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THERMOCHEMICAL CYCLE ANALYSIS USING LINKED CECS72 AND HYDRGN COMPUTER PROGRAMS

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16. Abstract

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SUMMARY

The Lewis Research Center chemical equilibrium computer program was coupled to the University of Kentucky thermochemical cycle analysis computer program. Input to the combined program is the same as input to the thermochemical cycle analysis program except that the extents of the reactions need not be specified.

The combined program is designed to be run interactively from a computer time-sharing terminal. This mode of operation allows correction or modification of the cycle to take place during cycle analysis.

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E-9191

INTRODUCTION

Closed thermochemical cycles have been proposed as a means of producing hydrogen and oxygen from water using a heat source, such as a nuclear reactor, for the thermal energy. Thermochemical cycles are currently of interest because they may provide a more efficient alternative to electrolysis.

Many new thermochemical cycles have been proposed in the recent literature (e. g., refs. 1 to 3). A number of ways for deciding if these cycles warrant further study have been developed. They do not require the detailed calculations and experimental data needed for an engineering design but are helpful as a preliminary screening to identify possibly interesting cycles and to eliminate those cycles with less potential. Some methods use only heats and free energies of formation. More involved methods require knowledge of other thermodynamic data as well as extents of reaction. Unfortunately, experimental values for extents of all reactions in a cycle are seldom known and estimated values must be used. Most cycles that have been analyzed for efficiency in this manner have supposedly used equilibrium extents of reaction.

The computer program HYDRGN was developed by Funk, et al. (ref. 4) for thermochemical cycle analysis. The program takes as input for each step in the cycle the chemical reaction occurring, the extent of the reaction, mole ratios of reactants, and temperature and pressure. The cycle evaluation program uses this information and appropriate thermodynamic data to calculate the work of separation of gaseous products, net heat required after as much heat exchange as possible between streams in the cycle, and finally, two figures of merit or efficiencies for the entire cycle. Results of calculations using this program have been reported in the literature (refs. 2, 5, and 6).

A sequence of computer programs for calculating thermodynamic equilibria has evolved over the years at the NASA Lewis Research Center. The latest version of this program (similar to the program documented in ref. 7), referred to as CECS72, has the ability to handle solid and liquid products but not aqueous solutions. Thermodynamic data included with the program are mostly taken from the JANAF tables (ref. 8).

Current interest in energy systems led us to the decision to link the existing chemical equilibrium computer program to the University of Kentucky's thermochemical cycle analysis computer program. This linking will allow checking of published cycles and facilitate evaluation of new cycles. For those steps in a cycle for which experimental values for extents of reaction are available, the equilibrium calculations can be bypassed.

Since both HYDRGN and CECS72 are occasionally updated, it was decided to link them in such a way that the integrity of neither program would be affected. Any information passed between them would be via data sets that are written by one program and read by the other. In this way updates of either program could be incorporated with a minimum of trouble, but the original linking would be more difficult.

LINKING PROGRAM

The original plan was for a rather straightforward linking of CECS72 and HYDRGN. It was only during evaluation of the first test cases that it became apparent that the user must easily be able to modify the cycle. Three kinds of problems dictated the final design. The first of these was computational; the other two were in cycle design.

Thermochemical cycles involve at least one solid or liquid in almost every reaction. In order for CECS72 to calculate equilibria with condensed species present, it is sometimes necessary to specify which of several possible condensed species the program should consider first (using the "insert" feature).

We have found it is better to consider all condensed products of a reaction first. However, to accommodate the cases in which this is not successful, the user is allowed to specify another choice of insert (including no insert at all).

At times products were encountered that were not anticipated - or were ignored - by a cycle designer. In some cases these extra products could be consumed as reactants in other steps. In other cases, the reactions were very temperature dependent; a 100 K change could alter the equilibrium composition significantly. It was found that the temperature of some steps needed to be changed in order to obtain the desired products.

Figure 1 shows a sketch of the flow of the program. The symbols used in the linking program are contained in appendix A and a listing of the program is given in appendix B. The program was designed to be run interactively from a time-sharing terminal. The user is notified whenever a difficulty arises and a course of action to be taken is suggested.

The linked programs, which are written in FORTRAN IV, run on an IBM 360/67 computer operating under TSS. Extensive use is made of system facilities, especially the command procedure facility (ref. 9) and the research editor (ref. 10). All changes to data sets are made with the research editor.

The linking program (which is actually two main programs), CECS72, and HYDRGN are executed from a procdef (CONTROL) requiring two parameters. The first parameter is the name of the input data set (in the form required by HYDRGN except that the extent of reaction need not be given). If the extent of reaction is known experimentally CECS72 can be bypassed for that reaction by specifying the second parameter. If this parameter, which acts as a two-way switch, is not blank program flow branches to a point immediately after the statement which executes CECS72. If the parameter is blank control passes to the next statement in the procdef.

The first linking program (CON1) reads (CONREA) the input data set, reformats (CONREF) each of the species names to be consistent with CECS72, and prepares (CONPRE) the input data set for CECS72. If any equation is not balanced, a message is typed at the terminal stating the problem and advising the user to correct the input data set and rerun the problem. Corrected data sets are checked until no more errors are detected.

CECS72 is run to determine the equilibrium composition for those reactions in which the extent of reaction was not specified. The second linking program (CON2) is next run. After again reading and reformatting the input data set, the CECS72 output data is read (CONS72) and checked for products not originally specified (CONEXT), the extents of reaction are calculated (CONEPS), and the

original input data set is modified to incorporate the equilibrium extents of reaction (CONMOD).

A final check for balanced equations is made. Also, the user is notified (default values are given here in parenthesis) if the concentration of unexpected products is too large (≥6 mole percent) or if the extent of reaction is too small (≤0.01). If so, the keyboard is unlocked and the user is invited to change the input data set and rerun the problem.

If the previous checkpoint is successfully traversed CECS72 output is checked for nonconvergence. If the equilibrium calculation for a reaction was not successful the user is advised to change inserts and rerun with the second parameter not defaulted.

Finally, HYDRGN is run to perform the cycle analysis and print the results. Also, printed in a separate listing for reference, are the warning messages that were printed at the terminal, a summary of CECS72 output, and a table of extents of reaction.

CYCLE EVALUATION

In a recent paper (ref. 2) Funk combined 26 reactions in different ways to create 13 new thermochemical cycles which were evaluated using HYDRGN. The high temperatures required by these cycles are beyond current nuclear reactor capability (process heat temperature of about 1100 K), but may be available in the future. These cycles were reevaluated to see how well the linked programs worked.

In the course of reevaluating these cycles a number of changes needed to be made to the reactions given in reference 2.

1. In some high temperature steps sulfur is given as the gaseous monatomic product S although equilibrium calculations indicate that S_2 is the correct form. Substitution of S_2 for S requires the introduction of another step to condense S_2 to S(ℓ) in order to balance the cycle. This step can be carried out at 718 K, the boiling point of sulfur.

2. Some cycles contain a low temperature step in which S(ℓ) appears as a product and a high temperature step involving S as a reactant. If one attempts to balance the cycle by introducing a step to vaporize S(ℓ) at 850 K, the temperature recommended in reference 5, equilibrium calculations indicate that approximately equimolar amounts of S_2 and S_8 are formed. Fortunately, however, the S_2 and S_8 can be used as reactants in place of S in the high temperature step.

3. In some cases, the reaction temperature needed to be changed in order to reduce the amount of side products to an acceptable level.

4. One reaction involved $CdSO_4(\ell)$ decomposition at 1300 K. Since we have no data on liquid $CdSO_4$, we substituted $CdSO_4(s)$ at its melting point, viz., 1273 K.

The cycles as originally reported and as revised are shown in table I.

Two reactions were unacceptable, thereby eliminating six cycles. The equilibrium pressure for

$$Bi_2S_3(s) \overset{1000\ K}{\rightleftharpoons} 2\ Bi(s) + 1.5\ S_2$$

was only 0.0028 atmosphere and 10 percent BiS was formed. For

$$CdSO_4(s) \overset{1273\ K}{\rightleftharpoons} CdO(s) + SO_2 + 0.5\ O_2$$

The extent of reaction was negligible ($<<0.01$).

A comparison of the results with those reported (ref. 2) for the seven cycles that were successfully calculated is given in table II. Molar recycle ratio for a step is the number of moles of gas that must be recycled at that step per mole of hydrogen produced by the cycle. The revised maximum molar recycle ratio is generally larger than that reported. Work of separation is calculated for gases only and assumes 100 percent separation efficiency. The reported and revised values are generally in agreement. Heat required after matching is the external heat input to the cycle. The reported and revised values agree quite well.

The η's are estimates of thermal efficiency, assuming an efficiency of 30 percent in converting heat to work. The first estimate, η_1, assumes total recovery of all exothermic heat and 100 percent efficiency for the work of separation. The reported and revised η_1's both average 0.53. In calculating the second estimate, η_2, it is assumed that the work of separation is 50 percent efficient and that work is generated from the exothermic heat (above 500 K) remaining after heat exchange matching. The revised η_2's are lower than the reported ones, averaging 0.31 as opposed to 0.36.

Some further information can be extracted by examining the detailed calculations. Table III shows the molar recycle ratio, work of separation, and extent of reaction, ϵ, for each step in the cycles successfully calculated. Some cycles can be improved significantly if the extent of reaction can be increased for certain steps. For example, the reaction

$$H_2S \overset{1300\ K}{\rightleftharpoons} H_2 + 0.5\ S_2$$

which occurs as step 3 of cycle 1 and step 2 in cycles 5, 7, and 10 consumes 50 to 60 percent of the 17 to 24 kcal of separation work. In addition, this reaction accounts for one-third to one-half of the total recycle ratio. The reaction

$$0.25\ BaS(s) + H_2O \overset{500\ K}{\rightleftharpoons} 0.25\ BaSO_4(s) + H_2$$

which occurs as step 1 of cycles 3 and 8, is responsible for almost the entire recycle ratio. Also, this reaction uses one-third to one-half of the work of separation of 7 to 11 kcal.

In order to determine the influence of the extents of reaction on cycle efficiency, the cycles that were successfully calculated using equilibrium values for extents of reaction were recalculated assuming complete conversion of reactants to products. The results are given in table IV. Examination of the table demonstrates that erroneous conclusions about cycle efficiency can be drawn unless reliable values for extents of reaction are known.

A simplified estimate of cycle efficiency that has been proposed (personal communication from M. G. Bowman) can be written as

$$\eta_E = \frac{\Delta H_{H_2O,\,298K}}{\sum_{endo} \Delta H_{298K} + \sum_{pos} \Delta G_T/0.3}$$

where the first summation is over all endothermic reactions at 298 K and the second summation is over all reactions with positive free energy changes at the temperature of the reaction. A comparison of this estimate with values calculated with the HYDRGN program using equilibrium values for extents of reaction is given in table V. This comparison indicates that efficiencies obtained from this estimate are probably overly optimistic.

