSS' 10X 'MBARSS' 10X 'AC' 12X 'VC' / 35X,E10.5,4X,
     X          E10.5,4X,E10.5,4X,E10.5,4X,E10.5 /)
104   READ (5,4) (AVSZ(I),I=1,4)
      NA = AVSZ(3)+4.
      NB = NA+1
      NC = 2.*AVSZ(3)+4.
      READ (5,4) (AVSZ(I),I=5,NA)
      READ (5,4) (AVSZ(I),I=NB,NC)
      WRITE (6,24)
24    FORMAT ('0' // 53X 'A, AP, DELTA VS Z TABLES')
      WRITE (6,21) (AVSZ(I),I=1,4)
      WRITE (6,22) (AVSZ(I),I=5,NA)
      WRITE (6,22) (AVSZ(I),I=NB,NC)
      WRITE (6,23)
      READ (5,4) (APVSZ(I),I=1,4)
      NA = APVSZ(3)+4.
      NB = NA+1
      NC = 2.*APVSZ(3)+4.
      READ (5,4) (APVSZ(I),I=5,NA)
      READ (5,4) (APVSZ(I),I=NB,NC)
      WRITE (6,21) (APVSZ(I),I=1,4)
      WRITE (6,22) (APVSZ(I),I=5,NA)
      WRITE (6,22) (APVSZ(I),I=NB,NC)
      WRITE (6,23)
      READ (5,4) (DELVSZ(I),I=1,4)
      NA = DELVSZ(3)+4.
      NB = NA+1
      NC = 2.*DELVSZ(3)+4.
      READ (5,4) (DELVSZ(I),I=5,NA)
      READ (5,4) (DELVSZ(I),I=NB,NC)
      WRITE (6,21) (DELVSZ(I),I=1,4)
      WRITE (6,22) (DELVSZ(I),I=5,NA)
      WRITE (6,22) (DELVSZ(I),I=NB,NC)
4     FORMAT (10E8.4)
20    FORMAT ('0' // 53X 'A, AP, DELTA VS Z TABLES' )
21    FORMAT (38X, 4E13.5)
22    FORMAT (1X, 10E13.5)
23    FORMAT ('0')
      IHOT = 0
```

```
      IF (PTI.GT.TI) IHOT=1
      CIH2O(1) = 0.
      CIH2OS(1) = 0.
      CIH2OL(1) = 0.
      CIH2OV(1) = 0.
      IF (PUNCH.EQ.2.OR.PUNCH.EQ.3) GO TO 90
C   SET INITIAL CONDITIONS THROUGHOUT REACTOR BED
      DO 50 I=2,NAXIAL
      CIH2(I) = CH2I
      CIO2(I) = CO2I
      CIH2O(I) = CH2OI
      CIH2OS(I) = CH2OI
      CIH2OL(I) = CH2OI
      CIH2OV(I) = CH2OI
      CIHE(I) = CHEI
      T(I) = TI
      PT(I) = PTI
 50   P(I) = PI
C   START REACTOR CALCULATIONS
 90   CALL MCALC (H2LEAD,DEBUG)
 91   CALL TMINS (TEND)
      TOTELT = TEND-TSTART
      IF (TOTELT.LT.0.) TOTELT=1440.-TSTART+TEND
      WRITE (6,100) TOTELT
 100  FORMAT ('0' /// 49X '****** OPERATIONS COMPLETE ******' /
     X       49X 'TOTAL EXECUTION TIME:',F5.1,' MINUTES' )
      GO TO 6
 99   STOP
      END
```

```
      SUBROUTINE MCALC (H2LEAD,DEBUG)
C
C     ROUTINE TO HANDLE MAIN BODY OF REACTOR CALCULATIONS
C
      LOGICAL DEBUG,H2LEAD,SSTATE
      INTEGER PASSNO,PUNCH,REGION
      REAL  MH2,MO2,MH2O,MHE,MUH2,MUO2,MUH2O,MUHE,MU,MBAR,MFH2,MFO2,
     X      MFH2O,MFHE,KAPPA,KP,KCH2,KCO2,KCH2O,MW,MU1VST,MU2VST,MU3VST,
     X      MU4VST,KCF,MBARSS
      PARAMETER NAX=70, NTI=40
      PARAMETER NPP=30, NRTS=200
      PARAMETER NX10=NAX*10
      COMMON /CB1/ TPP(NPP,NAX),CO2(NPP,NAX),CH2(NPP,NAX),CH2O(NPP,NAX),
     X      T(NAX),P(NAX),PT(NAX),H(NAX),CIH2(NAX),CIO2(NAX),CIH2O(NAX),
     X      CIH2OS(NAX),CIH2OL(NAX),CIH2OV(NAX),CIHE(NAX),DELT(NTI),
     X      PPT(NAX)
      COMMON /CB2/ Z(NAX),ZSSL(NTI),ZSLL(NTI),ZLLV(NTI),ZLVV(NTI)
      COMMON /CB3/ ALPHA,GAMMA,KAPPA,HC,KP,A,DELTT,KCH2,KCO2,KCH2O,TCH2,
     X      TCO2,TCH2O,PCH2,PCO2,PCH2O,MH2,MO2,MH2O,MHE,HR,HA,HA1,HA2,
     X      AW,CW,MW,DC,TA,D0H2,D0O2,D0H2O,ALPHAK,AP,DELTA,G,MU,HS,HL,
     X      HV,TW,RHOM,WH2,WO2,WH2OS,WH2OL,WH2OV,WHE,CFBAR,MBAR,CICP1,
     X      CICP2,CICP3,RHO,RHOV,DELHC,TITPS,DTDZ,DHDZ,TS,TL,DPDZ,DC1DZ,
     X      DC2DZ,DC3SDZ,DC3LDZ,DC3VDZ,DC4DZ,RHOP,CP,DELTP,DPTPS,SDTIME,
     X      PF,TSS,AC,VC,PREST,GSS,MBARSS
      COMMON /CB4/ NOFZ,NPASS,NAXIAL,INPERP,MODPC,MODNO,PUNCH,ITSTEP,
     X      JDP,ISHUT,IHOT
      COMMON /TABLES/ AVSZ(40),APVSZ(40),DELVSZ(40),HRVST(36),TC1(22),
     X      TC2(20),TC3V(20),TC4(18),MU1VST(34),MU2VST(34),MU3VST(32),
     X      MU4VST(34),CF1VST(34),CF2VST(34),CF3VST(34),CF3SVT(20),
     X      CF4VST(20),VPVST(60),TVSVP(48),DHCVST(24)
      DIMENSION MFH2(NAX),MFO2(NAX),MFH2O(NAX),MFHE(NAX),HW(NAX),
     X      MINT(NAX),TM(NTI),TWT(NTI),GT(NTI),PRESTT(NTI),PP(NX10),
     X      TT(NX10),TP(NX10),FH2(NX10),FO2(NX10),FH2O(NX10),FHE(NX10)
      DATA  R,PI,OMEGA,KM              /10.73, 3.1415927, 35800., 5       /
      DIF (D0,P,T) = 14.7*D0/P*(T/492.)**1.823
      KCF (G,RHO,AM,DI,AP) = .61*G/RHO*(AM/RHO/DI)**-.67*(G/AP/AM)**-.41
C     *****************************************************************
C
C     PROGRAM FLAGS AND INDICATORS
C
C              NOFZ  : NO. OF INPUT AXIAL STATIONS
C
C              NAXIAL: NOFZ+4 (ALLOWS FOR INTERFACE AXIAL STATIONS)
C
C              INPERP: NO. OF TIME INCREMENTS PER PASS THRU MESH
C
C              MODPC : MODULAR PASS COUNT INDICATOR USED TO DETERMINE WHEN
C                                      SUMMARY OUTPUT SHOULD BE CALLED
C
C              MODNO : MODULAR NUMBER OF INDEPENDENT VARIABLES USED FOR
C                                      PRINTER PLOT OUTPUT
C
C              IOCT  : PROGRAM COUNT OF THE NO. OF TIMES SUMMARY I/O HAS
C                                      BEEN CALLED
C
C              IT    : PROGRAM COUNT OF CURRENT TIME STEP INCREMENT
C
C              IZ    : PROGRAM COUNT OF CURRENT AXIAL STATION
```

```
C
C            PUNCH : AUXILIARY INPUT/OUTPUT INDICATOR ---
C                          =1 NO AUXILIARY I/O
C                          =2 READ AUXILIARY INPUT ONLY
C                          =3 PUNCH AUXILIARY OUTPUT ONLY
C                          =4 READ AUXILIARY INPUT, AND PUNCH AUXILIARY OUTPUT
C
C            ITSTEP: TIME INCREMENT INDICATOR ---
C                          =0 PROGRAM DETERMINES DELT INCREMENTS
C                          =1 DELT INCREMENTS ARE INPUT
C
C            IHOT  : HOT START INDICATOR ---
C                          =0 NORMAL START
C                          =1 HOT START
C
C            ISHUT : REACTOR SHUTDOWN INDICATOR ---
C                          =0 NORMAL REACTOR OPERATION
C                          =1 REACTOR SHUTDOWN HAS OCCURRED
C
C            JDP   : CONSTANT DELT INDICATOR (USED ONLY WHEN ITSTEP=0) ---
C                          =0 PROGRAM DETERMINES DELT AS USUAL
C                          =1 DELT SET CONSTANT AT .001 SEC
C
C            MINT3 : DIFFUSION CONTROL INDICATOR ---
C                          =0 REACTOR CALCULATIONS NOT YET DIFFUSION CONTROLLED
C                          =1 REACTOR CALCULATIONS ALL DIFFUSION CONTROLLED
C
C    ****************************************************************
C    INITIALIZE FLAGS AND COUNTERS
      IOCT = 0
      ITP = 0
      MINT3 = 0
      JDP = 0
      ISHUT = 0
      IT = 1
      IZ = 1
      K = 1
      N1 = 1
      PASSNO = 1
      M = 1
      MODPC = 10
      IF (NPASS.LT.10) MODPC=NPASS
      DCTEMP = (29160.-6.*P(1))/57.
      SSTATE = .FALSE.
      ZEND = Z(NOFZ)
C    INITIALLY ALL INTERFACES COINCIDE WITH END OF REACTOR BED
      DO 7 I=1,NTI
      ZSSL(I) = ZEND
      ZSLL(I) = ZEND
      ZLLV(I) = ZEND
  7   ZLVV(I) = ZEND
      GO TO (102,102,102,111), PUNCH
 102  ALPHA = 0.
      IF (IHOT.EQ.1) GO TO 33
      IF (T(1)-DCTEMP) 25,25,24
 24   SSTATE = .TRUE.
      GO TO 111
 25   DO 32 I=1,NAXIAL
 32   MINT(I) = 1
      GO TO 35
 33   DO 34 I=1,NAXIAL
 34   MINT(I) = 2
```

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      GO TO 35
 111  DO 112 I=1,NAXIAL
 112  MINT(I) = 3
C   DETERMINE APPROPRIATE DELTT
 35   IF (ITSTEP.EQ.1) GO TO 19
      TPSMAX = PT(2)
      CALL DELTAT
      GO TO 17
 19   DELTT = DELT(1)
 17   PT(1) = PT(2)
C    SET INITIAL PARTICLE SURFACE VALUES FOR TEMPERATURE, CONCENTRATION
      TPS = PT(1)
      TW = TPS
      CSH2 = CIH2(2)
      CSO2 = CIO2(2)
      CSH2O = CIH2O(2)
      IF (H2LEAD) GO TO 121
      G = GSS*SQRT((PF-PREST)/(PF-P(1)))
      CIO2(1) = CIO2(1)*PREST/P(1)
      CIH2(1) = CIH2(1)*PREST/P(1)
      CIHE(1) = CIHE(1)*PREST/P(1)
 121  TIME = 0.
      IF (PUNCH.NE.4) GO TO 113
      CALL PREVUS
 113  IF (PUNCH.EQ.2.OR.PUNCH.EQ.3) CALL RDPNCH(TIME,HW,MINT)
      CMSUM = CIH2(1)/MH2+CIO2(1)/MO2+CIH2O(1)/MH2O+CIHE(1)/MHE
      MFO2(1) = CIO2(1)/MO2/CMSUM
      REGION = 1
      CALL UNBAR (TVSVP,1,P(1),0.,TL,KK)
      IF (T(1)-TS) 1,1,8
 8    IF (T(1)-TL) 9,9,10
 9    REGION = 3
      GO TO 1
 10   REGION = 5
C
C    BEGIN STEPPING AXIALLY THROUGH THE REACTOR
C
 1    IZ = IZ+1
      IRHOM = 0
C    CHECK IF CALCULATIONS DIFFUSION CONTROLLED AT CURRENT AXIAL STATION
      MZ = MINT(IZ)
      GO TO (37,39,47), MZ
 39   IF (PASSNO.EQ.1.AND.IT.EQ.1) GO TO 38
      IF (PPT(IZ)-PT(IZ)) 37,37,36
 36   SSTATE = .FALSE.
      GO TO 38
 37   IF (PT(IZ)-DCTEMP) 31,30,30
 30   MINT(IZ) = 3
      GO TO 47
C    NOT DIFFUSION CONTROLLED ---
 31   SSTATE = .FALSE.
      MINT(IZ) = 1
      GO TO 38
C    DIFFUSION CONTROLLED ---
 47   SSTATE = .TRUE.
      IF (PUNCH.NE.4) REGION=5
 38   DELTZP = DELTZ
      DELTZ = Z(IZ)-Z(IZ-1)
      TAV = (PT(IZ-1)+T(IZ-1))/2.
      CALL UNBAR (AVSZ,1,Z(IZ-1),0.,A,KK)
      CALL UNBAR (APVSZ,1,Z(IZ-1),0.,AP,KK)
      CALL UNBAR (DELVSZ,1,Z(IZ-1),0.,DELTA,KK)
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```
      CALL UNBAR (HRVST,1,T(IZ-1),0.,HR,KK)
      CALL UNBAR (DHCVST,1,T(IZ-1),0.,DELHC,KK)
      CALL UNBAR (MU1VST,1,TAV,0.,MUH2,KK)
      CALL UNBAR (MU2VST,1,TAV,0.,MUO2,KK)
      CALL UNBAR (MU3VST,1,TAV,0.,MUH2O,KK)
      CALL UNBAR (MU4VST,1,TAV,0.,MUHE,KK)
      CALL UNBAR (CF1VST,1,T(IZ-1),0.,CFH2,KK)
      CALL UNBAR (CF2VST,1,T(IZ-1),0.,CFO2,KK)
      CALL UNBAR (CF4VST,1,T(IZ-1),0.,CFHE,KK)
      CALL UNBAR (TC1,1,TAV,0.,THH2,KK)
      CALL UNBAR (TC2,1,TAV,0.,THO2,KK)
      CALL UNBAR (TC3V,1,TAV,0.,THH2O,KK)
      CALL UNBAR (TC4,1,TAV,0.,THHE,KK)
      GO TO (2,2,3,4,5), REGION
2     CALL UNBAR (CF3SVT,1,T(IZ-1),0.,CFH2OS,KK)
      CFH2OL = 1.0
      CFH2OV = 0.
      RHOM = 0.
      GO TO 6
3     CFH2OS = 0.
      CFH2OL = 1.0
      CFH2OV = 0.
      RHOM = 0.
      GO TO 6
4     CALL UNBAR (CF3VST,1,T(IZ-1),0.,CFH2OV,KK)
      CFH2OS = 0.
      CFH2OL = 1.0
      RHOM = 0.
      GO TO 6
5     CALL UNBAR (CF3VST,1,T(IZ-1),0.,CFH2OV,KK)
      IF (IZ.EQ.2) GO TO 84
      IF (H(IZ-1).LT.H(IZ-2)) GO TO 83
84    IF (T(IZ-1)-TS) 81,81,82
81    CALL UNBAR (CF3SVT,1,T(IZ-1),0.,CFH2OV,KK)
      GO TO 83
82    IF (T(IZ-1).LT.TL) CFH2OV=1.0
83    CFH2OS = 0.
      CFH2OL = 0.