CONCLUDING REMARKS

The Lewis Research Center's chemical equilibrium computer program CECS72 was coupled to the University of Kentucky's thermochemical cycle analysis computer program HYDRGN. Input to the combined program is the same as input to HYDRGN except that the extents of reaction need not be specified. After CECS72 calculates equilibrium compositions for each reaction, the extents of reaction are calculated by the linking program and inserted into the

input data set for HYDRGN. If experimental values are known for some or all of the reactions, they can be specified in the input and the equilibrium calculations will be bypassed.

The combined program is designed to be run interactively from a computer time-sharing terminal. If the program encounters errors in the input or cycle design flaws, the user is notified at the terminal and invited to correct or modify the offending data set. Reactants and products can be added to or deleted from existing reactions, new reactions can be added, or temperatures can be changed to modify a defective cycle into a potentially useful one.

A group of 13 thermochemical cycles constructed from 26 chemical reactions were used to test the combined program. Equilibrium calculations showed that one reaction had an unacceptably low equilibrium partial pressure and one reaction had a negligible extent of reaction; six cycles were thus eliminated. Results for the remaining seven cycles were generally less favorable than reported values. The steps that would have the greatest impact in improving the cycles were pointed out.

APPENDIX A

SYMBOLS USED IN COMPUTER PROGRAM

F4CLC, F4TRT, and F4MVC are FORTRAN implementations of the assembly language commands CLC (compare logical character), TRT (translate and test), and MVC (move character).

The names of variables are the same as those used in HYDRGN, with the following additions:

1. NAMELIST/INPT2/uses CECS72 variable names.
2. In the list below, the letters A, I, L, R refer to alphameric, integer, logical, real.

Variable	Type	Description
ADDI	A	'ADDI'
BAL	L	TRUE if equation is balanced
BB	A	TRUE if equation is balanced
CMOLE	A	' MOLE'
CONV	L	TRUE if CECS72 matrix converges
CL, CS	L	used in search for letter
CS	A	' CAL'
DATA	R	temporary storage
DATT	R	dummy variable
DENOM	R	factor in extent of reaction calculation
EPSL	R	extent of reaction
FB	A	dummy variable
FRAC	R	mole fraction
GO	L	TRUE if CECS72 calculation is successful
IC	I	dummy variable
IDONE	I	message has been printed if = 0
IEP	I	index in implied DO loop
IH	I	upper limit in implied DO loop
II	I	reactant ratio

Variable	Type	Description
III	I	number of temperature schedules
IL	I	lower limit in implied DO loop
ILAST	I	number of reactant ratios
INS	L	TRUE if any products are solid or liquid
IP	I	number of products
IR	I	index in implied DO loop
IRR	I	number of reactant ratios
IS	I	index in DO loop
IT	I	number of steps
JL	I	number of temperature schedules
JT	I	index in DO loop
KB	I	base reactant
KBB	I	not used
KKLAST	I	number of products
KKP	I	sum of number of products and reactants
KP	I	number of products
KR	I	index in DO loop
LF, LL, LS	I	dummy variables
L1, L2	I	dummy variables
M	I	dummy variable
N	I	dummy variable
NCON	I	number of temperature schedules
NOCON	I	dummy variable
NOGO	L	TRUE if any step is unacceptable
NPR	I	number of products
NRE	I	number of reactants
NRR	I	number of reactant ratios
NT	I	reduced number of temperature schedules

Variable	Type	Description
PMF	R	product mole fraction
PR	R	pressure
PRO	A	'PROD'
PROD	R	not used
PROO	R	dummy variable
REAC	A	'REAC'
REACT	R	not used
RMF	R	reactant mole fraction
SB	R	temporary storage
SIG	R	sum of mole fractions
SING	A	' SIN'
STOP	A	' STO'
S1, S2, S3	R	temporary storage
T, TB, TLS	L	used in character search
TEM1, TEM2	R	temporary storage
THM	A	' THE'
TT	R	dummy variable
WARN	A	' WAR'
XDEN	R	factor in extent of reaction calculation
XL	L	not used
XLON	R	lowest acceptable extent of reaction
XMUL, XNUM	R	factors in extent of reaction calculation
XS	A	's'
XTRMAX	R	maximum allowed concentration
XMF	R	mole fraction

APPENDIX B

COMPUTER PROGRAM LISTING

```
PROCDEF CONTROL
PARAM $1,$2
RELEASE FT; RELEASE W; RELEASE X; RELEASE Y; RELEASE Z
DDEF FT03F001,VS,HYDIN.$1
DDEF FT04F001,VS,THDATA,DCB=(RECFM=V,LRECL=1500)
DDEF FT08F001,VS,$1
DDEF FT05F001,VS,CECIN.$1
DDEF FT06F001,VS,CECOUT.$1
DDEF W,VP,LERC,OPTION=JOBLIB
IF '$2'¬='': GOTO 'CK'
CON1
ERASE HYDIN.$1
QUALIFY CONREA; IF BAL; GOTO 'OK'
DISPLAY 'REDIT $1 AND RERUN'
GOTO XXX
'OK' DDEF X,VP,CECSUBS,OPTION=JOBLIB
DDEF Y,VP,CEQELT,OPTION=JOBLIB
LOAD CECBLD; CECS72
DDEF FT03F001,VS,HYDIN.$1
RELEASE FT05F001; DDEF FT05F001,VS,HGNIN.$1
RELEASE FT06F001; DDEF FT06F001,VS,HGNOUT.$1
DDEF FT07F001,VS,CECOUT.$1
UNLOAD CECS72
CON2
QUALIFY CONREA; IF BAL; GOTO 'NEXT'
DISPLAY 'REDIT $1 AND RERUN'
GOTO XXX
'NEXT' QUALIFY CONMOD; IF ¬NOGO; GOTO 'FINISH'
DISPLAY 'REDIT $1 TO CHANGE TEMPERATURES OR SPECIFY EXTENTS OF REACTION'
DISPLAY 'REDIT CECIN.$1 TO CHANGE INSERTS- THEN RERUN WITH SECOND KEYWORD NOT DEFAULTED'
GOTO XXX
'FINISH' PRINT HYDIN.$1,,,EDIT; PRINT HGNIN.$1; PRINT CECOUT.$1,,,EDIT
DDEF Z,VP,HGNSUBS,OPTION=JOBLIB
HYDRGN; PRINT HGNOUT.$1,,EDIT
```

```
CON1
0000100 C    READ INPUT DATA FOR HYDRGN
0000200      CALL READ
0000220 C    MAKE SPECIE NAMES COMPATIBLE
0000240      CALL REFMT
0000500 C    PREPARE CECS72 INPUT DATA
0000600      CALL PREPAR
0000650      STOP
0000700      END
```

```
0000020       SUBROUTINE READ
0000100 C     READ HYDRGN INPUT
0000200 C
0003100       INTEGER CARD,STEP,BASE,A,P
0003200       REAL NOTE
0003300       LOGICAL TEST15,BAL
0003400       LOGICAL TEST1,TEST2,TEST2C,PLINE,DRAW,SAME,THERM,H298
0003500       DOUBLE PRECISION XREACT,XPROD,SUMW,SUMRG,GASSUM
0003600       DOUBLE PRECISION H,S,G,HS,SS,GS,HTOT,STOT,GTOT,COEF,SUMPG,SUMPL
0003700       DIMENSION STOICR(11,5),STOICP(11,5),RATOM(11,5,4),PATOM(11,5,4),  -
0003800      1RATCO(11,5,4),PATCO(11,5,4),RATIO(10,5,4),P(50)
0003900       DIMENSION BASE(10),NSATOM(50),TEMP1(50,10),TEMP2(50,10),TRANGE(2,5-
0004000      10),T(20),TPHASE(11,5,4),TEST1(10),AREACT(10,5),APROD(10,5),       -
0004100      2NPROD(11),NREACT(11),NRATIO(10),DAT(25)     ,LNOTE(10),NOTE(10,100)-
0004200      3,HSTOCR(50),HSTOCP(50),FAZER(11,5),FAZEP(11,5),EP(10,4),EPSI(10,10-
0004300      4,4),HIM(10),HAM(10)
0004320       COMMON/CTL/RMF(10,4,10,5),PMF(10,4,10,5),REACT(11,5,4),PROD(11,5,4),JL(11),GO(11,4,13),IP(11,4),KBB(11,4)
0004400       COMMON/FNAME/STOICR,STOICP,RATOM,PATOM,RATCO,PATCO
0004500       COMMON/INDX/R,NR,NR1,NRXNS,NCTEMP,I,K,J,M,NRX,NTOT,BASE,NSATOM,NN
0004600       COMMON/TMP/TEMP1,TEMP2,TRANGE,TPHASE,TMID
0004700       COMMON/LOGIC/PLINE,TEST2C,DRAW,SAME,TEST1,THERM,H298
0004800       COMMON/PRESS/P
0004900       COMMON/MATL3/AREACT,APROD,RATIO,NCTE,HSTOCR,HSTOCP,NPROC,NREACT,  -
0005000      1NRATIO,LNOTE
0005100       COMMON/FZE/SUMPL,SUMPG,SUMPS,FAZER,FAZEP,NGASP,NLIQP,NSOLP,NGASR, -
0005200      1NLIQR,NSOLR
0005300       COMMON/WORK/HIM,HAM,EPSI
0005320       COMMON/PRD/PROD(11,4,10,3),FRAC(11,4,10,13),TITLE(20)
0005400       DATA  PRO/4HPROD/,REAC/4HREAC/,BLANK/4H    /,WEND/3HEND/          -
0005500      1,COMM/4HNOTE/,CHEM/4HCHEM/,CNAME/4HNAME/,THER/4HTHER/,BA/1HB/
0005520       DATA HYD/1HH/,FINI/4HFINI/
0005700       NAMELIST/NAM1/STEP,T,EP,PRES,DRAW,SAME,H298
0005720       BAL=.TRUE.
0005800       H298=.FALSE.
0005900       SAME=.FALSE.
0006000       TRY=0.0
0006100       DRAW=.FALSE.
0006200       THERM=.FALSE.
0006300       TEST15=.FALSE.
0006400       TEST20=.FALSE.
0006500       DO 40 I=1,10
0006600       BASE(I)=0
0006700       DO 20 J=1,10
0006800       JJ=J+10
0006900       T(JJ)=0.0
0007000       J5=J
0007100       IF(J.GT.5) J5=1
0007200       FAZER(I,J5)=BLANK
0007300       TEMP1(I,J)=0.0
0007400       TEMP2(I,J)=0.0
0007500    20 FAZEP(I,J5)=BLANK
0007600       TEST1(I)=.FALSE.
0007700       NREACT(I)=0
0007800       NPROD(I)=0
```

```
0007900          NRATIO(I)=C
0008000          LNOTE(I)=0
0008100       40 CONTINUE
0008200          NR=0
0008300 C
0008310          READ(8,50) (TITLE(I),I=1,20)
0008320       50 FORMAT(20A4)
0008330          IF(TITLE(1).EQ.FINI) RETURN
0008340          WRITE(3,55) (TITLE(I),I=1,20)
0008350       55 FORMAT('1','ORIGINAL INPUT DATA FOR  ',20A4)
0008360 C
0008400 C THIS SECTION READS THE CODE CARD INDICATING THE TYPE OF CARDS TO FOLLOW.
0008500 C **********************NOTE*************************
0008600 C THE ONLY STIPULATION AS TO THE ORDER OF EACH SECTION OF CARDS IS THAT THE
0008700 C CHEMICAL REACTION CARDS MUST BE READ BEFORE THE NAMELISTS.
0008800 C
0008900 C
0009000       60 READ(8,80) (DAT(I),I=1,10)
0009100       80 FORMAT(20A4)
0009200       90 WRITE(3,100) (DAT(I),I=1,10)
0009300      100 FORMAT(' ',20A4)
0009320      120 IF(DAT(1).EQ.WEND) GO TO 760
0009340          IF(DAT(1).EQ.BLANK) GO TO 60
0009600 C   TEST20=.TRUE. MEANS THAT AN ERROR HAS BEEN FOUND IN THE INPUT AND THE PROGRAM
0009700 C   SKIPS TO THE NEXT CYCLE.
0009800          IF(TEST20) GO TO 60
0009900          IF(DAT(1).EQ.COMM) GO TO 160
0010000          IF(DAT(1).EQ.CHEM) GO TO 240
0010100          IF(DAT(1).EQ.CNAME) GO TO 520
0010200          IF(DAT(1).EQ.THER) THERM=.TRUE.
0010300          IF(DAT(1).EQ.THER.AND.TEST15) GO TO 760
0010400          WRITE(3,140)
0010500      140 FORMAT('0','THE LAST CARD HAS AN UNRECOGNIZABLE CODE')
0010600          TEST20=.TRUE.
0010700          GO TO 60
0010800 C   THIS SECTION READS THE NOTE CARDS FOR EACH REACTION.  THE FIRST TWO ITEMS
0010900 C   ON EACH NOTE CARD ARE IN I2 FORMAT.  THE FIRST NUMBER IS THE NUMBER OF THE
0011000 C   CARD FOR THIS REACTION (1, 2, UP TO 5 FOR EACH REACTION). THE SECOND NUMBER
0011100 C   IS THE NUMBER OF THE CHEMICAL REACTION (UP TO 10).  THE REMAINDER OF EACH
0011200 C   CARD IS IN A4 FORMAT AND IS USED FOR THE COMMENTS.
0011300      160 READ(8,180) CARD,STEP,(DAT(I),I=1,19)
0011400      180 FORMAT(2I2,19A4)
0011500      190 WRITE(3,200) CARD,STEP,(DAT(I),I=1,19)
0011600      200 FORMAT(' ',2I2,19A4)
0011620          IF(CARD.EQ.0) GO TO 60
0011800          LNOTE(STEP)=CARD*19
0011900          DO 220 I=1,19
0012000          J=((CARD-1)*19)+I
0012100      220 NOTE(STEP,J)=DAT(I)
0012200          GO TO 160
0012300 C
0012400 C   THIS SECTION READS AND PROCESSES THE CHEMICAL REACTION CARDS.
0012500 C*****THESE CARDS MUST COME BEFORE THE NAMELISTS**********
0012600 C
```

```
0012700    240 READ(8,260) STEP,(DAT(I),I=1,17)
0012800    260 FORMAT(I2,2A4,4(A2,F3.0),A1,F9.4,A1,4F8.3,7X)
0012900        WRITE(3,280) STEP,(DAT(I),I=1,17)
0013000    280 FORMAT(' ',I2,2A4,4(A2,F3.0),A1,F9.4,A1,4F8.3,7X)
0013100        IF(DAT(1).EQ.BLANK) GO TO 500
0013200        IF(DAT(1).EQ.REAC) GO TO 320
0013300        IF(DAT(1).EQ.PROD)  GO TO 420
0013400        WRITE(3,300)
0013500    300 FORMAT('0','CODE FOR THIS CARD IS IN ERROR')
0013600        TEST20=.TRUE.
0013700        GO TO 120
0013750 C      REACTANTS
0013800    320 K=NREACT(STEP) + 1
0013900        NREACT(STEP)=K
0013920 C      K=REACTANT NUMBER,I=ELEMENT NUMBER,NREACT=NUMBER OF REACTANTS
0013940 C      RATOM=ATOMIC SYMBOL,RATCO=ATOMIC COEFFICIENT
0014000        DO 340 I=1,4
0014100        RATOM(STEP,K,I)=DAT(2*I+1)
0014200    340 RATCO(STEP,K,I)=DAT(2*I+2)
0014300        IF(STEP.GT.NR)  NR= STEP
0014400        NRXNS=NR
0014420 C      NR=NUMBER OF REACTIONS/CYCLE,AREACT=STOICHIOMETRIC COEFFICIENT
0014500        AREACT(STEP,K)=DAT(12)
0014600        IF(DAT(14).EQ.0.0) DAT(14)=AREACT(STEP,K)
0014620 C      K=REACTANT NUMBER,I=REACTANT RATIO SET NUMBER
0014640 C      RATIO=RELATIVE NUMBER OF MOLES,FAZER=ALPHA LETTER INDICATING PHASE
0014700        DO 360 I=1,4
0014800    360 RATIO(STEP,K,I)=DAT(I+13)
0014900    380 STOICR(STEP,K)=AREACT(STEP,K)
0015000        IF(DAT(13).EQ.BA) BASE(STEP)=K
0015100        FAZER(STEP,K)=DAT(11)
0015200        IF(NRATIO(STEP).GE.1) GO TO 240
0015300        DO 400 I=1,4
0015400    400 IF(RATIO(STEP,K,I).NE.0.0) NRATIO(STEP)=NRATIO(STEP)+1
0015500        GO TO 240
0015550 C      PRODUCTS
0015600    420 KK=NPROD(STEP)+1
0015700        NPROD(STEP)=KK
0015720 C      KK=PRODUCT NUMBER,I=ELEMENT NUMBER,NPROD=NUMBER OF PRODUCTS
0015740 C      PATOM=ATOMIC SYMBOL,PATCO=ATOMIC COEFFICIENT
0015800        DO 440 I=1,4
0015900        PATOM(STEP,KK,I)=DAT(2*I+1)
0016000    440 PATCO(STEP,KK,I)=DAT(2*I+2)
0016100        FAZEP(STEP,KK)=DAT(11)
0016120 C      APROD=STOICHIOMETRIC COEFFICIENT,FAZEP=ALPHA LETTER INDICATING PHASE
0016200        APROD(STEP,KK)=DAT(12)
0016220 C      KK=PRODUCT NUMBER,I=REACTANT RATIO SET NUMBER
0016300        DO 460 I=1,4
0016400    460 TPHASE(STEP,KK,I)=DAT(I+13)
0016500    480 STOICP(STEP,KK)=APROD(STEP,KK)
0016600        GO TO 240
0016700    500 CONTINUE
0016800        TEST15=.TRUE.
0016900        GO TO 60
```

```
0017000 C  THIS SECTION READS THE NAMELISTS.
0017100   520 IF(.NOT.TEST15) GO TO 720
0017200       DO 700 I=1,NR
0017300       PRES=1.0
0017400       DO 560 K=1,10
0017500       T(K)=0.0
0017600       DO 540 J=1,4
0017700   540 EP(K,J)=0.0
0017800   560 CONTINUE
0017900       READ(8,NAM1)
0017920       WRITE(3,NAM1)
0018100       P(STEP)=PPES
0018200       DO 620 J=1,10
0018300       DO 580 K=1,4
0018400       EPSI(STEP,J,K)=EP(J,K)
0018500       IF(EPSI(STEP,J,K).NE.0.0) TEST1(STEP)=.TRUE.
0018600   580 CONTINUE
0018700       IF(I.EQ.1) GO TO 600
0018800       IF(T(J).EQ.0.0.AND.(J-1).NE.NOTEMP) GO TO 640
0018900   600 IF(T(J).EQ.0.0.AND.I.EQ.1) NOTEMP=J-1
0019000       IF(T(J).EQ.0.0) GO TO 680
0019100       TEMP1(STEP,J)=T(J)
0019200   620 TEMP2(STEP,J)=T(J)
0019300       NOTEMP=10
0019400       GO TO 680
0019500   640 WRITE(3,660) STEP
0019600   660 FORMAT('1','ERROR IN NUMBER OF TEMPERATURES FOR STEP',I2)
0019700       TEST20=.TRUE.
0019720   680 NT=NOTEMP-1
0019740       DO 690 J=1,NT
0019760       JL(I)=J
0019780       IF((T(J).EQ.T(J+1)).OR.(T(J+1).EQ.0.0)) GO TO 700
0019800   690 CONTINUE
0019820       JL(I)=NOTEMP
0019900   700 CONTINUE
0020000       GO TO 60
0020100   720 WRITE(3,740)
0020200   740 FORMAT(' ','DATA CARDS ARE OUT OF ORDER, NAMELISTS MUST BE AFTER  -
0020300      1REACTION CARDS')
0020400       TEST20=.TRUE.
0020500       GO TO 60
0020600   760 CONTINUE
0020620 C
0020640 C  THIS SECTION CHECKS TO SEE IF THE REACTIONS ARE BALANCED.
0020660 C
0020680       DO 980 NRX=1,NR
0020700       NPR=NREACT(NRX)
0020720       DO 840 I=1,NPR
0020740       IF(RATOM(NRX,I,1).EQ.HYD.AND.RATOM(NRX,I,2).EQ.BLANK) TRY=TRY-     -
0020760      1STOICR(NRX,I)
0020780       DO 820 J=1,4
0020800       IF(RATOM(NRX,I,J).EQ.BLANK) GO TO 840
0020820       IF(I.EQ.1.AND.J.EQ.1) GO TO 800
0020840       DO 780 N=1,NN
```

```
      IF(RATOM(NRX,I,J).NE.DAT(N)) GO TO 780
      T(N)=T(N)+RATCO(NRX,I,J)*STOICR(NRX,I)
      GO TO 820
  780 CONTINUE
      NN=NN+1
      DAT(NN)=RATOM(NRX,I,J)
      T(NN)=RATCO(NRX,I,J)*STOICR(NRX,I)
      GO TO 820
  800 NN=1
      DAT(1)=RATOM(NRX,1,1)
      T(1)=RATCO(NRX,1,1)*STOICR(NRX,1)
  820 CONTINUE
  840 CONTINUE
      NPP=NPROD(NRX)
      DO 920 I=1,NPP
      IF(PATOM(NRX,I,1).EQ.HYD.AND.PATOM(NRX,I,2).EQ.BLANK) TRY=TRY+     -
     1 STOICP(NRX,I)
      DO 900 J=1,4
      IF(PATOM(NRX,I,J).EQ.BLANK) GO TO 920
      DO 860 N=1,NN
      IF(PATOM(NRX,I,J).NE.DAT(N)) GO TO 860
      T(N)=T(N)-PATCO(NRX,I,J)*STOICP(NRX,I)
      GO TO 900
  860 CONTINUE
      WRITE(3,880) PATOM(NRX,I,J),NRX
      WRITE(9,880) PATOM(NRX,I,J),NRX
      BAL=.FALSE.
  880 FORMAT('0','THE ELEMENT ',A2,' IS IN THE PRODUCTS OF REACTION',I3,-
     1', BUT IS NOT IN THE REACTANTS')
      IF(DRAW) TEST20=.TRUE.
  900 CONTINUE
  920 CONTINUE
      SMALL=0.00001
      DO 960 N=1,NN
      TAB=ABS(T(N))
      IF(TAB.LE.SMALL) GO TO 960
      WRITE(3,940) NRX,DAT(N)
      WRITE(9,940) NRX,DAT(N)
      BAL=.FALSE.
  940 FORMAT('0','REACTION ',I3,' IS NOT BALANCED IN REGARD TO THE ELEME-
     1NT ',A2)
      IF(DRAW) TEST20=.TRUE.
  960 CONTINUE
  980 CONTINUE
 1060 REWIND 8
      RETURN
      END
```

```
0000100       SUBROUTINE REFMT
0000200 C     REFORMAT HYDRGN INPUT SPECIE NAMES FOR COMPARISON WITH CECS72 OUTPUT NAMES
0000220       LOGICAL*1 DAT(21)/21*Z40/
0000221       LOGICAL*1 T(256)/64*Z00,ZC1,10*Z00,Z01,164*Z00,Z01,Z01,14*Z00/
0000224       LOGICAL*1 TB(256)/64*Z00,Z01,191*Z00/
0000226       LOGICAL*1 TLS(256)/211*Z00,ZD3,14*Z00,ZE2,29*Z00/
0000228       LOGICAL*1 CL(3)/Z4D,ZD3,Z5D/
0000229       LOGICAL*1 CS(3)/Z4D,ZE2,Z5D/
0000230       LOGICAL XL
0000231       LOGICAL F4TRT
0000232       DIMENSION M(20),IC(20),N(20)
0000250       LOGICAL TEST20,GO
0000300       INTEGER STEP
0000400       DIMENSION DATA(20),TEMP(5),KR(11),KP(11)
0000450       DIMENSION TITLE(20)
0000500       EQUIVALENCE (DAT(1),TEMP(1))
0000520       COMMON/INDX/R,NR,NR1,NRXNS,NOTEMP,I,K,J,M,NRX,NTOT,BASE,NSATOM,NN
0000600       COMMON/CTL/RMF(10,4,10,5),PMF(10,4,10,5),REACT(11,5,4),PROD(11,5,4),JL(11),GO(11,4,13),IP(11,4),KBB(11,4)
0000610       DATA FINI/'FINI'/,WEND/'END'/,CHEM/'CHEM'/,CNAME/'NAME'/,THER/'THER'/,COMM/'NOTE'/
0000640       DATA BLANK/'    '/,REAC/'REAC'/,PRO/'PROD'/
0000645       DO 9 I=1,11
0000650       KR(I)=0
0000660     9 KP(I)=0
0001400       READ(8,50) (TITLE(I),I=1,20)
0001420    50 FORMAT(20A4)
0001440       IF(TITLE(1).EQ.FINI) GO TO 422
0002200    60 READ(8,80) (DATA(I),I=1,10)
0002300    80 FORMAT(20A4)
0002600   120 IF(DATA(1).EQ.WEND) GO TO 422
0002700       IF(DATA(1).EQ.BLANK) GO TO 60
0003100       IF(DATA(1).EQ.COMM) GO TO 60
0003200       IF(DATA(1).EQ.CHEM) GO TO 240
0003300       IF(DATA(1).EQ.CNAME) GO TO 60
0003900       GO TO 60
0003902 C     READ A REACTANT OR PRODUCT CARD
0003910   240 READ(8,11) STEP,DATA(1),DATA(2),(DAT(I),I=1,21)
0003920       IF(DATA(1).EQ.BLANK) GO TO 60
0003930       IF(DATA(1).EQ.REAC) ISP=1
0003940       IF(DATA(1).EQ.PRO) ISP=2
0003960       I=1
000398C       LF=1
0004000       LL=20
0004020 C     FIND SPACES,ZEROS,DECIMAL POINTS AND ONES
0004025 C     AND CLOSE UP STRING
0004040    20 IF(.NOT.F4TRT(DAT,LF,LL,T,M(I),IC(I),N(I))) GO TO 21
0004045       LF=M(I)
000405C       LL=LL-1
0004055       L1=LF+1
000406C       L2=20-LF
0004065       CALL F4MVC(DAT,L1,DAT,LF,L2)
0004100       GO TO 20
0004110    21 CONTINUE
00042RC       I=1
0004300       LF=21
```