      RHOM = ALPHA*CIH2(IZ-1)*CIO2(IZ-1)*EXP(-OMEGA/T(IZ-1))
6     RHO = CIH2(IZ-1)+CIO2(IZ-1)+CIH2OS(IZ-1)+CIH2OL(IZ-1)+CIH2OV(IZ-1)
     X      +CIHE(IZ-1)
      RHOS = RHO-CIH2OL(IZ-1)-CIH2OV(IZ-1)
      RHOL = RHO-CIH2OS(IZ-1)-CIH2OV(IZ-1)
      RHOV = RHO-CIH2OS(IZ-1)-CIH2OL(IZ-1)
      SUM = CIH2(IZ-1)/MH2+CIO2(IZ-1)/MO2+(CIH2OS(IZ-1)+CIH2OL(IZ-1)+
     X      CIH2OV(IZ-1))/MH2O+CIHE(IZ-1)/MHE
      MU = (MUH2*CIH2(IZ-1)/MH2+MUO2*CIO2(IZ-1)/MO2+MUH2O*(CIH2OS(IZ-1)+
     X      CIH2OL(IZ-1)+CIH2OV(IZ-1))/MH2O+MUHE*CIHE(IZ-1)/MHE) / SUM
      MBAR = RHOV/(CIH2(IZ-1)/MH2+CIO2(IZ-1)/MO2+CIH2OV(IZ-1)/MH2O+
     X      CIHE(IZ-1)/MHE)
      CFBAR = (CFH2*CIH2(IZ-1)+CFO2*CIO2(IZ-1)+CFH2OS*CIH2OS(IZ-1)+
     X      CFH2OL*CIH2OL(IZ-1)+CFH2OV*CIH2OV(IZ-1)+CFHE*CIHE(IZ-1)) /
     X      RHO
      DIH2 = DIF(D0H2,P(IZ-1),T(IZ-1))
      DIO2 = DIF(D0O2,P(IZ-1),T(IZ-1))
      DIH2O = DIF(D0H2O,P(IZ-1),T(IZ-1))
      KCH2 = KCF(G,RHO,MU,DIH2,AP)
      KCO2 = KCF(G,RHO,MU,DIO2,AP)
      KCH2O = KCF(G,RHO,MU,DIH2O,AP)
      SUMC = CIH2(IZ-1)/MH2+CIO2(IZ-1)/MO2+CIH2O(IZ-1)/MH2O+CIHE(IZ-1)/
     X                                                          MHE
      THERMC = (THH2*CIH2(IZ-1)/MH2+THO2*CIO2(IZ-1)/MO2+THH2O*
```

```
     X             CIH2O(IZ-1)/MH2O+THHE*CIHE(IZ-1)/MHE)/SUMC
      HC = .61*CFBAR*G*(G/(AP*MU))**-.41*(CFBAR*MU/THERMC)**-.667
      HW(IZ) = HC
      HW(1) = HW(2)
 58   IF (SSTATE) GO TO 60
C   PARTICLE ANALYSIS --- TRANSIENT
      CALL PCALCT (CSH2,CSO2,CSH2O,TPS,DCTEMP,IT,ITP,IZ,PASSNO,NC,DEBUG)
      ITP = IT
      IF (NC.EQ.0) GO TO 59
      TPST = (PT(IZ)-PPT(IZ))/DELTP*(DELTP+DELTT)+PPT(IZ)
      IF (TPST.LT.DCTEMP) TPST=DCTEMP
      TPS = TPST
      CSO2 = CIO2(IZ)-HC/(HR*KCO2)*(T(IZ)-TPS)
      CSH2 = CIH2(IZ)-2.*KCO2/KCH2*MH2/MO2*(CIO2(IZ)-CSO2)
      CSH2O = 0.
      GO TO 59
C   PARTICLE ANALYSIS --- STEADY STATE
 60   CALL PCALCS (TPS,CSO2,CSH2,CSH2O,CIO2PR,IZ,MINT)
 59   TITPS = T(IZ-1)-TPS
      CICP1 = CIH2(IZ-1)-CSH2
      CICP2 = CIO2(IZ-1)-CSO2
      CICP3 = CIH2OV(IZ-1)-CSH2O
      IF (CSH2O) 85,85,86
 85   CICP3 = 0.
 86   WH2 = CIH2(IZ-1)/RHO
      WO2 = CIO2(IZ-1)/RHO
      WH2OS = CIH2OS(IZ-1)/RHO
      WH2OL = CIH2OL(IZ-1)/RHO
      WH2OV = CIH2OV(IZ-1)/RHO
      IF (REGION.NE.5) GO TO 87
      WH2OS = 0.
      WH2OL = 0.
 87   WHE = CIHE(IZ-1)/RHO
C   MAKE DERIVATIVE CALCULATIONS
 900  CALL DERIV (CIO2PR,DELTZ,IZ,REGION)
      CIO2(IZ) = CIO2(IZ-1)+DC2DZ*DELTZ
      IF (CIO2(IZ).LT.0..AND.RHOM.GT.0.) GO TO 901
      IF (IRHOM.EQ.1) CIO2(IZ)=0.
      GO TO 903
 901  RHOM = 0.
      IRHOM = 1
      GO TO 900
 903  P(IZ) = P(IZ-1)+DPDZ*DELTZ
C   TEST FOR NEGATIVE PRESSURE
      IF (P(IZ)) 905,61,61
 61   T(IZ) = T(IZ-1)+DTDZ*DELTZ
      IF (T(IZ).LT.T(1)) T(IZ)=T(1)
      PPT(IZ) = PT(IZ)
      PT(IZ) = TPS
      PT(1) = PT(2)
      H(IZ) = H(IZ-1)+DHDZ*DELTZ
      IF (H(IZ).LT.H(IZ-1)) REGION=5
      IF (H(IZ).LT.0.) H(IZ)=0.
      CIH2(IZ) = CIH2(IZ-1)+DC1DZ*DELTZ
      CIH2OS(IZ) = CIH2OS(IZ-1)+DC3SDZ*DELTZ
      CIH2OL(IZ) = CIH2OL(IZ-1)+DC3LDZ*DELTZ
      CIH2OV(IZ) = CIH2OV(IZ-1)+DC3VDZ*DELTZ
      IF (REGION.NE.5) GO TO 88
      CIH2OS(IZ) = 0.
      CIH2OL(IZ) = 0.
 88   CIHE(IZ) = CIHE(IZ-1)+DC4DZ*DELTZ
      IF (CIH2(IZ).LT.0.) CIH2(IZ)=0.
```

```
      IF (CIO2(IZ).LT.0.) CIO2(IZ)=0.
      IF (CIH2OV(IZ).LT.0.) CIH2OV(IZ)=0.
      IF (CIHE(IZ).LT.0.) CIHE(IZ)=0.
      CIH2O(IZ) = CIH2OS(IZ)+CIH2OL(IZ)+CIH2OV(IZ)
      CALL UNBAR (TVSVP,1,P(IZ),0.,TL,KK)
      CMSUM = CIH2(IZ)/MH2+CIO2(IZ)/MO2+CIH2O(IZ)/MH2O+CIHE(IZ)/MHE
      MFO2(IZ) = CIO2(IZ)/MO2/CMSUM
      IF ((MFO2(IZ).LT..01*MFO2(1)).AND.(PT(IZ).GT.(T(1)+30.))) MINT(IZ)
     X                                                              = 3
      DO 91 I=2,NAXIAL
      IF (MINT(I)-3) 140,91,140
 91   CONTINUE
C
C   BEGIN TESTING FOR INTERFACE LOCATIONS
C
      GO TO (100,110,120,130,140), REGION
C   SOLID/SOLID-LIQUID INTERFACE
 100  IF (T(IZ)-TS) 51,101,101
 101  CALL OVSTEP (ZEND,IZ,PASSNO,REGION)
      GO TO 140
C   SOLID-LIQUID/LIQUID INTERFACE
 110  IF (CIH2OS(IZ)) 101,101,51
C   LIQUID/LIQUID-VAPOR INTERFACE
 120  IF (T(IZ)-TL) 51,101,101
C   LIQUID-VAPOR/VAPOR INTERFACE
 130  IF (CIH2OL(IZ)) 101,101,51
C   END OF REACTOR BED
 140  IF (Z(IZ)-ZEND) 51,70,101
 51   IF (IZ.LT.NOFZ) GO TO 1
 70   NM1 = NOFZ-1
      DTWDT = (PI*DC*RSUM(NM1)-AW*(HA*(TW-TA)+HA1*(TW-TA)**1.25+HA2*
     X        (TW**4-TA**4)))/(MW*CW)
      TW = TW+DTWDT*DELTT
C   CALCULATE MOLE FRACTIONS
 54   DO 53 I=1,NAXIAL
      CMSUM = CIH2(I)/MH2+CIO2(I)/MO2+CIH2O(I)/MH2O+CIHE(I)/MHE
      MFH2(I) = CIH2(I)/MH2/CMSUM
      MFO2(I) = CIO2(I)/MO2/CMSUM
      MFH2O(I) = CIH2O(I)/MH2O/CMSUM
 53   MFHE(I) = CIHE(I)/MHE/CMSUM
      IF (H2LEAD.OR.TIME.GT.SDTIME) GO TO 118
      DPDT = R*T(IZ)/MBAR*AC/VC*(G-PREST*GSS*SQRT(MBAR*TSS/(T(IZ)*MBARSS
     X       ))/P(1))
      PPP = R*AC*GSS/(VC*P(1)*SQRT(MBARSS/TSS))*SQRT(T(IZ)/MBAR)
      DPDT = DPDT*(1.-EXP(-PPP*DELTT))/(PPP*DELTT)
      PREST = PREST+DPDT*DELTT
      G = GSS*SQRT((PF-PREST)/(PF-P(1)))
      CIO2(1) = CIO2(1)*PREST/P(1)
      CIH2(1) = CIH2(1)*PREST/P(1)
      CIHE(1) = CIHE(1)*PREST/P(1)
C   END OF REACTOR HAS BEEN REACHED FOR CURRENT TIME STEP
 118  TIME = TIME+DELTT
C   CHECK FOR DEBUG PRINT
      IF (DEBUG) CALL DEBUG3(TIME,IT)
      IF (PUNCH.EQ.4) GO TO 104
      DO 107 I=2,NAXIAL
      IF (MINT(I)-3) 104,107,104
 107  CONTINUE
      CALL RPNCH4 (TIME)
      MINT3 = 1
      NPASS = PASSNO
      GO TO 108
```

```
 104  IF (ISHUT.EQ.1) GO TO 42
C   TEST IF SHUTDOWN TIME HAS BEEN REACHED
      IF (TIME-SDTIME) 42,42,40
C   SHUTDOWN ---
 40   ISHUT = 1
      READ (5,41) CIH2(1),CIO2(1)
 41   FORMAT (2E10.5)
 42   IT = IT+1
      IZ = 1
      REGION = 1
      IF (T(1)-TS) 78,78,76
 76   IF (T(1)-TL) 74,74,75
 74   REGION = 3
      GO TO 78
 75   REGION = 5
 78   IF (PUNCH.NE.4) GO TO 89
      CALL DELETE (PASSNO)
      NOFZ = NAXIAL-4
C   DETERMINE APPROPRIATE DELTT FOR NEXT TIME STEP
 89   DELTP = DELTT
      TPSMAX = FMAX(PT,NAXIAL,NAX,1)
      CALL DELTAT
      IF (ITSTEP.NE.1.OR.JDP.EQ.1) GO TO 26
      IF (TPSMAX-380.) 26,23,23
 23   JDP = 1
      DELTT = .001
      DPTPS = TPSMAX
 26   IF (IT.LE.INPERP) GO TO 1
C   COMPLETION OF A PASS --- CHECK OUTPUT REQUIREMENTS
 108  IT = 1
      N2 = PASSNO
C   MODPC = NO. OF COLUMNS OF PRINT ON SUMMARY OUTPUT PAGES --- MUST BE
C   RESET AS PASS NUMBER COUNT (PASSNO) EXCEEDS 10 --- MAX. NO. OF OUTPUT
C   COLUMNS PER PAGE IS 10 --- IOCT IS COUNT OF HOW MANY TIMES SUMMARY
C   OUTPUT HAS BEEN PRINTED --- MAX. OF 3 TIMES (IOCT = 0,1,2)
      IF (IOCT.EQ.0) GO TO 55
      GO TO (56,57), IOCT
 56   MODPC = NPASS-10
      GO TO 55
 57   MODPC = NPASS-20
 55   TWT(PASSNO) = TW
      TM(PASSNO) = TIME
      IF (H2LEAD.OR.TIME.GT.SDTIME) GO TO 28
      GT(PASSNO) = G
      PRESTT(PASSNO) = PREST
C   PASS COMPLETE --- SET UP TEMP, PRESSURE, MOLE FRACTION CURVES FOR
C   PRINTER PLOTS
 28   CALL SETUP (TM,MFH2,MFO2,MFH2O,MFHE,PASSNO,K,KM)
C   STORE TEMP, PRESSURE, MOLE FRACTION PROFILES FOR LATER PRINTOUT
      DO 62 I=1,NOFZ
      MKT = M+MODPC*(I-1)
      TT(MKT) = T(I)
      TP(MKT) = PT(I)
      PP(MKT) = P(I)
      FH2(MKT) = MFH2(I)
      FO2(MKT) = MFO2(I)
      FH2O(MKT) = MFH2O(I)
 62   FHE(MKT) = MFHE(I)
      M = M+1
      IF (ITSTEP.EQ.0) GO TO 27
      DELTT = DELT(PASSNO)
C   CALL OUTPUT EVERY 10TH PASS AND AFTER LAST PASS
```

```
 27   IF (MOD(PASSNO,10).EQ.0.OR.PASSNO.EQ.NPASS) GO TO 63
      PASSNO = PASSNO+1
C   RETURN TO INLET
      GO TO 1
 63   NNAX = NAXIAL
      NAXIAL = NOFZ
      CALL OUTPUT (TM,TT,TP,PP,FH2,FO2,FH2O,FHE,N1,N2,IOCT)
      CALL TMPRNT (TM,TWT,N1,N2)
      IF (.NOT.H2LEAD.AND.TIME.LT.SDTIME) CALL TMPRP(TM,GT,PRESTT,N1,N2)
      NAXIAL = NNAX
      M = 1
      N1 = N2+1
      PASSNO = PASSNO+1
      IF (MINT3.EQ.0) GO TO 73
      WRITE (6,79) TIME
 79   FORMAT ('1' 46X 38('*') / 47X '* GO TO ALL DIFFUSION-CONTROLLED RU
     XN *'  /  47X '*            TIME =',E9.4,' SEC', 7X'*' / 47X, 38('*')
     X      )
      IF (ISHUT.EQ.1) GO TO 72
C   DUMMY READ STATEMENT POSITIONS PAST FINAL INPUT CARD IF SHUTSOWN TIME
C   HAS NOT BEEN REACHED
 71   READ (5,41) DUMMY1,DUMMY2
C   RETURN TO MAIN PROGRAM IF CASE HAS REACHED ALL DIFFUSION CONTROLLED
C   STATUS (MINT3=1) --- EVEN IF AMIDST A PASS
 72   RETURN
 73   IF (PASSNO.GT.NPASS) GO TO 77
C   RETURN TO INLET
      GO TO 1
 77   IF (PUNCH.EQ.1.OR.PUNCH.EQ.3) CALL RPNCH3(TIME,HW,MINT)
      IF (ISHUT.EQ.0) GO TO 71
      RETURN
C
C   ERROR MESSAGES FOLLOW ---
 905  WRITE (6,902) P(IZ),DPDZ,IT,PASSNO,IZ,REGION
 902  FORMAT ('0' 5X, 120('*') // 58X  'ERROR --- ERROR' / 53X 'PRESSURE
     X HAS GONE NEGATIVE' / 48X 'P =',E11.5, 5X 'DPDZ =',E11.5 /
     X        52X 'TIME INCREMENT',I3,' OF PASS',I3 /
     X  51X 'AXIAL STATION', I4, ' ... REGION', I2 // 5X,120('*') )
      CALL EXIT
C
C
C
C    INTERNAL FUNCTION AND SUBROUTINE SUB-PROGRAMS FOLLOW ---
C
C
C
      FUNCTION RSUM (NM1)
      RSUM = 0.
      DO 101 I=1,NM1
 101  RSUM = RSUM+.5*(HW(I+1)*(T(I+1)-TW)+HW(I)*(T(I)-TW))*(Z(I+1)-Z(I))
      RETURN
C
C
      SUBROUTINE PREVUS
C
C   ROUTINE TO SET UP AND INTERPOLATE TEMP, PRESSURE, CONCENTRATION VS Z
C
      DIMENSION  TABLE1(84),TABLE2(84),TABLE3(84),TABLE4(84),ZT(40),
     X           PTT(40),CO2T(40),CH2T(40),CH2OT(40),TABLE5(84),TTI(40)
      DATA (TABLE1(I),I=1,4) / 0., 1., 0., 0. /
      DATA (TABLE2(I),I=1,4) / 0., 1., 0., 0. /
      DATA (TABLE3(I),I=1,4) / 0., 1., 0., 0. /
```

```
      DATA (TABLE4(I),I=1,4) / 0., 1., 0., 0. /
      DATA (TABLE5(I),I=1,4) / 0., 1., 0., 0. /
      CALL RPNCH2 (TIME,NAXT,ZT,PTT,CO2T,CH2T,CH2OT,TTI)
      TABLE1(3) = NAXT
      TABLE2(3) = NAXT
      TABLE3(3) = NAXT
      TABLE4(3) = NAXT
      TABLE5(3) = NAXT
      DO 1 I=1,NAXT
      TABLE1(I+4) = ZT(I)
      TABLE2(I+4) = ZT(I)
      TABLE3(I+4) = ZT(I)
      TABLE4(I+4) = ZT(I)
 1    TABLE5(I+4) = ZT(I)
      DO 2 I=1,NAXT
      TABLE1(I+4+NAXT) = PTT(I)
      TABLE2(I+4+NAXT) = CO2T(I)
      TABLE3(I+4+NAXT) = CH2T(I)
      TABLE4(I+4+NAXT) = CH2OT(I)
 2    TABLE5(I+4+NAXT) = TTI(I)
      DO 3 I=1,NAXIAL
      CALL UNBAR (TABLE1,1,Z(I),0.,PT(I),KK)
      CALL UNBAR (TABLE2,1,Z(I),0.,CIO2(I),KK)
      CALL UNBAR (TABLE3,1,Z(I),0.,CIH2(I),KK)
      CALL UNBAR (TABLE4,1,Z(I),0.,CIH2O(I),KK)
      CALL UNBAR (TABLE5,1,Z(I),0.,T(I),KK)