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0000100       SUBROUTINE REFMT
0000200 C     REFORMAT HYDRGN INPUT SPECIE NAMES FOR COMPARISON WITH CECS72 OUTPUT NAMES
0000220       LOGICAL*1 DAT(21)/21*Z40/
0000221       LOGICAL*1 T(256)/64*Z00,ZC1,10*Z00,Z01,164*Z00,Z01,701,14*Z00/
0000224       LOGICAL*1 TB(256)/64*Z00,Z01,191*Z00/
0000226       LOGICAL*1 TLS(256)/211*Z00,ZD3,14*Z00,ZE2,29*Z00/
0000228       LOGICAL*1 CL(3)/Z4D,ZD3,Z5D/
0000229       LOGICAL*1 CS(3)/Z4D,ZE2,Z5D/
0000230       LOGICAL XL
0000231       LOGICAL F4TRT
0000232       DIMENSION M(20),IC(20),N(20)
0000250       LOGICAL TEST20,GO
0000300       INTEGER STEP
0000400       DIMENSION DATA(20),TEMP(5),KR(11),KP(11)
0000450       DIMENSION TITLE(20)
0000500       EQUIVALENCE (DAT(1),TEMP(1))
0000520       COMMON/INDX/R,NR,NR1,NRXNS,NOTEMP,I,K,J,M,NRX,NTOT,BASE,NSATOM,NN
0000600       COMMON/CTL/RMF(10,4,10,5),PMF(10,4,10,5),REACT(11,5,4),PROD(11,5,4),JL(11),GO(11,4,13),IP(11,4),KBB(11,4)
0000610       DATA FINI/'FINI'/,WEND/'END'/,CHEM/'CHEM'/,CNAME/'NAME'/,THER/'THER'/,COMM/'NOTE'/
0000640       DATA BLANK/'    '/,REAC/'REAC'/,PRO/'PROD'/
0000645       DO 9 I=1,11
0000650       KR(I)=0
0000660     9 KP(I)=0
0001400       READ(8,50) (TITLE(I),I=1,20)
0001420    50 FORMAT(20A4)
0001440       IF(TITLE(1).EQ.FINI) GO TO 422
0002200    60 READ(8,80) (DATA(I),I=1,10)
0002300    80 FORMAT(20A4)
0002600   120 IF(DATA(1).EQ.WEND) GO TO 422
0002700       IF(DATA(1).EQ.BLANK) GO TO 60
0003100       IF(DATA(1).EQ.COMM) GO TO 60
0003200       IF(DATA(1).EQ.CHEM) GO TO 240
0003300       IF(DATA(1).EQ.CNAME) GO TO 60
0003900       GO TO 60
0003902 C     READ A REACTANT OR PRODUCT CARD
0003910   240 READ(8,11) STEP,DATA(1),DATA(2),(DAT(I),I=1,21)
0003920       IF(DATA(1).EQ.BLANK) GO TO 60
0003930       IF(DATA(1).EQ.REAC) ISP=1
0003940       IF(DATA(1).EQ.PRO) ISP=2
0003960       I=1
0003980       LF=1
0004000       LL=20
0004020 C     FIND SPACES,ZEROS,DECIMAL POINTS AND ONES
0004025 C     AND CLOSE UP STRING
0004040    20 IF(.NOT.F4TRT(DAT,LF,LL,T,M(I),IC(I),N(I))) GO TO 21
0004045       LF=M(I)
0004050       LL=LL-1
0004055       L1=LF+1
0004060       L2=20-LF
0004065       CALL F4MVC(DAT,L1,DAT,LF,L2)
0004100       GO TO 20
0004110    21 CONTINUE
0004280       I=1
0004300       LF=21
```

```
0004320       LL=21
0004340 C     LIQUID OR SOLID?
0004360    23 IF(.NOT.F4TRT(DAT,LF,LL,TLS,M(I),IC(I),N(I))) GO TO 326
0004380       LS=N(I)
0004400 C     FIND FIRST BLANK
0004402       I=1
0004404       LF=1
0004415       LL=20
0004416       IF(.NOT.F4TRT(DAT,LF,LL,TB,M(I),IC(I),N(I))) GO TO 326
0004425       L1=M(I)
0004440    26 IF(LS.EQ.226) GO TO 27
0004500 C     LIQUID
0004520       CALL F4MVC(CL,1,DAT,L1,3)
0004540       GO TO 326
0004560 C     SOLID
0004580    27 CALL F4MVC(CS,1,DAT,L1,3)
0006100   326 GO TO (327,420), ISP
0006200 C     REACTANTS
0006220 C     KR=NUMBER OF REACTANTS/STEP
0006300   327 KR(STEP)=KR(STEP)+1
0006400       K=KR(STEP)
0006500       DO 328 I=1,3
0006600   328 REACT(STEP,K,I)=TEMP(I)
0006700       GO TO 240
0006800 C     PRODUCTS
0006820 C     KP=NUMBER OF PRODUCTS/STEP
0006900   420 KP(STEP)=KP(STEP)+1
0007000       KK=KP(STEP)
0007100       DO 421 I=1,3
0007200   421 PROD(STEP,KK,I)=TEMP(I)
0007300       GO TO 240
0007400   422 REWIND 8
0007500       RETURN
0007600    11 FORMAT(I2,2A4,21A1)
0007700       END
```

```
0000020       SUBROUTINE PREPAR
0000040 C     PREPARE INPUT DATA FOR CECS72
0003100       INTEGER CARD,STEP,BASE,A,R
0003200       REAL NOTE
0003300       LOGICAL TEST15,INS,GO
0003400       LOGICAL TEST1,TEST2,TEST20,PLINE,DRAW,SAME,THERM,H298
0003500       DOUBLE PRECISION XREACT,XPROD,SUMW,SUMRG,GASSUM
0003600       DOUBLE PRECISION H,S,G,HS,SS,GS,HTOT,STOT,GTOT,COEF,SUMPG,SUMPL
0003700       DIMENSION STOICR(11,5),STOICP(11,5),RATOM(11,5,4),PATOM(11,5,4),  -
0003800      1RATCO(11,5,4),PATCO(11,5,4),RATIO(10,5,4),P(50)
0003900       DIMENSION BASE(10),NSATOM(50),TEMP1(50,10),TEMP2(50,10),TRANGE(2,5-
0004000      10),T(20),TPHASE(11,5,4),TEST1(10),AREACT(10,5),APROD(10,5),      -
0004100      2NPROD(11),NREACT(11),NRATIO(10),DAT(25)     ,LNOTE(10),NOTE(10,100)-
0004200      3,HSTOCR(50),HSTOCP(50),FAZER(11,5),FAZEP(11,5),EP(10,4),EPSI(10,10-
0004300      4,4),HIM(10),HAM(10)
0004320       DIMENSION TITLE(20),INS(5)
0004400       COMMON/FNAME/STOICP,STOICP,RATOM,PATOM,RATCO,PATCO
0004500       COMMON/INDX/R,NR,NR1,NRXNS,NOTEMP,I,K,J,M,NRX,NTOT,BASE,NSATOM,NN
0004600       COMMON/TMP/TEMP1,TEMP2,TRANGE,TPHASE,TMID
0004700       COMMON/LOGIC/PLINE,TEST20,DRAW,SAME,TEST1,THERM,H298
0004800       COMMON/PRESS/P
0004900       COMMON/MATL3/AREACT,APROD,RATIO,NOTE,HSTOCR,HSTOCP,NPROD,NREACT,  -
0005000      1NRATIO,LNOTE
0005100       COMMON/FZE/SUMPL,SUMPG,SUMPS,FAZER,FAZEP,NGASP,NLIQP,NSOLP,NGASR, -
0005200      1NLIQR,NSOLR
0005300       COMMON/WORK/HIM,HAM,EPSI
0005320       COMMON/CTL/PMF(10,4,10,5),PMF(10,4,10,5),REACT(11,5,4),PROD(11,5,4),JL(11),GO(11,4,13),IP(11,4),KBB(11,4)
0005340       DATA XL/'L'/,XS/'S'/
0005900 C     REACTIONS
0006000       DO 8 STEP=1,NR
0006100       ILAST=NRATIO(STEP)
0006200       KLAST=NREACT(STEP)
0006220       KKLAST=NPROD(STEP)
0006300 C     REACTANT RATIOS
0006400       DO 7 I=1,ILAST
0006420 C-----IF INPUT EP.NE.0., DON'T CALCULATE EQUILIBRIUM WITH CECS72
0006440       IF(EPSI(STEP,1,I).NE.0.) GO TO 7
0006500 C     REACTANTS
0006520       WRITE(5,11)
0006600       DO 6 K=1,KLAST
0006700 C     ELEMENTS AND COEFFICIENTS IN A REACTANT
0006900       WRITE(5,12) (RATOM(STEP,K,IR),RATCO(STEP,K,IR),IR=1,4),RATIO(STEP,K,I)
0007000     6 CONTINUE
0007010 C     CHECK FOR LIQUID OR SOLID PRODUCTS
0007020       DO 4 KK=1,KKLAST
0007030       IF((FAZEP(STEP,KK).EQ.XL).OR.(FAZEP(STEP,KK).EQ.XS)) INS(KK)=.TRUE.
0007040     4 CONTINUE
0007100       WRITE(5,13)
0007110 C     ADD ANY INSERT CARDS REQUIRED
0007120       DO 5 KK=1,KKLAST
0007130       IF(INS(KK)) WRITE(5,18) (PROD(STEP,KK,IEP),IEP=1,3)
0007132       INS(KK)=.FALSE.
0007140     5 CONTINUE
0007200       WRITE(5,14)
```