 3    CIH2OV(I) = 0.
      RETURN
C
C
      SUBROUTINE DELTAT
C
C    ROUTINE TO DETERMINE APPROPRIATE DELTA T INCREMENT BASED ON TEMPERATURE
C                                                             AND PRESSURE
C
      IF (ITSTEP.EQ.1) GO TO 9
      IF (57.*TPSMAX+12.*P(1)-17280.) 10,10,1
 1    IF (57.*TPSMAX+12.*P(1)-19990.) 11,11,2
 2    IF (100.*TPSMAX+21.*P(1)-38000.) 12,12,3
 3    IF (TPSMAX-380.) 13,13,14
 14   DELTT = .001
      JDP = 1
      DPTPS = TPSMAX
      GO TO 9
 13   DELTT = .002
      GO TO 9
 12   DELTT = .01
      GO TO 9
 11   DELTT = .05
      GO TO 9
 10   DELTT = .10
 9    RETURN
      END
```

```
      SUBROUTINE DERIV (CIO2PR,DELTZ,IZ,REGION)
C
C   ROUTINE TO CALCULATE DERIVATIVE EXPRESSIONS IN EACH REGION
C
      INTEGER REGION
      REAL KCH2,KCO2,KCH2O,MH2,MO2,MH2O,MHE,MU,MBAR
      PARAMETER NAX=70, NTI=40
      PARAMETER NPP=30
      COMMON /CB1/ TPP(NPP,NAX),CO2(NPP,NAX),CH2(NPP,NAX),CH2O(NPP,NAX),
     X       T(NAX),P(NAX),PT(NAX),H(NAX),CIH2(NAX),CIO2(NAX),CIH2O(NAX),
     X       CIH2OS(NAX),CIH2OL(NAX),CIH2OV(NAX),CIHE(NAX),DELT(NTI),
     X       PPT(NAX)
      COMMON /CB2/ Z(NAX),ZSSL(NTI),ZSLL(NTI),ZLLV(NTI),ZLVV(NTI)
      COMMON /CB3/ ALPHA,GAMMA,KAPPA,HC,KP,A,DELTT,KCH2,KCO2,KCH2O,TCH2,
     X       TCO2,TCH2O,PCH2,PCO2,PCH2O,MH2,MO2,MH2O,MHE,HR,HA,HA1,HA2,
     X       AW,CW,MW,DC,TA,D0H2,D0O2,D0H2O,ALPHAK,AP,DELTA,G,MU,HS,HL,
     X       HV,TW,RHOM,WH2,WO2,WH2OS,WH2OL,WH2OV,WHE,CFBAR,MBAR,CICP1,
     X       CICP2,CICP3,RHO,RHOV,DELHC,TITPS,DTDZ,DHDZ,TS,TL,DPDZ,DC1DZ,
     X       DC2DZ,DC3SDZ,DC3LDZ,DC3VDZ,DC4DZ,RHOP,CP,DELTP,DPTPS,SDTIME,
     X       PF,TSS,AC,VC,PREST,GSS,MBARSS
      COMMON /CB4/ NOFZ,NPASS,NAXIAL,INPERP,MODPC,MODNO,PUNCH,ITSTEP,
     X       JDP,ISHUT,IHOT
      DATA  DELHF/143.4/
      IF (IZ.EQ.NOFZ) GO TO 10
      DZPR = Z(IZ+1)-Z(IZ-1)
10    FACT1 = (1.-EXP(-KCH2*AP*RHOV*DELTZ/G))/(KCH2*AP*RHOV*DELTZ/G)
      FACT2 = (1.-EXP(-KCO2*AP*RHOV*DELTZ/G))/(KCO2*AP*RHOV*DELTZ/G)
      FACT3 = (1.-EXP(-KCH2O*AP*RHOV*DELTZ/G))/(KCH2O*AP*RHOV*DELTZ/G)
      FACT2P = (1.-EXP(-KCO2*AP*RHOV*DZPR/G))/(KCO2*AP*RHOV*DZPR/G)
      DW1DZ = (-(RHOM*DELTA+KCH2*AP*CICP1)/G)*FACT1
      DW2DZ = (-(RHOM*DELTA*.5*MO2/MH2+KCO2*AP*CICP2)/G)*FACT2
      DW3DZ = ((RHOM*DELTA*MH2O/MH2-KCH2O*AP*CICP3)/G)*FACT3
      DW2DZP = DW2DZ*FACT2P/FACT2
      DW4DZ = 0.
      DPDZ = (DELTA-1.)/(144.*DELTA**3)*(1.75+75.*MU*(1.-DELTA)/(A*G)*
     X       (G*G/(64.4*A*RHO)))
      GO TO (1,2,3,4,5), REGION
C   ICE REGION
 1    HRD = 0.
      DELTAH = DELHC+DELHF
      DW3DZ = DW3DZ/FACT3
      DWDZ3 = 0.
      DW3SDZ = DW3DZ
      DW3LDZ = 0.
      DW3VDZ = 0.
      W3 = 0.
      HFACT = 0.
      RHO1 = RHO/(1.-WH2OS)
      DWJDZ = DW3DZ
      RHO2 = RHOV/RHO
      GO TO 6
C   ICE-LIQUID REGION
 2    HRD = 0.
      HSL = H(IZ-1)+DELHF*WH2OS
      DELTAH = DELHC+DELHF*(HSL-H(IZ-1))/(HSL-HS)
      DW3DZ = DW3DZ/FACT3
      DWDZ3 = 0.
      DW3SDZ = DW3DZ*((HSL-H(IZ-1))/(HSL-HS))-DHDZ/(HSL-HS)
```

```
      SUBROUTINE PCALCT (CSH2,CSO2,CSH2O,TPS,DCTEMP,IT,ITP,IZ,PASSNO,
     X         NCON,DEBUG)
C
C     ROUTINE TO DO PARTICLE ANALYSIS OF TEMP, CONCENTRATION DISTRIBUTIONS
C     AT PRE-STEADY STATE (TRANSIENT) CONDITIONS
C
      LOGICAL DEBUG
      INTEGER PASSNO,PUNCH
      REAL  LAMDA,LAMDA0,KAPPA,KP,KCO2,KCH2,KCH2O,MO2,MH2,MH2O
      PARAMETER NAX=70, NTI=40
      PARAMETER NPP=30, NRTS=200
      COMMON /CB1/ TPP(NPP,NAX),CO2(NPP,NAX),CH2(NPP,NAX),CH2O(NPP,NAX),
     X         T(NAX),P(NAX),PT(NAX),H(NAX),CIH2(NAX),CIO2(NAX),CIH2O(NAX),
     X         CIH2OS(NAX),CIH2OL(NAX),CIH2OV(NAX),CIHE(NAX),DELT(NTI),
     X         PPT(NAX)
      COMMON /CB3/ ALPHA,GAMMA,KAPPA,HC,KP,A,DELTT,KCH2,KCO2,KCH2O,TCH2,
     X         TCO2,TCH2O,PCH2,PCO2,PCH2O,MH2,MO2,MH2O,MHE,HR,HA,HA1,HA2,
     X         AW,CW,MW,DC,TA,DOH2,DOO2,DOH2O,ALPHAK,AP,DELTA,G,MU,HS,HL,
     X         HV,TW,RHOM,WH2,WO2,WH2OS,WH2OL,WH2OV,WHE,CFBAR,MBAR,CICP1,
     X         CICP2,CICP3,RHO,RHOV,DELHC,TITPS,DTDZ,DHDZ,TS,TL,DPDZ,DC1DZ,
     X         DC2DZ,DC3SDZ,DC3LDZ,DC3VDZ,DC4DZ,RHOP,CP,DELTP,DPTPS,SDTIME,
     X         PF,TSS,AC,VC,PREST,GSS,MBARSS
      COMMON /CB4/ NOFZ,NPASS,NAXIAL,INPERP,MODPC,MODNO,PUNCH,ITSTEP,
     X         JDP,ISHUT,IHOT
      DIMENSION GRT(NPP,NPP),GRTI(NPP,NPP),GRTTI(NPP,NPP),GRO2(NPP,NPP),
     X         GRO2I(NPP,NPP),GRO2TI(NPP,NPP),GRH2(NPP,NPP),GRH2I(NPP,NPP),
     X         GRH2TI(NPP,NPP),TP(NPP,2),CPO2(NPP,2),CPH2(NPP,2),CPH2O(NPP,
     X         2),RHET(NPP,2),LAMDA(NPP),LAMDA0(NPP),RATE(NPP),RTT(NRTS),
     X         RTO2(NRTS),RTH2(NRTS),F(NPP)
      DATA  PI/3.1415927/,RAOP/.656E-7/,TOL/.0001/,MAX/25/
C
C     PARTICLE ANALYSIS NOMLNCLATURE FOR  O2 + 2H2 --- 2H2O  REACTION
C
C          CSO2  : PARTICLE SURFACE CONCENTRATION OF O2
C          CSH2  : PARTICLE SURFACE CONCENTRATION OF H2
C          CSH2O : PARTICLE SURFACE CONCENTRATION OF H2O
C          TS    : PARTICLE SURFACE TEMPERATURE
C          CPO2(I,1)   : PARTICLE CONCENTRATION DISTRIBUTION OF O2 AT TIME 1
C          CPH2(I,1)   : PARTICLE CONCENTRATION DISTRIBUTION OF H2 AT TIME 1
C          CPH2O(I,1)  : PARTICLE CONCENTRATION DISTRIBUTION OF H2O AT TIME 1
C          TP(I,1)     : PARTICLE TEMPERATURE DISTRIBUTION AT TIME 1
C          CPO2(I,2)   : PARTICLE CONCENTRATION DISTRIBUTION OF O2 AT TIME 2
C                                                                   (GUESSED)
C          CPO2A(I)    : PARTICLE CONCENTRATION DISTRIBUTION OF O2 AT TIME 2
C                                                                   (CALCULATED)
C          CPH2(I,2)   : PARTICLE CONCENTRATION DISTRIBUTION OF H2 AT TIME 2
C          CPH2O(I,2)  : PARTICLE CONCENTRATION DISTRIBUTION OF H2O AT TIME 2
C          TP(I,2)     : PARTICLE TEMPERATURE DISTRIBUTION AT TIME 2
C
C          CIH2  : INTERSTITIAL CONCENTRATION OF H2
C          CIO2  : INTERSTITIAL CONCENTRATION OF O2
C          CIH2O : INTERSTITIAL CONCENTRATION OF H2O
C          T     : INTERSTITIAL TEMPERATURE
C          P     : INTERSTITIAL PRESSURE
C
C          DO2   : KNUDSEN
C          DH2   :  DIFFUSION
C          DH2O  :   COEFFICIENTS
```

```
C
C         RTO2(N) : ARRAYS CONTAINING
C         RTH2(N) :  CHARACTERISTIC ROOTS OF
C         RTH2O(N):   THE EQUATION   X*COT(X)+(PHI*A-1) = 0
C         RTT(N)  :    HEAT TRANSFER (RTT), AND MASS TRANSFER (RTO2,RTH2,RTH2O)
C
C         LAMDA(I) : NORMALIZED RADIAL POSITIONS
C         LAMDAO(I):  WITHIN THE CATALYST PARTICLE
C
C         GRT    : GREEN'S FUNCTIONS USED IN PARTICLE
C         GRTI   :  TEMPERATURE DISTRIBUTION CALCULATIONS
C         GRO2   : GREEN'S FUNCTIONS USED IN PARTICLE CALCULATION
C         GRO2I  :  OF OXYGEN DISTRIBUTION
C         GRH2   : GREEN'S FUNCTIONS USED IN PARTICLE CALCULATION
C         GRH2I  :  OF HYDROGEN DISTRIBUTION
C         GRH2O  : GREEN'S FUNCTIONS USED IN PARTICLE CALCULATION
C         GRH2OI:  OF H2O DISTRIBUTION
C
C         RADP   : PORE RADIUS OF CATALYST PELLET
C         TOL    : TOLERANCE USED FOR CONVERGENCE CHECK ON O2 PROFILE
C         MAX    : MAXIMUM NO. OF ITERATIONS ALLOWED
C         NPP    : NO. OF POINTS/PROFILE WITHIN CATALYST PELLET
C         NRTT   : MAXIMUM NUMBER OF TERMS USED IN SERIES EXPANSION FOR
C         NRTO2 :  OBTAINING GREEN'S FUNCTIONS ...
C         NRTH2 :   NRTT --- TEMPERATURE,  NRTO2 --- OXYGEN,
C         NRTH2O:    NRTH2 --- HYDROGEN,  NRTH2O --- WATER
C
      DKF(RADP,T,WT) = 237.*RADP*SQRT(T/WT)
      DF(PC,PCH2,WT,WTH2,T,P,TC,TCH2) = .442E-6*CBRT(PC*PCH2)*SQRT(1./W
     X      +1./WTH2)*T**1.823 / (P*(TC*TCH2)**.495)
      R = A
      DT = DELTT
      CAPPA = KAPPA
      NP1 = NPP-1
      ITER = 0
      KOUNT = 0
      NCON = 0
      IRATE = 0
      NEWDT = 0
      IF (PASSNO.EQ.1.AND.IT.EQ.1) GO TO 21
      IF (ITSTEP.EQ.1.AND.PASSNO.EQ.1) GO TO 20
      IF (ITSTEP.EQ.1.AND.JDP.EQ.0) GO TO 25
      IF (JDP.EQ.0) GO TO 28
      TPSX = DPTPS+50.
      IF (PT(IZ).GT.TPSX) GO TO 23
C   CHECK TIME INCREMENT WITH PREVIOUS DELTT --- MUST CALCULATE NEW GREEN'S
C   FUNCTIONS IF DIFFERENT
 28   IF (DELTP-DELTT) 21,20,21
 25   IF (DELT(PASSNO)-DELT(PASSNO-1)) 21,20,21
C   NEWDT IS INDICATOR FOR NEW TIME INCREMENT ...
C            NEWDT = 0 --- INCREMENT UNCHANGED
C            NEWDT = 1 --- NEW INCREMENT IN USE
 23   DPTPS = PT(IZ)
 21   NEWDT = 1
 20   IF (PUNCH.EQ.2.OR.PUNCH.EQ.3) GO TO 93
      IF (PASSNO.EQ.1.AND.IT.EQ.1) GO TO 43
C   SET PARTICLE CONCENTRATION, TEMP, RHET PROFILES FROM SURFACE VALUES
C   CALCULATED AT PREVIOUS TIME INCREMENT
 93   DO 42 I=1,NPP
      CPO2(I,1) = CO2(I,IZ)
      CPH2(I,1) = CH2(I,IZ)
      CPH2O(I,1) = CH2O(I,IZ)
```

```
      TP(I,1) = TPP(I,IZ)
      RHET(I,1) = ALPHAK*CPO2(I,1)**.8*EXP(-GAMMA/TP(I,1))
 42   RHET(I,2) = RHET(I,1)
      GO TO 44
 43   DO 1 I=1,NPP
      CPO2(I,1) = CSO2
      CPH2(I,1) = CSH2
      CPH2O(I,1) = CSH2O
      RHET(I,1) = ALPHAK*CPO2(I,1)**.8*EXP(-GAMMA/TP(I,1))
      RHET(I,2) = RHET(I,1)
 1    TP(I,1) = TPS
 44   NRTT = A*SQRT(23.03/(KAPPA*DELTT))/PI+.5
      IF (NRTT.GT.NRTS) NRTT=NRTS
      PHIT = HC/KP
     SOLVE FOR ROOTS OF EQUATION X*COT(X)+C = 0.   ... C=HC/KP*A-1.
      C = PHIT*A-1.
C                                                    HEAT TRANSFER
      RLOWER = PI/2.
      RUPPER = PI
      DO 2 N=1,NRTT
      CALL ROOT (RLOWER,RUPPER,C,RTT(N),N)
      RLOWER = RLOWER+PI
 2    RUPPER = RTT(N)+PI
      DKO2 = DKF(RADP,T(IZ),MO2)
      DKH2 = DKF(RADP,T(IZ),MH2)
      IF (P(IZ).LT..001) GO TO 18
      IF (PUNCH.EQ.2.OR.PUNCH.EQ.3) GO TO 71
      IF (PASSNO.EQ.1.AND.IT.EQ.1) GO TO 26
 71   TEMP = PT(IZ)
      GO TO 24
 26   TEMP = T(IZ)
 24   DO2 = DF(PCO2,PCH2,MO2,MH2,TEMP,P(IZ),TCO2,TCH2)
      DH2 = DF(PCH2,PCH2,MH2,MH2,TEMP,P(IZ),TCH2,TCH2)
      DO2 = DO2*(1.-EXP(-DKO2/DO2))
      DH2 = DH2*(1.-EXP(-DKH2/DH2))
      GO TO 50
 18   DO2 = DKO2
      DH2 = DKH2
 50   PHIO2 = KCO2/DO2
      PHIH2 = KCH2/DH2
C    SOLVE FOR ROOTS OF THE EQUATION X*COT(X)+C = 0. --- C=KCH2/DH2*A-1.,
C                                                    C=KCO2/DO2*A-1.,
C                                                    C=KCH2O/DH2O*A-1.
 6    NRTO2 = A*SQRT(23.03/(DO2*DELTT))/PI+.5
      NRTH2 = A*SQRT(23.03/(DH2*DELTT))/PI+.5
      IF (NRTO2.GT.NRTS) NRTO2=NRTS
      IF (NRTH2.GT.NRTS) NRTH2=NRTS
      RLOWER = PI/2.
      RUPPER = PI
C                                                    MASS TRANSFER
      CA = PHIO2*A-1.
      DO 3 N=1,NRTO2
      CALL ROOT (RLOWER,RUPPER,CA,RTO2(N),N)
      RLOWER = RLOWER+PI
 3    RUPPER = RTO2(N)+PI
      CB = PHIH2*A-1.
      RLOWER = PI/2.
      RUPPER = PI
      DO 4 N=1,NRTH2
      CALL ROOT (RLOWER,RUPPER,CB,RTH2(N),N)
      RLOWER = RLOWER+PI
 4    RUPPER = RTH2(N)+PI
```

```
C   SET UP RADIAL STATIONS WITHIN PARTICLE ON FIRST ENTRY TO ROUTINE
      DEL = 1./FLOAT(NPP)
      LAMDA(1) = 0.
      LAMDA0(1) = 0.
      DO 8 I=2,NP1
      LAMDA(I) = LAMDA(I-1)+DEL
 8    LAMDA0(I) = LAMDA(I)
      LAMDA(NPP) = 1.0
      LAMDA0(NPP) = 1.0
C
C   CALCULATE INITIAL GUESS FOR PARTICLE CONCENTRATION DISTRIBUTION OF O2
C
 19   NT = NRTO2
      DO 150 L=1,NPP
      DO 100 I=2,NPP
      IF (NEWDT.EQ.0.OR.ITP.EQ.IT.OR.ITER.GT.0) GO TO 9
      IF (I.LT.L) GO TO 7
      CALL GREEN (LAMDA(L),LAMDA0(I),RTO2,DO2,PHIO2,GRO2(L,I),
     X                    GRO2I(L,I),GRO2TI(L,I),DT,R,NT,L)
      GO TO 9
C   GREEN'S FUNCTIONS SYMMETRIC W.R.T. LAMDA, LAMDA0 --- G(L,L0)=G(L0,L)
 7    GRO2(L,I) = GRO2(I,L)
      GRO2I(L,I) = GRO2I(I,L)
      GRO2TI(L,I) = GRO2TI(I,L)
 9    IF (L.EQ.1) GO TO 30
      F(I) = 2.*LAMDA0(I)/LAMDA(L)*(-A**4/DO2**2*(RHET(I,2)-RHET(I,1))/
     X        DELTT*GRO2TI(L,I)-A**2/DO2*RHET(I,1)*GRO2I(L,I)+
     X        (CPO2(I,1)-CIO2(IZ))*GRO2(L,I))
      GO TO 100
 30   F(I) = 2.*(-A**4/DO2**2*(RHET(I,2)-RHET(I,1))/DELTT*GRO2TI(L,I)-A*
     X        *2/DO2*RHET(I,1)*GRO2I(L,I)+(CPO2(I,1)-CIO2(IZ))*GRO2(L,I))
 100  CONTINUE
      RSUM = 0.
      DO 133 I=1,NP1
 133  RSUM = RSUM+.5*(F(I)+F(I+1))*(LAMDA(I+1)-LAMDA(I))
      CPO2(L,2) = CIO2(IZ)+RSUM
      IF (CPO2(L,2).LT.0.) CPO2(L,2) = 0.
      CO2(L,IZ) = CPO2(L,2)
 150  CONTINUE
C
C   CALCULATE PARTICLE TEMPERATURE DISTRIBUTION
C
 15   NT = NRTT
      DO 650 L=1,NPP
      DO 600 I=2,NPP
      IF (NEWDT.EQ.0.OR.ITP.EQ.IT.OR.ITER.GT.0) GO TO 10
      IF (I.LT.L) GO TO 11
      CALL GREEN (LAMDA(L),LAMDA0(I),RTT,CAPPA,PHIT,GRT(L,I),
     X                    GRTI(L,I),GRTTI(L,I),DT,R,NT,L)
      GO TO 10
C   GREEN'S FUNCTIONS SYMMETRIC W.R.T. LAMDA AND LAMDA0 --- G(L,L0)=G(L0,L)
 11   GRT(L,I) = GRT(I,L)
      GRTI(L,I) = GRTI(I,L)
      GRTTI(L,I) = GRTTI(I,L)
C   CALCULATE INTEGRAND FUNCTION
 10   IF (L.EQ.1) GO TO 31
      F(I) = 2.*LAMDA0(I)/LAMDA(L)*((-HR*A**4/(KAPPA*KP))*(RHET(I,2)-
     X        RHET(I,1))/DELTT*GRTTI(L,I)-HR*A**2/KP*RHET(I,1)*GRTI(L,I)+
     X        (TP(I,1)-T(IZ))*GRT(L,I))
      GO TO 600
 31   F(I) = 2.*((-HR*A**4/(KAPPA*KP))*(RHET(I,2)-RHET(I,1))/DELTT*
     X        GRTTI(L,I)-HR*A**2/KP*RHET(I,1)*GRTI(L,I)+(TP(I,1)-T(IZ))*
```

```
     X        GRT(L,I))
 600  CONTINUE
C   CALCULATE INTEGRAL EXPRESSION FOR GIVEN LAMDA, ALL LAMDA0'S.
      RSUM = 0.
      DO 55 I=1,NP1
 55   RSUM = RSUM+.5*(F(I)+F(I+1))*(LAMDA(I+1)-LAMDA(I))
      TP(L,2) = T(IZ)+RSUM
      TPP(L,IZ) = TP(L,2)
      RATE(L) = ALPHAK*CPO2(L,2)**.8*EXP(-GAMMA/TP(L,2))
 650  CONTINUE
C
C   CHECK FOR CONVERGENCE
C
      DO 49 I=1,NPP
      IF (ABS(RHET(I,2)-RATE(I))-.02*RATE(I)) 49,49,32
 32   IF (RATE(I)-.02*RATE(NPP)) 49,49,27
 49   CONTINUE
C
C   CONVERGENCE --- CALCULATE CONCENTRATIONS FOR H2, H20
C   CALCULATE PARTICLE CONCENTRATION DISTRIBUTION FOR H2
C
      NT = NRTH2
      DO 550 L=1,NPP
      DO 500 I=2,NPP
      IF (NEWDT.EQ.0.OR.ITP.EQ.IT) GO TO 13
      IF (I.LT.L) GO TO 12
      CALL GREEN (LAMDA(L),LAMDA0(I),RTH2,DH2,PHIH2,GRH2(L,I),
     X                GRH2I(L,I),GRH2TI(L,I),DT,R,NT,L)
      GO TO 13
C   GREEN'S FUNCTIONS SYMMETRIC W.R.T. LAMDA AND LAMDA0 --- G(L,L0)=G(L0,L)
 12   GRH2(L,I) = GRH2(I,L)
      GRH2I(L,I) = GRH2I(I,L)
      GRH2TI(L,I) = GRH2TI(I,L)
 13   IF (L.EQ.1) GO TO 33
      F(I) = 2.*LAMDA0(I)/LAMDA(L)*(-A**4/DH2**2*2.*MH2/MO2*
     X        (RHET(I,2)-RHET(I,1))/DELTT*GRH2TI(L,I)-A**2/DH2*2.*MH2/
     X        MO2*RHET(I,1)*GRH2I(L,I)+(CPH2(I,1)-CIH2(IZ))*GRH2(L,I))
      GO TO 500
 33   F(I) = 2.*(-A**4/DH2**2*2.*MH2/MO2*(RHET(I,2)-RHET(I,1))/DELTT
     X        *GRH2TI(L,I)-A**2/DH2*2.*MH2/MO2*RHET(I,1)*GRH2I(L,I)
     X        +(CPH2(I,1)-CIH2(IZ))*GRH2(L,I))
 500  CONTINUE
      RSUM = 0.
      DO 75 I=1,NP1
 75   RSUM = RSUM+.5*(F(I)+F(I+1))*(LAMDA(I+1)-LAMDA(I))
      CPH2(L,2) = CIH2(IZ)+RSUM
      CH2(L,IZ) = CPH2(L,2)
 550  CONTINUE
      CPH20(NPP,2) = 0.
C   SAVE SURFACE VALUES OF TEMP, CONCENTRATION
      CS02 = CPO2(NPP,2)
      CSH2 = CPH2(NPP,2)
      CSH20 = CPH20(NPP,2)
      TPS = TP(NPP,2)
      ITER = ITER+1
      IF (TPS-DCTEMP) 77,77,78
 78   NCON = 1
      GO TO 99
 77   IF (CS02) 880,76,76
 76   IF (CSH2) 881,99,99
 99   RETURN
C
```

```
C   NO CONVERGENCE ..... SAVE CALC. RHET PROFILE AND REPEAT TEMP AND CPO2 CALCS
C
 27    IF (KOUNT.EQ.1) GO TO 38
       IF (ITER.GT.0) GO TO 35
       IF (RATE(NPP).GT.RHET(NPP,2)) IRATE=1
       GO TO 36
 35    IF ((RATE(NPP).GT.RHET(NPP,2).AND.IRATE.EQ.0).OR.(RATE(NPP).LT.
      X       RHET(NPP,2).AND.IRATE.EQ.1)) GO TO 38
 36    DO 37 I=1,NPP
 37    RHET(I,2) = RATE(I)
       GO TO 41
 38    DO 39 I=1,NPP
 39    RHET(I,2) = .5*(RATE(I)+RHET(I,2))
       KOUNT = 1
 41    ITER = ITER+1
       IF (ITER.GE.MAX) GO TO 86
       GO TO 19
 86    CSO2 = CPO2(NPP,2)
       CSH2 = CPH2(NPP,2)
       CSH2O = CPH2O(NPP,2)
       TPS = TP(NPP,2)
       IF (TPS-DCTEMP) 161,161,162
 162   NCON = 1
       RETURN
 161   IF (CSO2) 880,90,90
 90    IF (CSH2) 881,92,92
 92    RETURN
C
C   ERROR STATEMENTS FOLLOW ...
C
 880   WRITE (6,890) CSO2,CSH2,CSH2O,TPS,IT,PASSNO
 890   FORMAT ('0' 5X, 120('*') // 58X 'ERROR --- ERROR' / 38X 'PARTICLE
      XSURFACE CONCENTRATION OF O2 HAS GONE NEGATIVE' / 24X 'CSO2 =',
      X        E11.5, 5X, 'CSH2 =',E11.5, 5X, 'CSH2O =',E11.5, 5X, 'TPS =',
      X        E11.5 / 52X 'TIME INCREMENT',I3,' OF PASS',I3 // 120('*') )
       CALL EXIT
 881   WRITE (6,891) CSH2,CSO2,CSH2O,TPS,IT,PASSNO
 891   FORMAT ('0' 5X, 120('*') // 58X 'ERROR --- ERROR' / 38X 'PARTICLE
      XSURFACE CONCENTRATION OF H2 HAS GONE NEGATIVE' / 24X 'CSH2 =',
      X        E11.5, 5X, 'CSO2 =',E11.5, 5X, 'CSH2O =',E11.5, 5X, 'TPS =',
      X        E11.5 / 52X 'TIME INCREMENT',I3,' OF PASS',I3 // 120('*') )
       CALL EXIT
       END
```

```
      SUBROUTINE PCALCS (TPS,CSO2,CSH2,CSH2O,CIO2PR,IZ,MINT)
C
C    ROUTINE TO DO PARTICLE SURFACE TEMPERATURE CALCULATIONS AT STEADY STATE
C
      INTEGER PUNCH
      REAL KCO2,KCH2,KCH2O,MO2,MH2,MH2O
      PARAMETER NAX=70, NTI=40
      PARAMETER NPP=30, NRTS=200
      COMMON /CB1/ TPP(NPP,NAX),CO2(NPP,NAX),CH2(NPP,NAX),CH2O(NPP,NAX),
     X       T(NAX),P(NAX),PT(NAX),H(NAX),CIH2(NAX),CIO2(NAX),CIH2O(NAX),
     X       CIH2OS(NAX),CIH2OL(NAX),CIH2OV(NAX),CIHE(NAX),DELT(NTI),
     X       PPT(NAX)
      COMMON /CB3/ ALPHA,GAMMA,KAPPA,HC,KP,A,DELTT,KCH2,KCO2,KCH2O,TCH2,
     X       TCO2,TCH2O,PCH2,PCO2,PCH2O,MH2,MO2,MH2O,MHE,HR,HA,HA1,HA2,
     X       AW,CW,MW,DC,TA,DOH2,DOO2,DOH2O,ALPHAK,AP,DELTA,G,MU,HS,HL,
     X       HV,TW,RHOM,WH2,WO2,WH2OS,WH2OL,WH2OV,WHE,CFBAR,MBAR,CICP1,
     X       CICP2,CICP3,RHO,RHOV,DELHC,TITPS,DTDZ,DHDZ,TS,TL,DPDZ,DC1DZ,
     X       DC2DZ,DC3SDZ,DC3LDZ,DC3VDZ,DC4DZ,RHOP,CP,DELTP,DPTPS,SDTIME,
     X       PF,TSS,AC,VC,PREST,GSS,MBARSS
      COMMON /CB4/ NOFZ,NPASS,NAXIAL,INPERP,MODPC,MODNO,PUNCH,ITSTEP,
     X       JDP,ISHUT,IHOT
      COMMON /TABLES/ AVSZ(40),APVSZ(40),DELVSZ(40),HRVST(36),TC1(22),
     X       TC2(20),TC3V(20),TC4(18),MU1VST(34),MU2VST(34),MU3VST(32),
     X       MU4VST(34),CF1VST(34),CF2VST(34),CF3VST(34),CF3SVT(20),
     X       CF4VST(20),VPVST(60),TVSVP(48),DHCVST(24)
      CALL UNBAR (HRVST,1,PT(IZ),0.,HR,KK)
      GO TO (1,1,1,2), PUNCH
    2 IF (IZ.NE.2) GO TO 3
      CIO2(IZ) = CIO2(IZ-1)
      GO TO 1
    3 CIO2(IZ) = CIO2PR
    1 IF (CIO2(IZ).LT.0.) CIO2(IZ)=0.
      DTPSDT = 3./(A*RHOP*CP)*(HC*(T(IZ)-PT(IZ))-HR*KCO2*CIO2(IZ-1))
      EXTRM = (1.-EXP(-3.*HC*DELTT/(A*RHOP*CP)))/(3.*HC/(A*RHOP*CP))
      TPS = PT(IZ)+DTPSDT*(1.-EXP(-3.*HC*DELTT/(A*RHOP*CP)))/
     X                    (3.*HC/(A*RHOP*CP))
      CSO2  = 0.
      CSH2  = CIH2(IZ-1)-(KCO2/KCH2*MH2/(MO2*.5)*(CIO2(IZ-1)-CSO2))
      CSH2O = CIH2OV(IZ-1)-(KCO2/KCH2O*MH2O/(MO2*.5)*(CSO2-CIO2(IZ-1)))
      RETURN
      END
```

```
      DW3LDZ = DW3DZ*((H(IZ-1)-HS)/(HSL-HS))+DHDZ/(HSL-HS)
      DW3VDZ = 0.
      W3 = 0.
      HFACT = -KCO2*AP*CICP3*DELHF/(G*(HSL-H(IZ-1)))
      RHO1 = RHO/(1.-WH2OS-WH2OL)
      DWJDZ = DW3SDZ+DW3LDZ
      RHO2 = RHOV/RHO
      GO TO 6
C     LIQUID REGION
3     HRD = 0.
      DELTAH = DELHC
      DW3DZ = DW3DZ/FACT3
      DWDZ3 = 0.
      DW3SDZ = 0.
      DW3LDZ = DW3DZ
      DW3VDZ = 0.
      W3 = 0.
      HFACT = 0.
      RHO1 = RHO/(1.-WH2OL)
      DWJDZ = DW3DZ
      RHO2 = RHOV/RHO
      GO TO 6
C     LIQUID-VAPOR REGION
4     HRD = 0.
      HLV = H(IZ-1)+DELHC*WH2OL
      DELTAH = DELHC*(HLV-H(IZ-1))/(HLV-HL)
      DW3DZ = DW3DZ/FACT3
      DW3SDZ = 0.
      DW3LDZ = DW3DZ*((HLV-H(IZ-1))/(HLV-HL))-DHDZ/(HLV-HL)
      DW3VDZ = DW3DZ*((H(IZ-1)-HL) /(HLV-HL))+DHDZ/(HLV-HL)
      DWDZ3 = DW3VDZ
      W3 = WH2OV
      HFACT = -KCO2*AP*CICP3*DELHC/(G*(HLV-H(IZ-1)))
      RHO1 = RHO/(1.-WH2OL)
      DWJDZ = DW3LDZ
      RHO2 = RHOV/RHO
      GO TO 6
C     VAPOR REGION
5     HRD = HR*RHOM*DELTA/G
      DELTAH = 0.
      DWDZ3 = DW3DZ
      DW3SDZ = 0.
      DW3LDZ = 0.
      DW3VDZ = DW3DZ
      W3 = WH2OV
      HFACT = 0.
      RHO1 = RHO
      DWJDZ = 0.
      RHO2 = 1.