```
0007220        J=JL(STEP)
0007300     21 WRITE(5,15) STEP,P(STEP),(TEMP2(STEP,JT),JT=1,J)
0007320        WRITE(5,17)
0007400      7 CONTINUE
0007500      8 CONTINUE
0007600        WRITE(5,16)
0007700        RETURN
0007800     11 FORMAT('REACTANT')
0007900     12 FORMAT(4(A2,F7.5),9X,F7.5,'M')
0008000     13 FORMAT(' ')
0008100     14 FORMAT('NAMELIST')
0008200     15 FORMAT(' &INPT2 KASE= ',I2,',TP=T,P= ',F7.3,',T= ',10(F6.1,','))
0008220     17 FORMAT(' &END')
0008300     16 FORMAT('STOP')
0008320     18 FORMAT('INSERT',9X,3A4)
0008400        END
```

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               CON2

0000200 C      READ INPUT DATA FOR HYDRGN
0000300        CALL READ
0000600 C      MAKE SPECIE NAMES COMPATIBLE
0000700        CALL REFMT
0000800 C      READ CECS72 OUTPUT
0000900        CALL READ72
0000920 C      CHECK CECS72 OUTPUT FOR PRODUCTS NOT IN HYDRGN INPUT
0000940        CALL EXTRA
0000960 C      CALCULATE EPSILON
0000980        CALL EPSLN
0001000 C      MODIFY HYDRGN INPUT
0001020        CALL MODIFY
0001100        STOP
0001200        END
```

```
      SUBROUTINE READ72
C     READ CEC572 OUTPUT DATA
      LOGICAL*1 DATA(4)
      DIMENSION TEM1(3),TEM2(13),XMF(13)
      DIMENSION IRR(4)
      COMMON/INDX/R,NR,NP1,NRXNS,NOTEMP,I,K,J,M,NRX,NTOT,BASE,NSATOM,NN
      COMMON/TMP/TEMP1,TEMP2,TRANGE,TPHASE,TMIC
      COMMON/PRD/PRO(11,4,10,3),FRAC(11,4,10,13),TITLE(20)
      COMMON/PRESS/PR
      DIMENSION BASE(10),NSATOM(50),TEMP1(50,10),TEMP2(50,10),TRANGE(2,5-
     10),TT(20),TPHASE(11,5,4),TEST1(10),AREACT(10,5),APROD(10,5),
     2NPROD(11),NREACT(11),NRATIO(10),DATT(25)    ,LNOTE(10),NOTE(10,100)-
     3,HSTOCR(50),HSTOCP(50),FAZER(11,5),FAZEP(11,5),EP(10,4),EPSI(10,10-
     4,4),HIM(10),HAM(10)
      DIMENSION T(26),P(26),V(13),RHO(26),EQPGM(10),PR(50)
      REAL MIX(15)
      LOGICAL GO,CONV
      LOGICAL PSIA,MMHG,NSQM,ERATIO,OF,FPCT,FA,TP,HP,SP,TV,UV,SV,RKT,SHOCK,DETN,OTTO,IONS,SIUNIT,PHI,INHG
      DATA REAC/' REA'/,CMOLE/'OMOL'/,STOP/' STO'/,ADDI/'ADDI'/,CNAME/' NAM'/,WARN/'OWAR'/
      INTEGER STEP
      COMMON/CTL/RMF(10,4,10,5),PMF(10,4,10,5),REACT(11,5,4),PROD(11,5,4),JL(11),GO(11,4,13),IP(11,4),KBB(11,4)
      COMMON/CONVG/ CONV(11,4,10)
      NAMELIST/INPT2/KASE,T,P,PSIA,MMHG,NSQM,V,RHO,ERATIO,OF,FPCT,FA,-
     1MIX,TP,HP,SP,TV,UV,SV,RKT,SHOCK,DETN,OTTO,CR,SO,SD,IONS,IDEBUG,-
     2TRACE,SIUNIT,EQPGM,PHI,INHG
      EQUIVALENCE (DATA(1),DAT)
      DATA CS/'OCAL'/,SING/'OSIN'/,THM/'OTHE'/
      DO 16 JT=1,13
      DO 16 K=1,4
      DO 16 STEP=1,NP
      CONV(STEP,K,JT)=.TRUE.
   16 GO(STEP,K,JT)=.FALSE.
    1 READ(7,10) (DATA(J),J=1,4)
      IF(DAT.EQ.STOP) GO TO 21
C     FIND THE REACTANT CARD
      IF(DAT.NE.REAC) GO TO 1
    5 READ(7,10) (DATA(J),J=1,4)
      IF(DAT.EQ.STOP) GO TO 21
C     FIND THE NAMELIST CARD
      IF(DAT.NE.CNAME) GO TO 6
      READ(7,INPT2)
      STEP=KASE
C     IRR=NUMBER OF REACTANT RATIOS/STEP
      IRR(STEP)=IRR(STEP)+1
      II=IRR(STEP)
      GO TO 5
C     CHECK FOR WARNING MESSAGE THAT CONDENSED PRODUCTS MAY NOT BE CORRECT
    6 IF(DAT.NE.WARN) GO TO 13
      WRITE(3,29) STEP,II
      WRITE(9,29) STEP,II
   13 IF(DAT.NE.CS) GO TO 15
C     NO CONVERGENCE OR SINGULAR MATRIX
      BACKSPACE 7
      READ(7,32) NOCON
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```
0001160        NCON=NOCON+1
0001180        WRITE(3,31) STEP,II,NCON
0001185        WRITE(9,31) STEP,II,NCON
0001200        JL(STEP)=NCON
0001220        DO 14 J=NCON,NOTEMP
0001240        CONV(STEP,II,J)=.FALSE.
0001260     14 IF(NOCON.NE.0) TEMP1(STEP,J)=TEMP1(STEP,NOCON)
0001280        GO TO 5
0001290 C      FIND THE THERMODYNAMIC PROPERTIES CARD
0001295     15 IF(DAT.NE.THM) GO TO 17
0001300        READ(7,10) (DATA(J),J=1,4)
0001305        READ(7,10) (DATA(J),J=1,4)
0001310 C      READ THE PRESSURES AND TEMPERATURES
0001320        READ(7,34) PR(STEP)
0001380        READ(7,34) (TEMP2(STEP,I),I=1,10)
0001385        GO TO 5
0002120 C      FIND THE MOLE FRACTION CARD
0002140     17 IF(DAT.NE.CMOLE) GO TO 5
0002160        KK=1
0002180      3 DO 12 IT=1,13
0002200        TEM2(IT)=0.
0002220     12 XMF(IT)=0.
0002240        IIT=JL(STEP)
0002260        READ(7,10) (DATA(J),J=1,4)
0002280        READ(7,10) (DATA(J),J=1,4)
0002300 C      READ PRODUCTS AND MOLE FRACTIONS
0002320      4 READ(7,11) (TEM1(IR),IR=1,3),FB,(TEM2(IT),IT=1,IIT)
0002340 C      IP=NUMBER OF PRODUCTS FOR THIS STEP AND REACTANT RATIO
0002360        IP(STEP,II)=KK
0002380 C      II=REACTANT RATIO, KK=PRODUCT NUMBER
0002400        DO 2 I=1,3
0002420      2 PRO(STEP,II,KK,I)=TEM1(I)
0002440        DO 7 I=1,IIT
0002460      7 FRAC(STEP,II,KK,I)=TEM2(I)
0002480        KK=KK+1
0002500 C      CHECK TO SEE IF ALL PRODUCTS FOR THIS REACTANT RATIO HAVE BEEN READ
0002520        DO 8 IT=1,IIT
0002540      8 XMF(IT)=XMF(IT)+TEM2(IT)
0002560        DO 9 IT=1,IIT
0002580        IF(((1.0-XMF(IT)).GE.0.00002).AND.(XMF(IT).NE.0.0)) GO TO 4
0002600        GO(STEP,II,IT)=.TRUE.
0002620      9 CONTINUE
0002860        GO TO 1
0002880 C      PRINT THE PRODUCTS AND MOLE FRACTIONS
0002900     21 WRITE(3,30)
0002920        DO 25 IS=1,STEP
0002925        IF(JL(IS).EQ.0.) GO TO 25
0002940        IIT=JL(IS)
0002960        WRITE(3,33) IS,(TEMP1(IS,JT),JT=1,IIT)
0002965        WRITE(3,35) PR(IS)
0002980        IF(IIT.EQ.0) GO TO 25
0003000        II=IRR(IS)
0003020        DO 24 IR=1,II
0003040        IF(II.NE.1) WRITE(3,26) IR
```

```
      KP=IP(IS,IR)
      DO 23 K=1,KP
      WRITE(3,28) (PRO(IS,IR,K,IN),IN=1,3),(FRAC(IS,IR,K,IT),IT=1,IIT)
   23 CONTINUE
   24 CONTINUE
   25 CONTINUE
      RETURN
   10 FORMAT(4A1)
   11 FORMAT(1X,3A4,A2,13F9.0)
   26 FORMAT(1X,'REACTANT RATIO  ',I1)
   28 FORMAT(3X,3A4,9X,13F9.5)
   29 FORMAT('0','***  WARNING- CONDENSED PRODUCTS MAY NOT BE CORRECT FOR STEP ',I2,' REACTANT RATIO ',I1,'***')
   30 FORMAT('1','THE EQUILIBRIUM MOLE FRACTION  DISTRIBUTION OF SPECIES CALCULATED BY CECS72')
   31 FORMAT('1','*NO CONVERGENCE OR SINGULAR MATRIX FOR STEP ',I2,', REACTANT RATIO ',I1,-
     1', TEMPERATURE SCHEDULE ',I1,'*'/1X,'TRY A DIFFERENT INSERT')
   32 FORMAT(33X,I3)
   33 FORMAT(1X,'STEP ',I2,'   TEMPERATURE= ',10(3X,F6.1))
   34 FORMAT(15X,13F9.0)
   35 FORMAT(14X,'PRESSURE= ',10(3X,F6.2))
      END
```

```
      SUBROUTINE MODIFY
C     MODIFY HYDRGN INPUT BASED ON CECS72 RESULTS
      INTEGER CARD,STEP,BASE,A,B
      REAL NOTE
      DOUBLE PRECISION XREACT,XPROD,SUMW,SUMRG,GASSUM
      DOUBLE PRECISION H,S,G,HS,SS,GS,HTOT,STOT,GTOT,COEF,SUMPG,SUMPL
      DIMENSION STOICR(11,5),STOICP(11,5),RATOM(11,5,4),PATOM(11,5,4),  -
     1RATCO(11,5,4),PATCO(11,5,4),RATIO(10,5,4),P(50)
      DIMENSION BASE(10),NSATOM(50),TEMP1(50,10),TEMP2(50,10),TRANGE(2,5-
     10),TMID(10),TPHASE(11,5,4),TEST1(10),AREACT(10,5),APROD(10,5),   -
     2NPROD(11),AREACT(11),NRATIO(10),DAT(25)    ,LNOTE(10),NOTE(10,100)-
     3,HSTOCR(50),HSTOCP(50),FAZEP(11,5),FAZEP(11,5),EP(10,4),EPSI(10,10-
     4,4),HIM(10),HAM(10)
      DIMENSION RR(11),PP(11),NC(4)
      LOGICAL GO,NOGO,NC,CONV
      LOGICAL DRAW,SAME,H298
      COMMON/CTL/RMF(10,4,10,5),PMF(10,4,10,5),REACT(11,5,4),PROD(11,5,4),JL(11),GO(11,4,13),IP(11,4),KBB(11,4)
      COMMON/ENAME/STOICR,STOICP,RATOM,PATOM,RATCO,PATCO
      COMMON/INDX/R,NR,NR1,NRXNS,NCTEMP,I,K,J,M,NRX,NTOT,BASE,NSATOM,NN
      COMMON/LOGIC/PLINE,TEST20,DRAW,SAME,TEST1,THERM,H298
      COMMON/CONVG/CONV(11,4,10)
      COMMON/PRESS/P
      COMMON/TMP/TEMP1,TEMP2,TRANGE,TPHASE,TMID
      COMMON/MATL3/AREACT,APROD,RATIO,NOTE,HSTOCR,HSTOCP,NPROD,NREACT,  -
     1NRATIO,LNOTE
      COMMON/FZE/SUMPL,SUMPG,SUMPS,FAZEP,FAZEP,NGASP,NLIQP,NSOLP,NGASP, -
     1NLIQP,NSOLP
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0002100       COMMON/WORK/HIM,HAM,EPSI
0002200       COMMON/PRD/PRO(11,4,10,3),FRAC(11,4,10,13),TITLE(20)
0002205       DATA BA/'B'/,BB/' '/,XLOW/.01/
0002220       NAMELIST/NAM1/STEP,T,EP,PRES,DRAW,SAME,H298
0002240       DO 4 STEP=1,NR
0002260       NT=JL(STEP)
0002280       NRR=NRATIO(STEP)
0002300       DO 3 K=1,NRR
0002320       DO 2 J=1,NT
0002340       IF(CO(STEP,K,J)) GO TO 5
0002360       NOGO=.TRUE.
0002380       IF(CONV(STEP,K,J)) WRITE(3,40) STEP,K,TEMP1(STEP,J)
0002381       IF(CONV(STEP,K,J)) WRITE(9,40) STEP,K,TEMP1(STEP,J)
0002382       GO TO 2
0002384     5 IF(EPSI(STEP,J,K).GE.XLOW) GO TO 2
0002386       NOGO=.TRUE.
0002388       WRITE(3,43) STEP,K,TEMP1(STEP,J)
0002390       WRITE(9,43) STEP,K,TEMP1(STEP,J)
0002400     2 CONTINUE
0002420     3 CONTINUE
0002440     4 CONTINUE
0003322 C     WRITE INPUT DATA SET FOR HYDRGN
0003324       WRITE(5,31) (TITLE(I),I=1,20)
0003326 C     CHEMICAL REACTIONS
0003328       WRITE(5,32)
0003330       DO 25 STEP=1,NR
0003332       KB=BASE(STEP)
0003334       NRE=NREACT(STEP)
0003336       NPR=NPROD(STEP)
0003338       NRR=NRATIO(STEP)
0003340 C     REACTANTS
0003360       DO 23 K=1,NRE
0003380       IF(K.EQ.KB) SB=BA
0003400       WRITE(5,33) STEP,(RATCM(STEP,K,IR),RATCO(STEP,K,IR),IR=1,4),FAZER(STEP,K),-
0003420      1AREACT(STEP,K),SB,(RATIO(STEP,K,IR),IR=1,4)
0003440       SB=BB
0003460    23 CONTINUE
0003480 C     PRODUCTS
0003500       DO 24 KK=1,NPR
0003520    24 WRITE(5,34) STEP,(PATCM(STEP,KK,IR),PATCO(STEP,KK,IR),IR=1,4),FAZEP(STEP,KK),-
0003540      1APROD(STEP,KK),BB,(TPHASE(STEP,KK,IR),IR=1,4)
0003560    25 CONTINUE
0003565       WRITE(5,39)
0003580 C     NOTES
0003585       WRITE(5,35)
0003600       DO 27 STEP=1,NR
0003620 C     IF ANY LNOTE.NE.0 WRITE NOTE
0003640       IF(LNOTE(STEP).EQ.0) GO TO 27
0003660       LN=LNOTE(STEP)/19
0003680       DO 26 L=1,LN
0003700       IL=1
0003720       IH=19
0003740       WRITE(5,36) STEP,L,(NOTE(STEP,I),I=IL,IH)
0003760       IL=IL+19
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0003780        IH=IH+19
0003800     26 CONTINUE
0003920     27 CONTINUE
0003921        WRITE(5,39)