6     FACTOR = (1.-EXP(-(HC*AP/(G*CFBAR)+HFACT)*DELTZ))/((HC*AP/(G*
     X        CFBAR)+HFACT)*DELTZ)
      DHDZ = (-HRD-HC*AP*TITPS/G-KCH2O*AP*CICP3*DELTAH/G-4.*HC
     X          *(T(IZ-1)-TW)/(G*DC))*FACTOR
      DTDZ = DHDZ/CFBAR
      GO TO (7,8,7,8,7), REGION
7     TDZ = DTDZ/T(IZ-1)
      GO TO 9
8     TDZ = 0.
9     DMBRDZ = -MBAR*(DW1DZ/MH2+DW2DZ/MO2+DWDZ3/MH2O)/(WH2/MH2+WO2/MO2+
     X        W3/MH2O+WHE/MHE)
      DRHODZ = RHO1*(DWJDZ+RHO2*(DPDZ/P(IZ-1)+DMBRDZ/MBAR -TDZ))
      RCOR = -RHO1/RHO*(DWJDZ+RHO2*(DPDZ/P(IZ-1)+DMBRDZ/MBAR-TDZ))
```

```
DRODZP = DRHODZ*(1.-EXP(-RCOR*DZPR))/(RCOR*DZPR)
DC2DZP = RHO*DW2DZP+WO2*DRODZP
CIO2PR = CIO2(IZ-1)+DC2DZP*DZPR
DRHODZ = DRHODZ*(1.-EXP(-RCOR*DELTZ))/(RCOR*DELTZ)
DC1DZ = RHO*DW1DZ+WH2*DRHODZ
DC2DZ = RHO*DW2DZ+WO2*DRHODZ
DC3SDZ = RHO*DW3SDZ+WH2OS*DRHODZ
DC3LDZ = RHO*DW3LDZ+WH2OL*DRHODZ
DC3VDZ = RHO*DW3VDZ+WH2OV*DRHODZ
DC4DZ = WHE*DRHODZ
RETURN
END
```

```
      SUBROUTINE GREEN (LAMDA,LAMDA0,RT,D,PHI,GR,GRI,GRTI,DT,A,NR,LL)
C
C     ROUTINE TO CALCULATE GREEN'S FUNCTIONS NEEDED FOR TRANSIENT
C     PARTICLE ANALYSIS
C
      REAL LAMDA,LAMDA0
      DIMENSION RT(1)
      SUM1 = 0.
      SUM2 = 0.
      SUM3 = 0.
      SUML1 = 0.
      SUML2 = 0.
      SUML3 = 0.
      DO 2 I=1,NR
      RTERM = (RT(I)**2+(PHI*A-1.)**2)/(RT(I)**2+PHI*A*(PHI*A-1.))
      RAD = RT(I)*LAMDA
      RAD0 = RT(I)*LAMDA0
      SINL = SIN(RAD)
      SINL0 = SIN(RAD0)
      EXTRM1 = EXP(-(RT(I)/A)**2*D*DT)
      EXTRM2 = EXTRM1/RT(I)**2
      EXTRM3 = (1.-EXTRM1)/RT(I)**4
      IF (LL.EQ.1) GO TO 1
      SUM1 = SUM1+RTERM*SINL*SINL0*EXTRM1
      SUM2 = SUM2+RTERM*SINL*SINL0*EXTRM2
      SUM3 = SUM3+RTERM*SINL*SINL0*EXTRM3
      GO TO 2
    1 SUML1 = SUML1+LAMDA0*RTERM*RT(I)*SINL0*EXTRM1
      SUML2 = SUML2+LAMDA0*RTERM*1./RT(I)*SINL0*EXTRM1
      SUML3 = SUML3+LAMDA0*RTERM*1./RT(I)**3*SINL0*(1.-EXTRM1)
    2 CONTINUE
      IF (LL.EQ.1) GO TO 4
      GR = SUM1
      IF (LAMDA0.GT.LAMDA) GO TO 3
      S = 0.5*LAMDA*LAMDA0*(1./LAMDA-(PHI*A-1.)/(PHI*A))
      GRI = S - SUM2
      GRTI = D*DT/A**2*S - SUM3
      RETURN
    3 S = 0.5*LAMDA*LAMDA0*(1./LAMDA0-(PHI*A-1.)/(PHI*A))
      GRI = S - SUM2
      GRTI = D*DT/A**2*S - SUM3
      RETURN
    4 GR = SUML1
      S = LAMDA0/2.-LAMDA0**2/2.*((PHI*A-1.)/(PHI*A))
      GRI = S - SUML2
      GRTI = D*DT/A**2*S - SUML3
      RETURN
      END
```

```
      SUBROUTINE ROOT (RLOWER,RUPPER,C,RTO,N)
C
C   ROUTINE TO FIND ROOTS OF THE CHARACTERISTIC EQUATION X*COT(X)+C = 0.
C                     MODIFIED METHOD OF SUCCESSIVE SUBSTITUTIONS
C
      I = 0
      RTLO = RLOWER
      RTHI = RUPPER
 1    IF (ABS(RTHI-RTLO).LT.2.E-5) GO TO 9
      I = I+1
      IF (I.GT.25) GO TO 7
      RTO = (RTLO+RTHI)/2.
      RT = -C*TAN(RTO)
      IF (RT-RUPPER) 2,2,4
 2    IF (RT-RLOWER) 5,3,3
 3    IF (ABS((RT-RTO)/RT)-.00005) 9,9,6
 4    RTLO = RTO
      GO TO 1
 5    RTHI = RTO
      GO TO 1
 6    IF (RT.LT.RTO) RTHI=RTO
      IF (RT.GT.RTO) RTLO=RTO
      GO TO 1
 7    WRITE (6,8) N
 8    FORMAT ('0' // 21X, 'NO CONVERGENCE ON ROOT NUMBER',I3,' AFTER 25
     XITERATIONS --- USE VALUE CALCULATED ON 25TH ITERATION')
 9    RETURN
      END
```

```
      CIO2(K) = CCIO2(I)
      CIH2O(K) = CCH2O(I)
      K = K-1
   50 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE INSERT (ZIF,IZ)
C
C   ROUTINE TO INSERT INTERFACE AXIAL POSITIONS INTO ORIGINAL Z ARRAY
C
      PARAMETER NAX=70, NTI=40
      PARAMETER NPP=30
      COMMON /CB1/ TPP(NPP,NAX),CO2(NPP,NAX),CH2(NPP,NAX),CH2O(NPP,NAX),
     X       T(NAX),P(NAX),PT(NAX),H(NAX),CIH2(NAX),CIO2(NAX),CIH2O(NAX),
     X       CIH2OS(NAX),CIH2OL(NAX),CIH2OV(NAX),CIHE(NAX),DELT(NTI),
     X       PPT(NAX)
      COMMON /CB2/ Z(NAX),ZSSL(NTI),ZSLL(NTI),ZLLV(NTI),ZLVV(NTI)
      COMMON /CB3/ ALPHA,GAMMA,KAPPA,HC,KP,A,DELTT,KCH2,KCO2,KCH2O,TCH2,
     X       TCO2,TCH2O,PCH2,PCO2,PCH2O,MH2,MO2,MH2O,MHE,HR,HA,HA1,HA2,
     X       AW,CW,MW,DC,TA,DOH2,DOO2,DOH2O,ALPHAK,AP,DELTA,G,MU,HS,HL,
     X       HV,TW,RHOM,WH2,WO2,WH2OS,WH2OL,WH2OV,WHE,CFBAR,MBAR,CICP1,
     X       CICP2,CICP3,RHO,RHOV,DELHC,TITPS,DTDZ,DHDZ,TS,TL,DPDZ,DC1DZ,
     X       DC2DZ,DC3SDZ,DC3LDZ,DC3VDZ,DC4DZ,RHOP,CP,DELTP,DPTPS,SDTIME,
     X       PF,TSS,AC,VC,PREST,GSS,MBARSS
      COMMON /CB4/ NOFZ,NPASS,NAXIAL,INPERP,MODPC,MODNO,PUNCH,ITSTEP,
     X       JDP,ISHUT,IHOT
      DIMENSION ZZ(NAX),PTZ(NAX),TIZ(NAX),CIO2Z(NAX),CIH2Z(NAX)
      DO 50 I=1,NOFZ
      PTZ(I) = PT(I)
      TIZ(I) = T(I)
      CIO2Z(I) = CIO2(I)
      CIH2Z(I) = CIH2(I)
 50   ZZ(I) = Z(I)
      DO 51 I=IZ,NOFZ
      PT(I+1) = PTZ(I)
      T(I+1) = TIZ(I)
      CIO2(I+1) = CIO2Z(I)
      CIH2(I+1) = CIH2Z(I)
 51   Z(I+1) = ZZ(I)
      Z(IZ) = ZIF
      NOFZ = NOFZ+1
 52   RETURN
      END
```

```
      SUBROUTINE DELETE (PASSNO)
C
C   ROUTINE TO DELETE INTERFACE AXIAL STATIONS FROM INITIAL INPUT Z ARRAY
C
      INTEGER PASSNO
      PARAMETER NAX=70, NTI=40, NPP=30
      COMMON /CB1/ TPP(NPP,NAX),CO2(NPP,NAX),CH2(NPP,NAX),CH2O(NPP,NAX),
     X       T(NAX),P(NAX),PT(NAX),H(NAX),CIH2(NAX),CIO2(NAX),CIH2O(NAX),
     X       CIH2OS(NAX),CIH2OL(NAX),CIH2OV(NAX),CIHE(NAX),DELT(NTI),
     X       PPT(NAX)
      COMMON /CB2/ Z(NAX),ZSSL(NTI),ZSLL(NTI),ZLLV(NTI),ZLVV(NTI)
      COMMON /CB4/ NOFZ,NPASS,NAXIAL,INPERP,MODPC,MODNO,PUNCH,ITSTEP,
     X       JDP,ISHUT,IHOT
      DIMENSION ZZ(NAX),TT(NAX),CCIH2(NAX),CCIO2(NAX),CCH2O(NAX)
C   SAVE CURRENT Z ARRAY AND CORRESPONDING TEMPS, CONCENTRATIONS
      DO 5 I=1,NOFZ
      ZZ(I) = Z(I)
      TT(I) = T(I)
      PPT(I) = PT(I)
      CCIH2(I) = CIH2(I)
      CCIO2(I) = CIO2(I)
 5    CCH2O(I) = CIH2O(I)
C   LOCATE INTERFACE POSITIONS
      NOFZ1 = NOFZ-1
      DO 10 I=1,NOFZ1
      IF (Z(I)-ZSSL(PASSNO)) 10,1,10
 10   CONTINUE
      RETURN
 1    IF1 = I
      DO 20 I=IF1,NOFZ1
      IF (Z(I)-ZSLL(PASSNO)) 20,2,20
 20   CONTINUE
      IF2 = NAXIAL+1
      IF3 = NAXIAL+1
      IF4 = NAXIAL+1
      GO TO 6
 2    IF2 = I
      DO 30 I=IF2,NOFZ1
      IF (Z(I)-ZLLV(PASSNO)) 30,3,30
 30   CONTINUE
      IF3 = NAXIAL+1
      IF4 = NAXIAL+1
      GO TO 6
 3    IF3 = I
      DO 40 I=IF3,NOFZ1
      IF (Z(I)-ZLVV(PASSNO)) 40,4,40
 40   CONTINUE
      IF4 = NAXIAL+1
      GO TO 6
 4    IF4 = I
C   ADJUST Z ARRAY TO INITIAL VALUES
 6    K = NAXIAL-4
      DO 50 I=NOFZ,1,-1
      IF (I.EQ.IF4.OR.I.EQ.IF3.OR.I.EQ.IF2.OR.I.EQ.IF1) GO TO 50
      Z(K) = ZZ(I)
      T(K) = TT(I)
      PT(K) = PPT(I)
      CIH2(K) = CCIH2(I)
```

```
      SUBROUTINE OVSTEP (ZEND,IZ,PASSNO,REGION)
C
C     THIS ROUTINE MAKES APPROPRIATE ADJUSTMENTS TO TEMPERATURE, PRESSURE,
C     CONCENTRATION ETC. WHEN AXIAL POSITIONING HAS OVERSTEPPED INTERFACE
C     BOUNDARIES FROM ONE REGION TO ANOTHER
C
      INTEGER PASSNO,REGION
      PARAMETER NAX=70, NTI=40
      PARAMETER NPP=30
      COMMON /CB1/ TPP(NPP,NAX),CO2(NPP,NAX),CH2(NPP,NAX),CH2O(NPP,NAX),
     X       T(NAX),P(NAX),PT(NAX),H(NAX),CIH2(NAX),CIO2(NAX),CIH2O(NAX),
     X       CIH2OS(NAX),CIH2OL(NAX),CIH2OV(NAX),CIHE(NAX),DELT(NTI),
     X       PPT(NAX)
      COMMON /CB2/ Z(NAX),ZSSL(NTI),ZSLL(NTI),ZLLV(NTI),ZLVV(NTI)
      COMMON /CB3/ ALPHA,GAMMA,KAPPA,HC,KP,A,DELTT,KCH2,KCO2,KCH2O,TCH2,
     X       TCO2,TCH2O,PCH2,PCO2,PCH2O,MH2,MO2,MH2O,MHE,HR,HA,HA1,HA2,
     X       AW,CW,MW,DC,TA,DOH2,DOO2,DOH2O,ALPHAK,AP,DELTA,G,MU,HS,HL,
     X       HV,TW,RHOM,WH2,WO2,WH2OS,WH2OL,WH2OV,WHE,CFBAR,MBAR,CICP1,
     X       CICP2,CICP3,RHO,RHOV,DELHC,TITPS,DTDZ,DHDZ,TS,TL,DPDZ,DC1DZ,
     X       DC2DZ,DC3SDZ,DC3LDZ,DC3VDZ,DC4DZ,RHOP,CP,DELTP,DPTPS,SDTIME,
     X       PF,TSS,AC,VC,PREST,GSS,MBARSS
      COMMON /CB4/ NOFZ,NPASS,NAXIAL,INPERP,MODPC,MODNO,PUNCH,ITSTEP,
     X       JDP,ISHUT,IHOT
      GO TO (1,2,3,4,5), REGION
C     SOLID/SOLID-LIQUID INTERFACE
 1    DELTZ = (TS-T(IZ))/DTDZ
      T(IZ) = TS
      H(IZ) = H(IZ)+DHDZ*DELTZ
      HS = H(IZ)
      CIH2OS(IZ) = CIH2OS(IZ)+DC3SDZ*DELTZ
      ZSSL(PASSNO) = Z(IZ)+DELTZ
      ZIF = ZSSL(PASSNO)
      PT(IZ) = (ZIF-Z(IZ-1))*(PT(IZ)-PT(IZ-1))/(Z(IZ)-Z(IZ-1))+PT(IZ-1)
      CALL INSERT (ZIF,IZ)
      REGION = 2
      GO TO 10
C     SOLID-LIQUID/LIQUID INTERFACE
 2    DELTZ = -CIH2OS(IZ)/DC3SDZ
      H(IZ) = H(IZ)+DHDZ*DELTZ
      CIH2OS(IZ) = 0.
      CIH2OL(IZ) = CIH2OL(IZ)+DC3LDZ*DELTZ
      ZSLL(PASSNO) = Z(IZ)+DELTZ
      ZIF = ZSLL(PASSNO)
      PT(IZ) = (ZIF-Z(IZ-1))*(PT(IZ)-PT(IZ-1))/(Z(IZ)-Z(IZ-1))+PT(IZ-1)
      CALL INSERT (ZIF,IZ)
      REGION = 3
      GO TO 10
C     LIQUID/LIQUID-VAPOR INTERFACE
 3    DELTZ = (TL-T(IZ))/DTDZ
      T(IZ) = TL
      H(IZ) = H(IZ)+DHDZ*DELTZ
      HL = H(IZ)
      CIH2OL(IZ) = CIH2OL(IZ)+DC3LDZ*DELTZ
      ZLLV(PASSNO) = Z(IZ)+DELTZ
      ZIF = ZLLV(PASSNO)
      PT(IZ) = (ZIF-Z(IZ-1))*(PT(IZ)-PT(IZ-1))/(Z(IZ)-Z(IZ-1))+PT(IZ-1)
      CALL INSERT (ZIF,IZ)
      REGION = 4
```

```
      GO TO 10
C     LIQUID-VAPOR/VAPOR INTERFACE
 4    DELTZ = -CIH2OL(IZ)/DC3LDZ
      H(IZ) = H(IZ)+DHDZ*DELTZ
      CIH2OL(IZ) = 0.
      CIH2OV(IZ) = CIH2OV(IZ)+DC3VDZ*DELTZ
      ZLVV(PASSNO) = Z(IZ)+DELTZ
      ZIF = ZLVV(PASSNO)
      PT(IZ) = (ZIF-Z(IZ-1))*(PT(IZ)-PT(IZ-1))/(Z(IZ)-Z(IZ-1))+PT(IZ-1)
      CALL INSERT (ZIF,IZ)
      REGION = 5
      GO TO 10
C     END OF REACTOR BED
 5    DELTZ = ZEND-Z(IZ)
      H(IZ) = H(IZ)+DHDZ*DELTZ
      CIH2OV(IZ) = CIH2OV(IZ)+DC3VDZ*DELTZ
      Z(IZ) = ZEND
      ZIF = ZEND
      PT(IZ) = (ZIF-Z(IZ-1))*(PT(IZ)-PT(IZ-1))/(Z(IZ)-Z(IZ-1))+PT(IZ-1)
C     ADJUST TEMP, PRESSURE, CONCENTRATIONS
 10   CIH2(IZ) = CIH2(IZ)+DC1DZ*DELTZ
      CIO2(IZ) = CIO2(IZ)+DC2DZ*DELTZ
      CIH2O(IZ) = CIH2OS(IZ)+CIH2OL(IZ)+CIH2OV(IZ)
      CIHE(IZ) = CIHE(IZ)+DC4DZ*DELTZ
      IF (REGION.EQ.2.OR.REGION.EQ.4) GO TO 12
      T(IZ) = T(IZ)+DTDZ*DELTZ
 12   P(IZ) = P(IZ)+DPDZ*DELTZ
      RETURN
      END
```

```
      FUNCTION FMAX (X,N,MAX,M)
C
C   ROUTINE TO FIND MAXIMUM VALUE OF ALL ELEMENTS IN ARRAY X
C
      DIMENSION X(MAX,M)
      FMAX = X(1,1)
      DO 10 J=1,M
      DO 10 I=1,N
      IF (X(I,J)-FMAX) 10,10,5
 5    FMAX = X(I,J)
 10   CONTINUE
      RETURN
      END
```

```
      FUNCTION FMIN (X,N,MAX,M)
C
C   ROUTINE TO FIND MINIMUM VALUE OF ALL ELEMENTS IN ARRAY X
C
      DIMENSION X(MAX,M)
      FMIN = X(1,1)
      DO 10 J=1,M
      DO 10 I=1,N
      IF (FMIN-X(I,J)) 10,10,5
 5    FMIN = X(I,J)
 10   CONTINUE
      RETURN
      END
```

```
      SUBROUTINE RDPNCH(TIME,HW,MINT)
C
C   ROUTINE TO READ AND PUNCH AUXILIARY INPUT
C
      INTEGER PUNCH
      PARAMETER NAX=70, NTI=40
      PARAMETER NPP=30, NRTS=200
      COMMON /CB1/ TPP(NPP,NAX),CO2(NPP,NAX),CH2(NPP,NAX),CH2O(NPP,NAX),
     X       T(NAX),P(NAX),PT(NAX),H(NAX),CIH2(NAX),CIO2(NAX),CIH2O(NAX),
     X       CIH2OS(NAX),CIH2OL(NAX),CIH2OV(NAX),CIHE(NAX),DELT(NTI),
     X       PPT(NAX)
      COMMON /CB2/ Z(NAX),ZSSL(NTI),ZSLL(NTI),ZLLV(NTI),ZLVV(NTI)
      COMMON /CB3/ ALPHA,GAMMA,KAPPA,HC,KP,A,DELTT,KCH2,KCO2,KCH2O,TCH2,
     X       TCO2,TCH2O,PCH2,PCO2,PCH2O,MH2,MO2,MH2O,MHE,HR,HA,HA1,HA2,
     X       AW,CW,MW,DC,TA,DOH2,DOO2,DOH2O,ALPHAK,AP,DELTA,G,MU,HS,HL,
     X       HV,TW,RHOM,WH2,WO2,WH2OS,WH2OL,WH2OV,WHE,CFBAR,MBAR,CICP1,
     X       CICP2,CICP3,RHO,RHOV,DELHC,TITPS,DTDZ,DHDZ,TS,TL,DPDZ,DC1DZ,
     X       DC2DZ,DC3SDZ,DC3LDZ,DC3VDZ,DC4DZ,RHOP,CP,DELTP,DPTPS,SDTIME,
     X       PF,TSS,AC,VC,PREST,GSS,MBARSS
      COMMON /CB4/ NOFZ,NPASS,NAXIAL,INPERP,MODPC,MODNO,PUNCH,ITSTEP,
     X       JDP,ISHUT,IHOT
      DIMENSION HW(1),CO2T(1),CH2T(1),CH2OT(1),PTT(1),TTI(1),ZT(1),
     X       MINT(1)
      READ (5,1) (Z(I),I=1,NAXIAL)
      READ (5,1) (PT(I),I=1,NAXIAL)
      READ (5,1) (T(I),I=2,NAXIAL)
      READ (5,1) (H(I),I=2,NAXIAL)
      READ (5,1) (P(I),I=2,NAXIAL)
      READ (5,1) (CIH2(I),I=2,NAXIAL)
      READ (5,1) (CIO2(I),I=2,NAXIAL)
      READ (5,1) (CIH2OV(I),I=2,NAXIAL)
      READ (5,1) (CIHE(I),I=2,NAXIAL)
      READ (5,1) (PPT(I),I=1,NAXIAL)
      READ (5,1) ((TPP(I,J),I=1,NPP),J=1,NAXIAL)
      READ (5,1) ((CO2(I,J),I=1,NPP),J=1,NAXIAL)
      READ (5,1) ((CH2(I,J),I=1,NPP),J=1,NAXIAL)
      READ (5,2) (MINT(I),I=1,NAXIAL)
      READ (5,1) TIME,TW,DELTT
 1    FORMAT (8E10.5)
      RETURN
      ENTRY RPNCH2 (TIME,NAXT,ZT,PTT,CO2T,CH2T,CH2OT,TTI)
      READ (5,2) NAXT
      READ (5,1) (ZT(I),I=1,NAXT)
      READ (5,1) (PTT(I),I=1,NAXT)
      READ (5,1) (CO2T(I),I=1,NAXT)
      READ (5,1) (CH2T(I),I=1,NAXT)
      READ (5,1) (CH2OT(I),I=1,NAXT)
      READ (5,1) (TTI(I),I=1,NAXT)
      READ (5,1) TIME,TW
      RETURN
      ENTRY RPNCH3(TIME,HW,MINT)
 10   WRITE (7,1) (Z(I),I=1,NAXIAL)
      WRITE (7,1) (PT(I),I=1,NAXIAL)
      WRITE (7,1) (T(I),I=2,NAXIAL)
      WRITE (7,1) (H(I),I=2,NAXIAL)
      WRITE (7,1) (P(I),I=2,NAXIAL)
      WRITE (7,1) (CIH2(I),I=2,NAXIAL)
      WRITE (7,1) (CIO2(I),I=2,NAXIAL)
```

```
      WRITE (7,1) (CIH2OV(I),I=2,NAXIAL)
      WRITE (7,1) (CIHE(I),I=2,NAXIAL)
      WRITE (7,1) (PPT(I),I=1,NAXIAL)
      WRITE (7,1) ((TPP(I,J),I=1,NPP),J=1,NAXIAL)
      WRITE (7,1) ((CO2(I,J),I=1,NPP),J=1,NAXIAL)
      WRITE (7,1) ((CH2(I,J),I=1,NPP),J=1,NAXIAL)
      WRITE (7,2) (MINT(I),I=1,NAXIAL)
      WRITE (7,1) TIME,TW,DELTT
2     FORMAT (40I2)
      RETURN
      ENTRY RPNCH4 (TIME)
      WRITE (7,2) NAXIAL
      WRITE (7,1) (Z(I),I=1,NAXIAL)
      WRITE (7,1) (PT(I),I=1,NAXIAL)
      WRITE (7,1) (CIO2(I),I=1,NAXIAL)
      WRITE (7,1) (CIH2(I),I=1,NAXIAL)
      WRITE (7,1) (CIH2O(I),I=1,NAXIAL)
      WRITE (7,1) (T(I),I=1,NAXIAL)
      WRITE (7,1) TIME,TW
      RETURN
      END
```

```
      SUBROUTINE OUTPUT (TM,TT,TP,PP,FH2,FO2,FH2O,FHE,N1,N2,IOCT)
C
C   ROUTINE TO PRINT TEMP, PRESSURE, MOLE FRACTION PROFILES IN SUMMARY FORM
C
      PARAMETER NAX=70, NTI=40
      INTEGER FORMT(9) / 54H      (11X,1H*,5X,3HSEC,       (9X,3HSEC)/11
     XX,1H*)      /
      COMMON /CB2/ Z(NAX),ZSSL(NTI),ZSLL(NTI),ZLLV(NTI),ZLVV(NTI)
      COMMON /CB4/ NOFZ,NPASS,NAXIAL,INPERP,MODPC,MODNO,PUNCH,ITSTEP,
     X     JDP,ISHUT,IHOT
      DIMENSION NUMBER(9)
      DIMENSION TM(1),TT(1),TP(1),PP(1),FH2(1),FO2(1),FH2O(1),FHE(1)
      DATA  NUMBER / '     1     2     3     4     5     6     7     8
     X   9' /
C   NO. OF COLUMNS OF OUTPUT = (N2-N1+1)
      FORMT(5) = NUMBER(N2-N1)
      WRITE (6,100)
 100  FORMAT ('1' / 36X 'TIME PROFILES OF INTERSTITIAL TEMPERATURE VS AX
     XIAL POSITION' // 3X 'AXIAL   *' 42X 'TEMPERATURE (DEGREES R)' /
     X      ' POSITION  *' / 3X '(FT)    *' )
      WRITE (6,101) (TM(I),I=N1,N2)
 101  FORMAT ( 11X '*   ' F8.4, 9(4X,F8.4) )
      WRITE (6,FORMT)
      K1 = 1
      K2 = MODPC
      DO 10 I=1,NAXIAL
      WRITE (6,102) Z(I),(TT(K),K=K1,K2)
      K1 = K2+1
 10   K2 = (I+1)*MODPC
 102  FORMAT ( E9.4, '  *', E11.5, 9(E12.5) )
      WRITE (6,109)
 109  FORMAT ('1' / 38X 'TIME PROFILES OF PARTICLE TEMPERATURE VS AXIAL
     XPOSITION' // 3X  'AXIAL   *' 43X 'TEMPERATURE (DEGREES R)' /
     X     ' POSITION  *' / 3X '(FT)    *' )
      WRITE (6,101) (TM(I),I=N1,N2)
      WRITE (6,FORMT)
      K1 = 1
      K2 = MODPC
      DO 70 I=1,NAXIAL
      WRITE (6,102) Z(I),(TP(K),K=K1,K2)
      K1 = K2+1
 70   K2 = (I+1)*MODPC
      WRITE (6,103)
 103  FORMAT ('1' / 40X 'TIME PROFILES OF CHAMBER PRESSURE VS AXIAL POSI
     XTION' // 3X 'AXIAL   *' 46X 'PRESSURE (PSIA)' /
     X      ' POSITION  *' / 3X '(FT)    *' )
      WRITE (6,101) (TM(I),I=N1,N2)
      WRITE (6,FORMT)
      K1 = 1
      K2 = MODPC
      DO 20 I=1,NAXIAL
      WRITE (6,102) Z(I), (PP(K),K=K1,K2)
      K1 = K2+1
 20   K2 = (I+1)*MODPC
      WRITE (6,104)
 104  FORMAT ('1' / 40X 'TIME PROFILES OF H2 MOLE FRACTION VS AXIAL POSI
```

```
     XTION' // 3X 'AXIAL     *' 38X 'H2 MOLE FRACTION (DIMENSIONLESS)' /
     X        ' POSITION   *' / 3X '(FT)       *' )
      WRITE (6,101) (TM(I),I=N1,N2)
      WRITE (6,FORMT)
      K1 = 1
      K2 = MODPC
      DO 30 I=1,NAXIAL
      WRITE (6,102) Z(I), (FH2(K),K=K1,K2)
      K1 = K2+1
30    K2 = (I+1)*MODPC
      WRITE (6,107)
107   FORMAT ('1' / 40X 'TIME PROFILES OF O2 MOLE FRACTION VS AXIAL POSI
     XTION' // 3X 'AXIAL     *' 38X 'O2 MOLE FRACTION (DIMENSIONLESS)' /
     X        ' POSITION   *' / 3X '(FT)       *' )
      WRITE (6,101) (TM(I),I=N1,N2)
      WRITE (6,FORMT)
      K1 = 1
      K2 = MODPC
      DO 40 I=1,NAXIAL
      WRITE (6,102) Z(I), (FO2(K),K=K1,K2)
      K1 = K2+1
40    K2 = (I+1)*MODPC
      WRITE (6,105)
105   FORMAT ('1' / 40X 'TIME PROFILES OF H2O MOLE FRACTION VS AXIAL POS
     XITION' // 3X 'AXIAL     *' 38X 'H2O MOLE FRACTION (DIMENSIONLESS)' /
     X        ' POSITION   *' / 3X '(FT)       *' )
      WRITE (6,101) (TM(I),I=N1,N2)
      WRITE (6,FORMT)
      K1 = 1
      K2 = MODPC
      DO 50 I=1,NAXIAL
      WRITE (6,102) Z(I), (FH2O(K),K=K1,K2)
      K1 = K2+1
50    K2 = (I+1)*MODPC
      WRITE (6,106)
106   FORMAT ('1' / 40X 'TIME PROFILES OF HE MOLE FRACTION VS AXIAL POSI
     XTION' // 3X 'AXIAL     *' 38X 'HE MOLE FRACTION (DIMENSIONLESS)' /
     X        ' POSITION   *' / 3X '(FT)       *' )
      WRITE (6,101) (TM(I),I=N1,N2)
      WRITE (6,FORMT)
      K1 = 1
      K2 = MODPC
      DO 60 I=1,NAXIAL
      WRITE (6,102) Z(I), (FHE(K),K=K1,K2)
      K1 = K2+1
60    K2 = (I+1)*MODPC
      IOCT = IOCT+1
      RETURN
      END
```

```
      SUBROUTINE SETUP (TM,MFH2,MFO2,MFH2O,MFHE,PASSNO,K,KM)
C
C     ROUTINE TO SET UP ARRAYS FOR PRINTER PLOTS
C
      INTEGER PASSNO
      REAL  MFH2,MFO2,MFH2O,MFHE
      PARAMETER NAX=70, NTI=40
      PARAMETER NPP=30, NRTS=200
      COMMON /CB1/ TPP(NPP,NAX),CO2(NPP,NAX),CH2(NPP,NAX),CH2O(NPP,NAX),
     X       T(NAX),P(NAX),PT(NAX),H(NAX),CIH2(NAX),CIO2(NAX),CIH2O(NAX),
     X       CIH2OS(NAX),CIH2OL(NAX),CIH2OV(NAX),CIHE(NAX),DELT(NTI),
     X       PPT(NAX)
      COMMON /CB2/ Z(NAX),ZSSL(NTI),ZSLL(NTI),ZLLV(NTI),ZLVV(NTI)
      COMMON /CB4/ NOFZ,NPASS,NAXIAL,INPERP,MODPC,MODNO,PUNCH,ITSTEP,
     X       JDP,ISHUT,IHOT
      DIMENSION LABEL(91),LBL(15),LABLY(91),LABLX(24),TZ(5)
      DIMENSION Z1(NAX,5),Y1(NAX,5),Y2(NAX,5),Y3(NAX,5),Y4(NAX,5),
     X           Y5(NAX,5),Y6(NAX,5),Y7(NAX,5)
      DIMENSION TM(1),MFH2(1),MFO2(1),MFH2O(1),MFHE(1)
C     LABELS FOR PRINTER PLOTS ARE IN FOLLOWING DATA STATEMENTS ...
      DATA LABEL/6*'       ','TIME PROFILES: INTERSTITIAL TEMPERATURE VS
     XAXIAL POSITION   ',6*'       ','TIME PROFILES: CHAMBER PRESSURE VS
     XAXIAL POSITION     ',6*'       ','TIME PROFILES: H2 MOLE FRACTION V
     XS AXIAL POSITION     ',6*'       ','TIME PROFILES: O2 MOLE FRACTION
     X VS AXIAL POSITION     ',6*'       ','TIME PROFILES: H2O MOLE FRACT
     XION VS AXIAL POSITION    ',6*'       ','TIME PROFILES: HE MOLE FRAC
     XTION VS AXIAL POSITION     '/
      DATA LBL/6*'       ','TIME PROFILES: PARTICLE TEMPERATURE VS AXIAL
     XPOSITION '/
      DATA LABLX/'AXIAL POSITION (FT)      ','     TIME (SECONDS)     ',
     X'    TIMES (IN SEC) REPRESENTED BY CURVES 1 THRU ','AXIAL POSITION
     XS (IN FT) REPRESENTED BY CURVES 1-'/
      DATA LABLY/' ',' ','T','E','M','P','E','R','A','T','U','R','E',' '
     X ,' ',' ',' ',' ','(','D','E','G','R','E','E','S',' ','R',')',' ',
     X ' ',' ','M','O','L','E',' ','F','R','A','C','T','I','O','N',' ',
     X '(','D','I','M','E','N','S','I','O','N','L','E','S','S',')',' ',
     X ' ',' ','P','R','E','S','S','U','R','E',' ',' ',' ',' ',' ',' ',
     X ' ',' ','(','P','S','I','A',')',' ',' ',' ',' ',' '/
      IF (K.GT.1) GO TO 5
      MAX = NAX
C     CALCULATE NUMBER OF POINTS PER PLOT
      NPTS = NAXIAL/MODNO
      IF (MOD(NAXIAL,MODNO).NE.0) NPTS=NPTS+1
 5    I = 1
      DO 10 J=1,NAXIAL,MODNO
      Z1(I,K) = Z(J)
      Y1(I,K) = T(J)
      Y7(I,K) = PT(J)
      Y2(I,K) = P(J)
      Y3(I,K) = MFH2(J)
      Y4(I,K) = MFO2(J)
      Y5(I,K) = MFH2O(J)
      Y6(I,K) = MFHE(J)
 10   I = I+1
      Z1(NPTS,K) = Z(NAXIAL)
      Y1(NPTS,K) = T(NAXIAL)
      Y7(NPTS,K) = PT(NAXIAL)
      Y2(NPTS,K) = P(NAXIAL)
```

```
      Y3(NPTS,K) = MFH2(NAXIAL)
      Y4(NPTS,K) = MFO2(NAXIAL)
      Y5(NPTS,K) = MFH2O(NAXIAL)
      Y6(NPTS,K) = MFHE(NAXIAL)
      K = K+1
      IF (PASSNO.NE.NPASS) GO TO 15
      KM = K-1
 15   IF (K.LE.KM) RETURN
      ITM = PASSNO-KM
      DO 20 I=1,KM
 20   TZ(I) = TM(ITM+I)
C   CALL PRINTER PLOT ROUTINE WHEN ALL Y1, Y2,...,Y6 ARRAYS FULL
      CALL PRPLOT (Z1,Y1,NPTS,KM,MAX,TZ,LABEL(1),LABLX(1),LABLX(9),
     X       LABLY(1),LABLY(17),16,0)
      CALL PRPLOT (Z1,Y7,NPTS,KM,MAX,TZ,LBL(1),LABLX(1),LABLX(9),
     X       LABLY(1),LABLY(17),15,0)
      CALL PRPLOT (Z1,Y2,NPTS,KM,MAX,TZ,LABEL(17),LABLX(1),LABLX(9),
     X       LABLY(62),LABLY(77),15,0)
      CALL PRPLOT (Z1,Y3,NPTS,KM,MAX,TZ,LABEL(32),LABLX(1),LABLX(9),
     X       LABLY(32),LABLY(47),15,0)
      CALL PRPLOT (Z1,Y4,NPTS,KM,MAX,TZ,LABEL(47),LABLX(1),LABLX(9),
     X       LABLY(32),LABLY(47),15,0)
      CALL PRPLOT (Z1,Y5,NPTS,KM,MAX,TZ,LABEL(62),LABLX(1),LABLX(9),
     X       LABLY(32),LABLY(47),15,0)
      CALL PRPLOT (Z1,Y6,NPTS,KM,MAX,TZ,LABEL(77),LABLX(1),LABLX(9),
     X       LABLY(32),LABLY(47),15,0)
      K = 1
      RETURN
      END
```

```
      SUBROUTINE PRPLOT (X,Y,NP,NV,MAX,TZ,LBL,LX1,LX2,LY1,LY2,NL,NC)
C
C   ROUTINE TO DEVELOP PRINTER PLOTS OF Y VS X
C   MAXIMUM OF FIVE SUPERIMPOSED CURVES PER PLOT
C
      DIMENSION X(1),Y(1),TZ(1)
      DIMENSION LBL(1),LX1(1),LX2(1),LY1(1),LY2(1)
      DIMENSION LINE(126),XGRAD(12),YGRAD(12),XSCAL(12),YSCAL(12)
      INTEGER NUMBR(10) /'1','2','3','4','5','6','7','8','9','0'/
      INTEGER ALPHA(26) /'A','B','C','D','E','F','G','H','I','J','K',
     X      'L','M','N','O','P','Q','R','S','T','U','V','W','X','Y','Z'/
      DATA KBLNK/' '/, IPLUS/'+'/, MINUS/'-'/, ICOLN/':'/
      WRITE (6,1000) (LBL(I),I=1,NL)
 1000 FORMAT ('1' // 20A6)
      NSCAL = 120
      LK = 12
      NTRS = 1
      NNN = 1
      XYMRGN = 0.