0003825 C      NAMELISTS
0003940        WRITE(5,37)
0003850        DO 30 STEP=1,NR
0003980        NRR=NRATIO(STEP)
0003900        DO 29 J=1,NOTEMP
0003920        T(J)=TEMP1(STEP,J)
0003930        DO 28 K=1,NRR
0003760     28 EP(J,K)=EPSI(STEP,J,K)
0003980     29 CONTINUE
0004000        PRES=P(STEP)
0004020        WRITE(5,NAM1)
0004022        DO 42 J=1,NOTEMP
0004024        T(J)=0.0
0004026        DO 41 K=1,NRR
0004028     41 EP(J,K)=0.0
0004030     42 CONTINUE
0004040     30 CONTINUE
0004060        WRITE(5,38)
0004080        RETURN
0004081     31 FORMAT(20A4)
0004084     32 FORMAT('CHEMICAL REACTIONS  ')
0004086     33 FORMAT(I2,'REACTANT',4(A2,F3.0),A1,F9.4,A1,4F8.3)
0004088     34 FORMAT(I2,'PRODUCT ',4(A2,F3.0),A1,F9.4,A1,4F8.3)
0004090     35 FORMAT('NOTES    ')
0004092     36 FORMAT(2I2,19A4)
0004094     37 FORMAT('NAMELISTS   ')
0004096     38 FORMAT('END ')
0004100     39 FORMAT(' ')
0004105     40 FORMAT('0','TOO LARGE A CONCENTRATION OF EXTRA PRODUCTS FOR STEP ',I2,-
0004110       1' REACTANT RATIO ',I1,' TEMPERATURE = ',F6.1,' K.  HYDRGN WILL NOT BE RUN.')
0004112     43 FORMAT('1','EXTENT OF REACTION FOR STEP ',I2,' REACTANT RATIO ',I1,-
0004114       1' TEMPERATURE ',F6.1,' K WAS TOO SMALL.  HYDRGN WILL NOT BE RUN.')
0004120        END



0000100        SUBROUTINE EPSLN
0000200 C      CALCULATE EPSILON BASED ON CEQS72 OUTPUT
0000300        INTEGER CARD,STEP,BASE,A,P
0000320        DOUBLE PRECISION XREACT,XPROD,SUMW,SUMRG,CASSUM
0000340        DOUBLE PRECISION H,S,G,HS,SS,GS,HTOT,STOT,GTOT,COEF,SUMPG,SUMPL
0000400        DIMENSION STOICP(11,5),STOICR(11,5),RATOM(11,5,4),PATOM(11,5,4),  -
0000500       1RATCO(11,5,4),PATCO(11,5,4),RATIO(10,5,4),P(50)
0000600        DIMENSION BASE(10),NSATOM(50),TEMP1(50,10),TEMP2(50,10),TRANGE(2,5-
0000700       10),T(20),TPHASE(11,5,4),TEST1(10),AREACT(10,5),APROD(10,5),      -
0000800       2APROD(11),NREACT(11),NRATIO(10),DAT(25)    ,LNOTE(10),NOTE(10,100)-
0000900       3,HSTOCP(50),HSTOCR(50),EAZER(11,5),EAZEP(11,5),EP(10,4),EPSI(10,10-
0001000       4,4),HIM(10),HAM(10)
0001200        LOGICAL CC,CONV
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0001300       COMMON/CTL/RMF(10,4,10,5),PMF(10,4,10,5),REACT(11,5,4),PROD(11,5,4),JL(11),GO(11,4,13),IP(11,4),KBB(11,4)
0001400       COMMON/ENAME/STOICR,STOICP,RATOM,PATOM,RATCO,PATCO
0001500       COMMON/INDX/R,NR,NR1,NRXNS,NOTEMP,I,K,J,M,NRX,NTOT,BASE,NSATOM,NN
0001600       COMMON/TMP/TEMP1,TEMP2,TRANGE,TPHASE,TMIC
0001700       COMMON/MATL3/AREACT,APROD,RATIO,NOTE,HSTOCR,HSTOCP,NPROD,NREACT,  -
0001800      1NRATIO,LNOTE
0001900       COMMON/FZE/SUMPL,SUMPC,SUMPS,FAZER,FAZEP,NGASP,NLIQP,NSOLP,NGASR,  -
0002000      1NLIQR,NSOLR
0002100       COMMON/WORK/HIM,HAM,EPSI
0002120       COMMON/PRD/PRO(11,4,10,3),FRAC(11,4,10,13),TITLE(20)
0002140       COMMON/CONVC/CONV(11,4,10)
0002145       COMMON/PRESS/PR
0002160       DIMENSION PR(50)
0002200       DIMENSION EPSL(11,4,13),XNUM(11,4),XDEN(11
0002220       IDONE=0
0002300       DO 5 STEP=1,NR
0002400       KB=BASE(STEP)
0002500       NRE=NREACT(STEP)
0002600       NPR=NPROD(STEP)
0002700       NRR=NRATIO(STEP)
0002800 C     REACTANT RATIOS
0002900       DO 2 I=1,NRR
0003000       S1=0.0
0003100 C     REACTANT MOLE RATIOS
0003200       DO 1 K=1,NRE
0003300     1 S1=S1+RATIO(STEP,K,I)
0003320       XNUM(STEP,I)=S1/RATIO(STEP,KB,I)
0003400     2 CONTINUE
0003500       S3=0.
0003600 C     REACTANT STOICHIOMETRIC COEFFICIENTS
0003700       DO 3 K=1,NRE
0003800     3 S3=S3+AREACT(STEP,K)
0003900       S2=0.
0004000 C     PRODUCT STOICHIOMETRIC COEFFICIENTS
0004100       DO 4 KK=1,NPR
0004200     4 S2=S2+APROD(STEP,KK)
0004300       XDEN(STEP)=(S2-S3)/AREACT(STEP,KB)
0004400     5 CONTINUE
0004500 C     CALCULATE EPSILON
0004600       DO 13 STEP=1,NR
0004800       NRR=NRATIO(STEP)
0004900       NT=JL(STEP)
0005000 C     REACTANT RATIOS
0005100       DO 12 K=1,NRR
0005220       KK=KBB(STEP,K)
0005300 C     TEMPERATURES
0005400       DO 11 J=1,NT
0005420       EPSL(STEP,K,J)=1.
0005422       IF(EPSI(STEP,J,K).EQ.0.) GO TO 33
0005424 C-----IF INPUT EP.NE.0.
0005425       IF(IDONE.NE.0) GO TO 34
0005426       WRITE(3,21)
0005427       IDONE=IDONE+1
0005428    34 XMUL=EPSI(STEP,J,K)/AREACT(STEP,KB)
0005430       DENOM=XNUM(STEP,K)+EPSI(STEP,J,K)*XDEN(STEP)
0005432 C-----REACTANTS
0005434       DO 31 KR=1,NRE
0005436       IF(KR.EQ.KB) GO TO 31
0005438       FRAC(STEP,K,KR,J)=(RATIO(STEP,K,KR)-XMUL*AREACT(STEP,KR))/DENOM
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0005442    31 CONTINUE
0005444 C-----BASE REACTANT
0005446       FRAC(STEP,K,KB,J)=(1.-EPSI(STEP,J,K))/DENOM
0005448 C-----PRODUCTS
0005450       DO 32 KP=1,NPR
0005451       KKP=NRE+KP
0005454       FRAC(STEP,K,KKP,J)=(XMUL*APROD(STEP,KP))/DENOM
0005458    32 CONTINUE
0005461       IF(CONV(STEP,J,K)) GO(STEP,J,K)=.TRUE.
0005464       WRITE(3,17) STEP,TEMP2(STEP,1)
0005466       WRITE(3,24) PR(STEP)
0005468       DO 35 KP=1,NRE
0005470    35 WRITE(3,25) (REACT(STEP,KP,I),I=1,3),FRAC(STEP,K,KP,J)
0005472       DO 36 KP=1,NPR
0005474       KKP=NRE+KP
0005476    36 WRITE(3,25) (PROD(STEP,KP,I),I=1,3),FRAC(STEP,K,KKP,J)
0005500    33 IF(KK.NE.0) EPSL(STEP,K,J)=(1.-FRAC(STEP,K,KK,J)*XNUM(STEP,K))/(1.+FRAC(STEP,K,KK,J)*XDEN(STEP))
0005520       IF(CONV(STEP,K,J)) EPSI(STEP,J,K)=EPSL(STEP,K,J)
0005700    11 CONTINUE
0005900    12 CONTINUE
0005950    13 CONTINUE
0005952 C     COPY EPSI FOR DUPLICATE TEMPERATURES THAT WERE NOT CALCULATED BY CECS72
0005954       DO 16 STEP=1,NR
0005956       NT=JL(STEP)
0005957       IF(NT.EQ.0) NT=NT+1
0005958       IF(NT.EQ.NOTEMP) GO TO 16
0005960       NRR=NRATIO(STEP)
0005962       NT=NT+1
0005964       DO 15 K=1,NRR
0005966       DO 14 J=NT,NOTEMP
0005967       GO(STEP,K,J)=GO(STEP,K,J-1)
0005968       EPSI(STEP,J,K)=EPSI(STEP,J-1,K)
0005969       TEMP1(STEP,J)=TEMP1(STEP,J-1)
0005970    14 CONTINUE
0005972    15 CONTINUE
0005974    16 CONTINUE
0005975 C     WRITE OUT THE EPSILONS
0005980       WRITE(3,20)
0006000       DO 23 STEP=1,NR
0006010       NT=JL(STEP)
0006040       WRITE(3,17) STEP,(TEMP2(STEP,JT),JT=1,NT)
0006060       NRR=NRATIO(STEP)
0006080       DO 22 K=1,NRR
0006100       IF(NRR.NE.1) WRITE(3,18) K
0006120    22 WRITE(3,19) (EPSI(STEP,J,K),J=1,NT)
0006140    23 CONTINUE
0006160       RETURN
0006180    17 FORMAT(1X,'STEP ',I2,'  TEMPERATURE= ',10(3X,F6.1))
0006200    18 FORMAT(1X,'REACTANT RATIO ',I1)
0006220    19 FORMAT(3X,'EPSILON',13X,11F9.5)
0006240    20 FORMAT('1','EXTENT OF REACTION BASED ON REACTION AS ORIGINALLY WRITTEN')
0006260    21 FORMAT('1','MOLE FRACTION DISTRIBUTION BASED ON INPUT EPSILON')
0006280    24 FORMAT(13X,'PRESSURE= ',3X,F6.2)
0006300    25 FORMAT(3X,3A4,9X,13F9.5)
0006400       END
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      SUBROUTINE EXTRA
C     CHECK FOR CEQS72 OUTPUT PRODUCTS THAT ARE NOT IN HYDRGN INPUT
      INTEGER CARD,STEP,BASE,A,P
      DOUBLE PRECISION XREACT,XPROD,SUMW,SUMRG,GASSUM
      DOUBLE PRECISION H,S,G,HS,SS,GS,HTOT,STOT,GTOT,COEF,SUMPG,SUMPL
      DIMENSION STOICP(11,5),STOICR(11,5),RATOM(11,5,4),PATOM(11,5,4),
     1RATCO(11,5,4),PATCO(11,5,4),RATIO(10,5,4),P(50)
      DIMENSION BASE(10),NSATOM(50),TEMP1(50,10),TEMP2(50,10),TRANGE(2,5
     10),T(20),TPHASE(11,5,4),TEST1(10),AREACT(10,5),APROD(10,5),
     2NPROD(11),NREACT(11),NRATIO(10),DAT(25)    ,LNOTE(10),NOTE(10,100)
     3,HSTOCR(50),HSTOCP(50),FAZER(11,5),FAZEP(11,5),EP(10,4),EPSI(10,10
     4,4),HIM(10),HAM(10)
      LOGICAL GO,FS,EP
      COMMON/CTL/PMF(10,4,10,5),PMF(10,4,10,5),REACT(11,5,4),PROD(11,5,4),JL(11),GO(11,4,13),IP(11,4),KBB(11,4)
      COMMON/ENAME/STOICR,STOICP,RATOM,PATOM,RATCO,PATCO
      COMMON/INDX/R,NR,NR1,NRXAS,NOTEMP,I,K,J,M,NRX,NTOT,BASE,NSATOM,NN
      COMMON/TMP/TEMP1,TEMP2,TRANGE,TPHASE,TMID
      COMMON/MATL3/AREACT,APROD,RATIO,NOTE,HSTOCR,HSTOCP,NPROD,NREACT,
     1NRATIO,LNOTE
      COMMON/FZE/SUMPL,SUMPG,SUMRS,FAZER,FAZEP,NGASP,NLIQP,NSOLP,NGASR,
     1NLIQR,NSOLR
      COMMON/WORK/HIM,HAM,EPSI
      LOGICAL F4CLC
      COMMON/PRD/PRO(11,4,10,3),FRAC(11,4,10,13),TITLE(20)
      DIMENSION S1(3),S2(3),SR(3),SIG(13)
      DATA X1RMAX/.06/
      FS=.TRUE.
      DO 12 STEP=1,NR
      KB=BASE(STEP)
      NRE=NREACT(STEP)
      NPR=NPROD(STEP)
      NRR=NRATIO(STEP)
      NT=JL(STEP)
      IF(NT.EQ.0) GO TO 12
      DO 9 I=1,3
    9 SR(I)=REACT(STEP,KB,I)
C     REACTANT RATIOS
      DO 11 KRR=1,NRR
      IF(EPSI(STEP,1,KRR).NE.0.) GO TO 11
      EP=.TRUE.
      KP=IP(STEP,KRR)
      DO 1 I=1,12
    1 SIG(I)=0.0
C     CEQS72 PRODUCTS
      DO 10 KK=1,KP
      DO 2 I=1,3
    2 S1(I)=PRO(STEP,KRR,KK,I)
C     HYDRGN REACTANTS
      DO 4 K=1,NRE
      DO 3 I=1,3
    3 S2(I)=REACT(STEP,K,I)
      IF(F4CLC(S1,1,SR,1,12)) KBB(STEP,KRR)=KK
      IF(F4CLC(S1,1,S2,1,12)) GO TO 10
    4 CONTINUE
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0001140 C      HYDRGN PRODUCTS
0001160        DO 6 KJ=1,KRR
0001180        DO 5 I=1,3
0001200      5 S2(I)=PROD(STEP,KJ,I)
0001220        IF(FACLC(S1,1,S2,1,12)) GO TO 10
0001240      6 CONTINUE
0001260 C      CECS72 PRODUCTS NOT IN HYDRGN INPUT
0001262        IF(FS) WRITE(3,21)
0001264        FS=.FALSE.
0001266        IF(FP) WRITE(3,22) STEP,KRR
0001268        FP=.FALSE.
0001280        WRITE(3,24) S1,(FRAC(STEP,KRR,KK,JT),JT=1,NT)
0001300 C      ADD UP MOLE FRACTIONS OF THESE PRODUCTS FOR EACH TEMPERATURE
0001320        DO 7 JT=1,NT
0001340      7 SIG(JT)=SIG(JT)+FRAC(STEP,KRR,KK,JT)
0001360     10 CONTINUE
0001380        DO 8 JT=1,NT
0001400        IF(SIG(JT).GE.XTRMAX) GC(STEP,KRR,JT)=.FALSE.
0001419      8 CONTINUE
0001440     11 CONTINUE
0001460     12 CONTINUE
0001480        RETURN
0001500     21 FORMAT('1','CECS72 PRODUCTS NOT IN HYDRGN INPUT')
0001520     22 FORMAT(1X,'STEP=',I2,'  REACTANT RATIO ',I1)
0001540     24 FORMAT(1X,3A4,13F9.5)
0001560        END
```