      XMAX = FMAX(X,NP,MAX,NV)
      XMIN = FMIN(X,NP,MAX,NV)
C   SCALE AXES FROM MAX AND MIN VALUES (SAME SCALING PROCEDURE FOR BOTH AXES)
C   LXSF: POWER OF 10 TO WHICH X VALUES ARE SCALED
C   LYSF: POWER OF 10 TO WHICH Y VALUES ARE SCALED
 920  IF (ABS(XMAX).LT.1.) GO TO 100
      DO 30 II=1,30
      IF (ABS(XMAX).LT.10.**II) GO TO 31
 30   CONTINUE
 31   LYSF = -(II-1)
      GO TO 22
 100  DO 40 II=1,10
      IF (ABS(XMAX).GT.10.**(-II)) GO TO 41
 40   CONTINUE
 41   LYSF = II
 22   MANT = IFIX(XMAX*10.**(LYSF+2))
      DO 302 K=1,10
      IF (MOD(MANT+K,5).EQ.0) GO TO 303
 302  CONTINUE
 303  AMM = FLOAT(MANT+K)/100.
      XSPAN = AMM-XMIN*10.**LYSF
      MANT = IFIX(XSPAN*100.)
      DO 304 K=1,NSCAL
      IF (MOD(MANT+K,NSCAL).EQ.0) GO TO 305
 304  CONTINUE
 305  XINCR = (FLOAT(MANT+K)/100.)/FLOAT(LK-1)
      HALFX = XINCR/2.
      IF ((XMIN-(AMM-FLOAT(LK-1)*XINCR)).GT.HALFX) XYMRGN=HALFX
C   ADD HALF A SCALING INCREMENT TO FORM MARGIN IF NEEDED
      YSCAL(LK) = AMM+XYMRGN
      DO 306 I=LK,2,-1
 306  YSCAL(I-1) = YSCAL(I)-XINCR
      IF (ABS(YSCAL(1)).LT.10.) GO TO 338
      LYSF = LYSF-1
      XINCR = XINCR/10.
      DO 339 I=1,LK
 339  YSCAL(I) = YSCAL(I)/10.
C   SCALING COMPLETE ON X-AXIS --- IF NTRS=0, SCALING COMPLETE ON Y-AXIS ALSO
 338  IF (NTRS.EQ.0) GO TO 42
```

```
C     XSCAL: SCALING GRADATIONS ON X-AXIS
C     YSCAL: SCALING GRADATIONS ON Y-AXIS
      LXSF = LYSF
      XINCX = XINCR
      DO 43 JJ=1,LK
      XGRAD(JJ) = YSCAL(JJ)
 43   XSCAL(JJ) = YSCAL(JJ)
C     RESET SCALING PARAMETERS TO SCALE FOR Y-AXIS
      NSCAL = 50
      LK = 6
      NTRS = 0
      MM = LK
      XYMRGN = 0.
      XMAX = FMAX(Y,NP,MAX,NV)
      XMIN = FMIN(Y,NP,MAX,NV)
      RANGE = ABS(XMAX-XMIN)
C     IF Y-AXIS RANGE LESS THAN 1 PERCENT OF MAX VALUE, ASSUME CURVE IS CONSTANT
      IF (RANGE.LT.ABS(.01*XMAX)) XMAX=XMIN
      GO TO 920
 42   DO 44 J=1,LK
 44   YGRAD(J) = YSCAL(J)*10.**(-LYSF)
C     GENERATE TOP AND BOTTOM LINES OF GRAPH
 9    DO 13 K=16,126
      IF (MOD(K-16,10)) 14,15,14
 14   LINE(K) = MINUS
      GO TO 13
 15   LINE(K) = IPLUS
 13   CONTINUE
      NMN = 11-NNN*5
      WRITE (6,52) YGRAD(NMN),(LINE(M),M=16,126)
 52   FORMAT (6X, E10.5, 1X, 111A1)
      IF (NNN.EQ.2) GO TO 712
C     GENERATE INTERNAL LINES OF GRAPH
      C = XINCR*10.**(-LYSF)/10.
      A = YSCAL(6)*10.**(-LYSF)+C/2.
      B = A-C
C     BEGIN LOOP TO SET UP EACH INTERNAL LINE OF GRAPH --- LINES ARE LABELED
C                                     1 THRU 49 FROM TOP TO BOTTOM
      DO 401 JS=1,49
      DO 403 K=1,126
 403  LINE(K) = KBLNK
      IF (MOD(JS,10)) 18,19,18
 18   LINE (16) = ICOLN
      LINE (126) = ICOLN
      GO TO 20
 19   LINE(16) = IPLUS
      LINE(126) = IPLUS
C     A, B ARE UPPER AND LOWER BRACKETING VALUES FOR Y-COORDINATE OF POINT
C     C IS SCALED HEIGHT OF PRINT CHARACTER (A, B ARE ADJUSTED BY THIS AMOUNT
C                                           ON EACH NEW PRINT LINE)
 20   A = A-C
      B = B-C
      DO 427 NN=1,NV
      DO 427 JR=1,NP
C     GET SUBSCRIPT OF JR TH POINT OF NN TH CURVE
      JD = JR+(NN-1)*MAX
C     TEST IF Y-COORDINATE LIES WITHIN RANGE OF A MINUS B OF LINE NO. JS
      IF (Y(JD).GT.A.OR.Y(JD).LE.B) GO TO 427
C     VALUE IS POSITIONING VALUE FOR X-COORDINATE OF POINT
      VALUE = X(JD)*10.**LXSF
      DD = XINCX
      NPOS = (VALUE-XSCAL(1))/DD*10.+16.5
```

```
C   TEST IF X-COORDINATE LIES WITHIN CHARACTER POSITIONS 17 THRU 125 OF LINE JS
      IF (NPOS.LT.17.OR.NPOS.GT.125) GO TO 427
C   CURVES IDENTIFIED WITH DIGITS IF NC=0
      LINE(NPOS) = NUMBR(NN)
      JRS = MOD(JR,26)
      IF (JRS.EQ.0) JRS=26
C   CURVES IDENTIFIED WITH SEQUENTIAL CHARACTERS OF ALPHABET IF NC=1
      IF (NC.EQ.1) LINE(NPOS)=ALPHA(JRS)
 427  CONTINUE
      IF (MOD(JS,10)) 25,24,25
 24   MM = MM-1
      WRITE (6,52) YGRAD(MM),(LINE(M),M=16,126)
      GO TO 401
 25   IF (JS.NE.25.AND.JS.NE.26) GO TO 36
      IF (JS.EQ.26) GO TO 27
      DO 33 I=1,15
 33   LINE(I) = LY1(I)
      GO TO 36
 27   DO 34 I=1,15
 34   LINE(I) = LY2(I)
 36   WRITE (6,55) (LINE(M),M=1,126)
 55   FORMAT ( 1X, 15A1, 1X, 111A1 )
 401  CONTINUE
      NNN = NNN+1
      GO TO 9
C   PRINT X-AXIS GRADATION MARKINGS
 712  WRITE (6,53) (XGRAD(M),KBLNK,M=1,11),XGRAD(12)
 53   FORMAT (14X, 11(F6.3, A4), F6.3)
      WRITE (6,56) (LX1(I),I=1,4)
 56   FORMAT ('0' 56X, 4A6 )
      WRITE (6,58) (LX2(I),I=1,8),NV,(TZ(I),I=1,NV)
 58   FORMAT ('+' 81X, 8A6, I1 / 86X, 5F8.4)
      IF (LXSF.EQ.0) GO TO 57
      WRITE (6,35) LXSF
 35   FORMAT ( '0' 50X 'X-AXIS SCALING:  X VALUES*10**',I2 )
 57   RETURN
      END
```

```
      SUBROUTINE TMPRNT (TM,TWT,N1,N2)
C
C    ROUTINE TO PRINT WALL TEMPERATURE AND AXIAL INTERFACE VS TIME PROFILES
C
      PARAMETER NAX=70, NTI=40
      COMMON /CB2/ Z(NAX),ZSSL(NTI),ZSLL(NTI),ZLLV(NTI),ZLVV(NTI)
      DIMENSION G(1),P(1),TM(1),TWT(1)
      WRITE (6,10)
 10   FORMAT ('1' //// 43X 'WALL TEMPERATURE, INTERFACE VARIATIONS VS TI
     XME' // 15X 'TIME     *      WALL TEMP      SOLID/SOLID-LIQUID    SOLID
     X-LIQUID/LIQUID   LIQUID/LIQUID-VAPOR   LIQUID-VAPOR/VAPOR' /
     X   15X '(SEC)    *     (DEGREES R)' 10X '(FT)' 3(18X '(FT)')  / 23X
     X    '*')
      DO 30 I=N1,N2
 30   WRITE (6,40) TM(I),TWT(I),ZSSL(I),ZSLL(I),ZLLV(I),ZLVV(I)
 40   FORMAT ( 13X, F8.4, '   *   ', E12.5, 5X, E12.5, 3(10X, E12.5) )
      RETURN
      ENTRY TMPRP (TM,G,P,N1,N2)
      WRITE (6,20)
 20   FORMAT ('0' // 44X 'PRESSURE, MASS FLOW RATE VARIATIONS VS TIME' /
     X       / 43X 'TIME     *    PRESSURE' 8X 'MASS FLOW RATE' / 43X
     X       '(SEC)    *     (PSIA)' 9X '(LB/FT**2-SEC)' / 51X '*' )
      DO 50 I=N1,N2
 50   WRITE (6,60) TM(I),P(I),G(I)
 60   FORMAT ( 41X, F8.4, 2X, '*', E12.5, 7X, E12.5 )
      RETURN
      END
```

```
      SUBROUTINE DEBUG3 (TIME,IT)
      REAL  MH2,MO2,MH2O,MHE,MU,MBAR,KAPPA,KP,KCH2,KCO2,KCH2O,MW,MU1VST,
     X      MU2VST,MU3VST,MU4VST
      PARAMETER NAX=70, NTI=40
      PARAMETER NPP=30
      COMMON /CB1/ TPP(NPP,NAX),CO2(NPP,NAX),CH2(NPP,NAX),CH2O(NPP,NAX),
     X      T(NAX),P(NAX),PT(NAX),H(NAX),CIH2(NAX),CIO2(NAX),CIH2O(NAX),
     X      CIH2OS(NAX),CIH2OL(NAX),CIH2OV(NAX),CIHE(NAX),DELT(NTI),
     X      PPT(NAX)
      COMMON /CB2/ Z(NAX),ZSSL(NTI),ZSLL(NTI),ZLLV(NTI),ZLVV(NTI)
      COMMON /CB3/ ALPHA,GAMMA,KAPPA,HC,KP,A,DELTT,KCH2,KCO2,KCH2O,TCH2,
     X      TCO2,TCH2O,PCH2,PCO2,PCH2O,MH2,MO2,MH2O,MHE,HR,HA,HA1,HA2,
     X      AW,CW,MW,DC,TA,DOH2,DOO2,DOH2O,ALPHAK,AP,DELTA,G,MU,HS,HL,
     X      HV,TW,RHOM,WH2,WO2,WH2OS,WH2OL,WH2OV,WHE,CFBAR,MBAR,CICP1,
     X      CICP2,CICP3,RHO,RHOV,DELHC,TITPS,DTDZ,DHDZ,TS,TL,DPDZ,DC1DZ,
     X      DC2DZ,DC3SDZ,DC3LDZ,DC3VDZ,DC4DZ,RHOP,CP,DELTP,DPTPS,SDTIME,
     X      PF,TSS,AC,VC,PREST,GSS,MBARSS
      COMMON /CB4/ NOFZ,NPASS,NAXIAL,INPERP,MODPC,MODNO,PUNCH,ITSTEP,
     X      JDP,ISHUT,IHOT
      COMMON /TABLES/ AVSZ(40),APVSZ(40),DELVSZ(40),HRVST(36),TC1(22),
     X      TC2(20),TC3V(20),TC4(18),MU1VST(34),MU2VST(34),MU3VST(32),
     X      MU4VST(34),CF1VST(34),CF2VST(34),CF3VST(34),CF3SVT(20),
     X      CF4VST(20),VPVST(60),TVSVP(48),DHCVST(24)
      NAXIAT = NAXIAL
      NAXIAL = NOFZ
      WRITE (6,90) (CIH2(I),I=1,NAXIAL)
      WRITE (6,91) (CIO2(I),I=1,NAXIAL)
      WRITE (6,92) (CIH2OS(I),I=1,NAXIAL)
      WRITE (6,93) (CIH2OL(I),I=1,NAXIAL)
      WRITE (6,94) (CIH2OV(I),I=1,NAXIAL)
      WRITE (6,95) (CIHE(I),I=1,NAXIAL)
      WRITE (6,96) (T(I),I=1,NAXIAL)
      WRITE (6,81) (PT(I),I=1,NAXIAL)
      WRITE (6,97) (H(I),I=1,NAXIAL)
      WRITE (6,98) (P(I),I=1,NAXIAL)
      WRITE (6,80) (Z(I),I=1,NAXIAL)
      WRITE (6,99) TIME,TW
80    FORMAT ('0' 57X 'AXIAL POSITIONS' / (1X,10E13.5))
81    FORMAT ('0' 50X 'PARTICLE SURFACE TEMPERATURES' / (1X,10E13.5))
90    FORMAT ('0'//48X'INTERSTITIAL CONCENTRATIONS OF H2' / (1X,10E13.5)
     X      )
91    FORMAT ('0' 48X 'INTERSTITIAL CONCENTRATIONS OF O2' / (1X,10E13.5)
     X      )
92    FORMAT ('0' 47X 'INTERSTITIAL CONCENTRATIONS OF H2O(S)' / (1X,
     X      10E13.5) )
93    FORMAT ('0' 47X 'INTERSTITIAL CONCENTRATIONS OF H2O(L)' / (1X,
     X      10E13.5) )
94    FORMAT ('0' 47X 'INTERSTITIAL CONCENTRATIONS OF H2O(V)' / (1X,
     X      10E13.5) )
95    FORMAT ('0' 48X 'INTERSTITIAL CONCENTRATIONS OF HE' / (1X,10E13.5)
     X      )
96    FORMAT ('0' 52X 'INTERSTITIAL TEMPERATURES' / (1X,10E13.5) )
97    FORMAT ('0' 60X 'ENTHALPIES' / (1X,10E13.5) )
98    FORMAT ('0' 53X 'INTERSTITIAL PRESSURES' / (1X,10E13.5) )
99    FORMAT ('0' 22X 'TIME =',E11.5, 3X 'WALL TEMP =',E11.5)
      NAXIAL = NAXIAT
      RETURN
      END
```

```
      SUBROUTINE UNBAR (T,IK,XIN,YIN,ZZ,KK)
C
C     THIS ROUTINE WILL DO LINEAR, QUADRATIC, OR CUBIC INTERPOLATION BETWEEN
C     TABULATED POINTS IN TABLE T --- INTERPOLATION MAY BE EITHER UNIVARIATE
C     OR BIVARIATE
C
      DIMENSION A(6),X(6),Y(6),T(1)
      II = IK+1
      N = 3
      N2 = 2
      IF (T(II)-3.) 700,701,702
  700 IF (T(II)) 60,701,704
  704 IF (T(II)-2.) 705,706,701
  705 N = 1
      GO TO 707
  706 N = 2
  707 N2 = 1
  701 II = II+1
  702 N1 = N+1
      DO 50 L=II,II
      IF (T(L)) 60,60,51
   60 KK = -1
      ZZ = 0.
      GO TO 9999
   51 NX = T(L)
      IF (T(L+1)) 60,52,50
   52 NY = 0
      GO TO 53
   50 NY = T(L+1)
   53 CONTINUE
      KK = 0
      KY = 0
      XX = XIN
      YY = YIN
      J1 = II+2
      J2 = NX+II+1
      IF (XX-T(J1)) 301,306,400
  400 DO 302 J=J1,J2
      IF (XX-T(J)) 304,304,302
  302 CONTINUE
  309 KK = 2
      XX = T(J2)
  308 JX1 = J2-N
      GO TO 305
  301 KK = 1
      XX = T(J1)
  306 JX1 = J1
      GO TO 305
  304 IF (J-J1-1) 301,306,307
  307 IF (J-J2) 303,308,309
  303 JX1 = J-N2
  305 CONTINUE
      XINT = XX
      IF (NY) 1500,1500,3000
 1500 DO 1599 L=1,N1
      X(L) = T(JX1)
      LY = JX1+NX
      Y(L) = T(LY)
```

```
1599 JX1 = JX1+1
     I = 1
     GO TO 54
3000 J1 = J1+NX
     J2 = J2+NY
     IF (YY-T(J1)) 311,316,401
401  DO 312 J=J1,J2
     IF (YY-T(J)) 314,314,312
312  CONTINUE
319  KY = 6
     YY = T(J2)
318  JY1 = J2-N
     GO TO 315
311  KY = 3
     YY = T(J1)
316  JY1 = J1
     GO TO 315
314  IF (J-J1-1) 311,316,317
317  IF (J-J2) 313,318,319
313  JY1 = J-N2
315  CONTINUE
     JX2 = JX1
     LY = JY1+NY*(JX2-II-1)
     LY1 = LY
     DO 3099 L=1,N1
     X(L) = T(JX2)
     Y(L) = T(LY1)
     LY1 = LY1+NY
3099 JX2 = JX2+1
     I = 0
     GO TO 54
3098 Y(1) = ZZ
     DO 4400 I=1,N
     LY1 = LY+I
     Y(I+1) = 0.
     DO 4050 MM=1,N1
     Y(I+1) = Y(I+1)+T(LY1)*X(MM)
4050 LY1 = LY1+NY
4400 CONTINUE
     DO 4199 L=1,N1
     X(L) = T(JY1)
4199 JY1 = JY1+1
     XINT = YY
     I = 1
54   D = 1.
     X(N+2) = X(1)
     X(N+3) = X(2)
     DO 55 J=1,N1
     A(J+1) = X(J+1)-X(J)
     TPAL1 = XINT-X(J)
     IF (TPAL1) 57,58,57
58   ZZ = Y(J)
     X(1) = 0.
     X(2) = 0.
     X(3) = 0.
     X(4) = 0.
     X(J) = 1.
     GO TO 59
57   D = D*TPAL1
     GO TO (711,712,713), N
711  X(J) = TPAL1/A(J+1)
     GO TO 55
```

```
 712  X(J) = -TPAL1
      GO TO 55
 713  X(J) = (X(J+2)-X(J))*TPAL1
 55   CONTINUE
      A(1) = A(N+2)
      ZZ = 0.
      DO 56 J=1,N1
      X(J) = D/(A(J)*A(J+1)*X(J))
      ZZ = ZZ+Y(J)*X(J)
 56   CONTINUE
 59   IF (I) 3098,3098,9999
 9999 KK = KK+KY
      RETURN
      END
```

```
      BLOCK DATA
C
C
      REAL  MU1VST,MU2VST,MU3VST,MU4VST
      COMMON /TABLES/ AVSZ(40),APVSZ(40),DELVSZ(40),HRVST(36),TC1(22),
     X      TC2(20),TC3V(20),TC4(18),MU1VST(34),MU2VST(34),MU3VST(32),
     X      MU4VST(34),CF1VST(34),CF2VST(34),CF3VST(34),CF3SVT(20),
     X      CF4VST(20),VPVST(60),TVSVP(48),DHCVST(24)
C
C   HEAT OF REACTION OF O2 VS TEMPERATURE (DEG R)
C
      DATA (HRVST(I),I=1,36) / 0. ,  1. , 16. , 0. ,
C   TEMPERATURES
     X    0.    ,    180.   ,    360.   ,    720.   ,   1080.   ,   1440.   ,
     X 1800.    ,   2160.   ,   2520.   ,   2880.   ,   3240.   ,   3600.   ,
     X 3960.    ,   4320.   ,   4680.   ,   5040.   ,
C   HEATS OF REACTION
     X -6423.   ,  -6461.   ,  -6478.   ,  -6529.   ,  -6581.   ,  -6626.   ,
     X -6665.   ,  -6696.   ,  -6720.   ,  -6740.   ,  -6755.   ,  -6766.   ,
     X -6777.   ,  -6786.   ,  -6794.   ,  -6801.   /
C
C   FOUR VISCOSITY TABLES FOLLOW ...
C
C
C   H2 VISCOSITY (LB/FT-SEC) VS TEMPERATURE (DEG R)
C
      DATA (MU1VST(I),I=1,34)/ 0. ,  1. , 15. , 0. ,
C   TEMPERATURES
     X  180.    ,    360.   ,    720.   ,   1080.   ,   1440.   ,   1800.   ,
     X 2160.    ,   2520.   ,   2880.   ,   3240.   ,   3600.   ,   3960.   ,
     X 4320.    ,   4680.   ,   5040.   ,
C   H2 VISCOSITIES
     X  2.54 E-6,  4.47 E-6,  7.30 E-6,  9.54 E-6, 11.48 E-6, 13.29 E-6,
     X 14.97 E-6, 16.54 E-6, 18.04 E-6, 19.47 E-6, 20.84 E-6, 22.16 E-6,
     X 23.45 E-6, 24.68 E-6, 25.89 E-6 /
C
C   O2 VISCOSITY (LB/FT-SEC) VS TEMPERATURE (DEG R)
C
      DATA (MU2VST(I),I=1,34)/ 0. ,  1. , 15. , 0. ,
C   TEMPERATURES
     X  180.    ,    360.   ,    720.   ,   1080.   ,   1440.   ,   1800.   ,
     X 2160.    ,   2520.   ,   2880.   ,   3240.   ,   3600.   ,   3960.   ,
     X 4320.    ,   4680.   ,   5040.   ,
C   O2 VISCOSITIES
     X  5.15 E-6,  9.94 E-6, 17.24 E-6, 22.94 E-6, 27.87 E-6, 32.30 E-6,
     X 36.33 E-6, 40.10 E-6, 43.74 E-6, 47.29 E-6, 50.65 E-6, 53.90 E-6,
     X 57.03 E-6, 60.08 E-6, 63.03 E-6 /
C
C   H2O VAPOR VISCOSITY (LB/FT-SEC) VS TEMPERATURE (DEG R)
C
      DATA (MU3VST(I),I=1,32)/ 0. ,  1. , 14. , 0. ,
C   TEMPERATURES
     X  360.    ,    720.   ,   1080.   ,   1440.   ,   1800.   ,   2160.   ,
     X 2520.    ,   2880.   ,   3240.   ,   3600.   ,   3960.   ,   4320.   ,
     X 4680.    ,   5040.   ,
C   H2O VAPOR VISCOSITIES
     X  5.18 E-6,  9.62 E-6, 14.44 E-6, 19.35 E-6, 24.10 E-6, 28.67 E-6,
     X 32.99 E-6, 37.07 E-6, 40.92 E-6, 44.60 E-6, 48.11 E-6, 51.49 E-6,
```

```
      X 54.73 E-6, 57.87 E-6 /
C
C     HE VISCOSITY (LB/FT-SEC) VS TEMPERATURE (DEG R)
C
       DATA (MU4VST(I),I=1,34)/ 0. ,  1. , 15. , 0. ,
C     TEMPERATURES
      X   180.    ,   360.    ,   720.    ,  1080.   ,  1440.   ,  1800.   ,
      X  2160.    ,  2520.    ,  2880.    ,  3240.   ,  3600.   ,  3960.   ,
      X  4320.    ,  4680.    ,  5040.    ,
C     HE VISCOSITIES
      X  6.71 E-6, 10.54 E-6, 16.50 E-6, 21.43 E-6, 25.80 E-6, 29.79 E-6,
      X 33.50 E-6, 37.01 E-6, 40.34 E-6, 43.52 E-6, 46.58 E-6, 49.54 E-6,
      X 52.40 E-6, 55.17 E-6, 57.87 E-6 /
C
C     FIVE SPECIFIC HEAT TABLES FOLLOW
C
C
C     H2 SPECIFIC HEAT (BTU/LB-DEG R) VS TEMPERATURE (DEG R)
C
       DATA (CF1VST(I),I=1,34)/ 0. ,  1. , 15. , 0. ,
C     TEMPERATURES
      X   180.    ,   360.    ,   720.    ,  1080.   ,  1440.   ,  1800.   ,
      X  2160.    ,  2520.    ,  2880.    ,  3240.   ,  3600.   ,  3960.   ,
      X  4320.    ,  4680.    ,  5040.    ,
C     H2 SPECIFIC HEATS
      X  2.675    ,  3.233    ,  3.460    ,  3.474   ,  3.509   ,  3.577   ,
      X  3.670    ,  3.772    ,  3.872    ,  3.966   ,  4.050   ,  4.126   ,
      X  4.193    ,  4.253    ,  4.306    /
C
C     O2 SPECIFIC HEATS (BTU/LB-DEG R) VS TEMPERATURE (DEG R)
C
       DATA (CF2VST(I),I=1,34)/ 0. ,  1. , 15. , 0. ,
C     TEMPERATURES
      X   180.    ,   360.    ,   720.    ,  1080.   ,  1440.   ,  1800.   ,
      X  2160.    ,  2520.    ,  2880.    ,  3240.   ,  3600.   ,  3960.   ,
      X  4320.    ,  4680.    ,  5040.    ,
C     O2 SPECIFIC HEATS
      X   .217    ,   .217    ,   .224    ,   .239   ,   .251   ,   .260   ,
      X   .266    ,   .270    ,   .274    ,   .278   ,   .281   ,   .285   ,
      X   .288    ,   .291    ,   .294    /
C
C     H2O VAPOR SPECIFIC HEATS (BTU/LB-DEG R) VS TEMPERATURE (DEG R)
C
       DATA (CF3VST(I),I=1,34)/ 0. ,  1. , 15. , 0. ,
C     TEMPERATURES
      X   180.    ,   360.    ,   720.    ,  1080.   ,  1440.   ,  1800.   ,
      X  2160.    ,  2520.    ,  2880.    ,  3240.   ,  3600.   ,  3960.   ,
      X  4320.    ,  4680.    ,  5040.    ,
C     H2O VAPOR SPECIFIC HEATS
      X  .4406    ,  .4411    ,  .453     ,  .480    ,  .512    ,  .546    ,
      X  .579     ,  .609     ,  .636     ,  .659    ,  .678    ,  .694    ,
      X  .709     ,  .721     ,  .731     /
C
C     H2O SOLID SPECIFIC HEATS (BTU/LB-DEG R) VS TEMPERATURE (DEG R)
C
       DATA (CF3SVT(I),I=1,16)/ 0. ,  1. ,  6. , 0. ,
C     TEMPERATURES
      X  200.     ,  300.     ,  350.     ,  400.    ,  450.    ,  491.4   ,
C     H2O SOLID (ICE) SPECIFIC HEATS
      X  .227     ,  .320     ,  .367     ,  .415    ,  .462    ,  .502    /
C
C     HE SPECIFIC HEAT (BTU/LB-DEG R) VS TEMPERATURE (DEG R)
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C
      DATA (CF4VST(I),I=1,16)/ 0. ,  1. ,  6. , 0. ,
C    TEMPERATURES
     X  180.     ,  720.      ,  1800.     ,  2880.     ,  3960.     ,  5040.     ,
C    HE SPECIFIC HEATS
     X  1.24     ,  1.24      ,  1.24      ,  1.24      ,  1.24      ,  1.24      /
C
C    VAPOR PRESSURE (PSIA) VS TEMPERATURE (DEG R)
C
      DATA (VPVST(I),I=1,60) / 0., 1., 28., 0.,
C    TEMPERATURES
     X     210.  ,     281.   ,     301.   ,     331.   ,     360.   ,     380.   ,
     X     401.  ,     420.   ,     440.   ,     460.   ,     480.   ,     492.   ,
     X     513.  ,     562.   ,     586.   ,     622.   ,     653.   ,     688.   ,
     X     727.  ,     768.   ,     788.   ,     818.   ,     842.   ,     877.   ,
     X     905.  ,     927.   ,    1005.   ,    1155.   ,
C    PRESSURES
     X  .17 E-11 , .441 E-8 , .588 E-7 , .147 E-5 , .232 E-4 ,  .00012   ,
     X  .00056   ,   .0019  ,   .0062  ,   .0185  ,   .0505  ,   .0885   ,
     X   0.2     ,  1.0     ,  2.0     ,  5.0     ,  10.     ,  20.      ,
     X   40.     ,  75.     ,  100.    ,  150.    ,  200.    ,  300.     ,
     X   400.    ,  500.    ,  1000.   ,  3000.   /
C
C    TEMPERATURE (DEG R) VS VAPOR PRESSURE (PSIA)
C
      DATA (TVSVP(I),I=1,48) / 0. , 1. , 22. , 0. ,
C    PRESSURES
     X   .20     ,  .50     ,  1.0     ,  2.0     ,  3.5     ,  5.0     ,
     X   7.5     ,  10.     ,  15.     ,  20.     ,  25.     ,  30.     ,
     X   40.     ,  50.     ,  75.     ,  100.    ,  150.    ,  200.    ,
     X   300.    ,  400.    ,  500.    ,  1000.   ,
C    TEMPERATURES
     X   513.    ,  540.    ,  562.    ,  586.    ,  608.    ,  622.    ,
     X   640.    ,  653.    ,  673.    ,  688.    ,  700.    ,  710.    ,
     X   727.    ,  741.    ,  768.    ,  788.    ,  818.    ,  842.    ,
     X   877.    ,  905.    ,  927.    ,  1005.   /
C
C    DELTA HEAT OF CONDENSATION VS TEMPERATURE
C
      DATA (DHCVST(I),I=1,24)/ 0. ,  1. , 10. , 0. ,
C    TEMPERATURES
     X   513.    ,  562.    ,  586.    ,  622.    ,  653.    ,  688.    ,
     X   710.    ,  741.    ,  768.    ,  788.    ,
C    DELTA HEATS OF CONDENSATION
     X   1064.   ,  1036.   ,  1022.   ,  1001.   ,  982.    ,  960.    ,
     X   945.    ,  924.    ,  904.    ,  889.    /
C
C   TABLE OF THERMAL CONDUCTIVITY OF H2 VS TEMPERATURE (DEG R)
      DATA (TC1(I),I=1,22) / 0., 1., 9., 0.,
C                                TEMPERATURES
     X     132.  ,     312.  ,     492.  ,     672.  ,     852.  ,    1032.  ,
     X    1200.  ,    1500.  ,    2000.  ,
C                          THERMAL CONDUCTIVITIES (H2)
     X   .614 E-5, 1.811 E-5, 2.683 E-5, 3.444 E-5, 4.122 E-5, 4.736 E-5,
     X 5.292 E-5, 6.194 E-5, 7.583 E-5/
C
C   TABLE OF THERMAL CONDUCTIVITY OF O2 VS TEMPERATURE (DEG R)
      DATA (TC2(I),I=1,20) / 0., 1., 8., 0.,
C                                TEMPERATURES
     X     132.  ,     312.  ,     492.  ,     582.  ,     672.  ,     800.  ,
     X    1000.  ,    2000.  ,
C                          THERMAL CONDUCTIVITIES (O2)
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     X  .106 E-5, .253 E-5, .394 E-5, .461 E-5, .522 E-5, .600 E-5,
     X  .714 E-5, 1.222 E-5/

C TABLE OF THERMAL CONDUCTIVITY OF H2O VAPOR VS TEMPERATURE (DEG R)
      DATA (TC3V(I),I=1,20) / 0., 1., 8., 0.,
C                           TEMPERATURES
     X    672.  ,    852.  ,   1032.  ,   1212.  ,   1392.  ,   1600.  ,
     X   1800.  ,   2000.  ,
C                    THERMAL CONDUCTIVITIES (H2O VAPOR)
     X  .378 E-5, .506 E-5, .639 E-5, .775 E-5, .911 E-5, 1.061 E-5,
     X 1.208 E-5, 1.356 E-5/

C TABLE OF THERMAL CONDUCTIVITY OF HELIUM VS TEMPERATURE (DEG R)
      DATA (TC4(I),I=1,18) / 0., 1., 7., 0.,
C                           TEMPERATURES
     X    132.  ,    312.  ,    492.  ,    672.  ,   1000.  ,   1500.  ,
     X   2000.  ,
C                     THERMAL CONDUCTIVITIES (HELIUM)
     X  .939 E-5, 1.700 E-5, 2.272 E-5, 2.744 E-5, 3.458 E-5, 4.347 E-5,
     X 5.139 E-5/

      END
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