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TABLE I. - DESCRIPTION OF CYCLES

Reported (ref. 2)			Revised		
1. Mg(A)					
$MgO(s) + SO_2 + H_2O + S(\ell)$	500 K	$MgSO_4(s) + H_2S$	$MgO(s) + SO_2 + H_2O + S(\ell)$	600 K	$MgSO_4(s) + H_2S$
$MgSO_4(s)$	1400 K	$MgO(s) + SO_2 + 0.5\ O_2$	$MgSO_4(s)$	1400 K	$MgO(s) + SO_2 + 0.5\ O_2$
H_2S	1300 K	$H_2 + S$	H_2S	1300 K	$H_2 + 0.5\ S_2$
			$0.5\ S_2$	718 K	$S(\ell)$
2. Mg(B)					
$MgO(s) + SO_2 + H_2O + S(\ell)$	500 K	$MgSO_4(s) + H_2S$	$MgO(s) + SO_2 + H_2O + S(\ell)$	600 K	$MgSO_4(s) + H_2S$
$MgSO_4(s)$	1400 K	$MgO(s) + SO_2 + 0.5\ O_2$	$MgSO_4(s)$	1400 K	$MgO(s) + SO_2 + 0.5\ O_2$
$H_2S + 0.67\ Bi(s)$	500 K	$0.33\ Bi_2S_3(s) + H_2$	$H_2S + 0.67\ Bi(s)$	500 K	$0.33\ Bi_2S_3(s) + H_2$
$0.33\ Bi_2S_3(s)$	1000 K	$0.67\ Bi(\ell) + S$	$0.33\ Bi_2S_3(s)$	1000 K	$0.67\ Bi(\ell) + 0.5\ S_2$
			$0.5\ S_2$	718 K	$S(\ell)$
3. Zn-Ba					
$0.25\ BaS(s) + H_2O$	500 K	$0.25\ BaSO_4(s) + H_2$	$0.25\ BaS(s) + H_2O$	500 K	$0.25\ BaSO_4(s) + H_2$
$0.25\ BaSO_4(s) + 0.5\ S$	1400 K	$0.25\ BaS(s) + 0.5\ SO_2$	$0.25\ BaSO_4(s) + 0.05\ S_2 + 0.05\ S_8$	1400 K	$0.25\ BaS(s) + 0.5\ SO_2$
$ZnO(s) + 1.5\ SO_2$	500 K	$ZnSO_4(s) + 0.5\ S(\ell)$	$ZnO(s) + 1.5\ SO_2$	500 K	$ZnSO_4(s) + 0.5\ S(\ell)$
$ZnSO_4(s)$	1300 K	$ZnO(s) + SO_2 + 0.5\ O_2$	$ZnSO_4(s)$	1300 K	$ZnO(s) + SO_2 + 0.5\ O_2$
			$0.5\ S(\ell)$	850 K	$0.05\ S_2 + 0.05\ S_8$
4. Zn-Ca(A)					
$0.25\ CaS(s) + S(\ell) + H_2O$	500 K	$0.25\ CaSO_4(s) + H_2S$	$0.25\ CaS(s) + S(\ell) + H_2O$	500 K	$0.25\ CaSO_4(s) + H_2S$
$0.25\ CaSO_4(s) + 0.5\ S$	1400 K	$0.25\ CaS(s) + 0.5\ SO_2$	$0.25\ CaSO_4(s) + 0.25\ S_2$	1400 K	$0.25\ CaS(s) + 0.5\ SO_2$
$H_2S + 0.67\ Bi(s)$	500 K	$0.33\ Bi_2S_3(s) + H_2$	$H_2S + 0.67\ Bi(s)$	500 K	$0.33\ Bi_2S_3(s) + H_2$
$0.33\ Bi_2S_3(s)$	1000 K	$0.67\ Bi(\ell) + S$	$0.33\ Bi_2S_3(s)$	1000 K	$0.67\ Bi(\ell) + 0.5\ S_2$
$ZnO(s) + 1.5\ SO_2$	500 K	$ZnSO_4(s) + 0.5\ S(\ell)$	$ZnO(s) + 1.5\ SO_2$	500 K	$ZnSO_4(s) + 0.5\ S(\ell)$
$ZnSO_4(s)$	1300 K	$ZnO(s) + SO_2 + 0.5\ O_2$	$ZnSO_4(s)$	1300 K	$ZnO(s) + SO_2 + 0.5\ O_2$
			$0.25\ S_2$	718 K	$0.5\ S(\ell)$

TABLE I. - Continued.

Reported (ref. 2)			Revised		
5. Zn(A)					
$H_2O + 1.5\ S$	850 K	$H_2S + 0.5\ SO_2$	$H_2O + 0.55\ S_2 + 0.05\ S_8$	850 K	$H_2S + 0.5\ SO_2$
H_2S	1300 K	$H_2 + S$	H_2S	1300 K	$H_2 + 0.5\ S_2$
$ZnO(s) + 1.5\ SO_2$	500 K	$ZnSO_4(s) + 0.5\ S(\ell)$	$ZnO(s) + 1.5\ SO_2$	500 K	$ZnSO_4(s) + 0.5\ S(\ell)$
$ZnSO_4(s)$	1300 K	$ZnO(s) + SO_2 + 0.5\ O_2$	$ZnSO_4(s)$	1300 K	$ZnO(s) + SO_2 + 0.5\ O_2$
			$0.5\ S(\ell)$	850 K	$0.05\ S_2 + 0.05\ S_8$
6. Zn-Ca(B)					
$0.5\ CaS(s) + 2S(\ell) + 2H_2O$	500 K	$0.5\ CaSO_4(s) + 2H_2S$	$0.5\ CaS(s) + 2S(\ell) + 2H_2O$	500 K	$0.5\ CaSO_4(s) + 2H_2S$
$0.5\ CaSO_4(s) + S$	1400 K	$0.5\ CaS(s) + SO_2$	$0.5\ CaSO_4(s) + 0.5\ S_2$	1400 K	$0.5\ CaS(s) + SO_2$
$H_2S + 0.67\ Bi(s)$	500 K	$0.33\ Bi_2S_3(s) + H_2$	$H_2S + 0.67\ Bi(s)$	500 K	$0.33\ Bi_2S_3(s) + H_2$
$0.33\ Bi_2S_3(s)$	1000 K	$0.67\ Bi(\ell) + S$	$0.33\ Bi_2S_3(s)$	1000 K	$0.67\ Bi(\ell) + 0.5\ S_2$
$ZnS(s) + 2SO_2$	500 K	$ZnSO_4(s) + 2S(\ell)$	$ZnS(s) + 2SO_2$	500 K	$ZnSO_4(s) + 2S(\ell)$
$ZnSO_4(s)$	1300 K	$ZnO(s) + SO_2 + 0.5\ O_2$	$ZnSO_4(s)$	1300 K	$ZnO(s) + SO_2 + 0.5\ O_2$
$ZnO(s) + H_2S$	600 K	$ZnS(s) + H_2O$	$ZnO(s) + H_2S$	600 K	$ZnS(s) + H_2O$
7. Zn(B)					
$2H_2O + 3S$	850 K	$2H_2S + S_2$	$2H_2O + 0.75\ S_2 + 0.2\ S_8$	850 K	$2H_2S + SO_2$
H_2S	1300 K	$H_2 + S$	H_2S	1300 K	$H_2 + 0.5\ S_2$
$ZnS(s) + 2SO_2$	500 K	$ZnSO_4(s) + 2S(\ell)$	$ZnS(s) + 2SO_2$	500 K	$ZnSO_4(s) + 2S(\ell)$
$ZnSO_4(s)$	1300 K	$ZnO(s) + SO_2 + 0.5\ O_2$	$ZnSO_4(s)$	1300 K	$ZnO(s) + SO_2 + 0.5\ O_2$
$ZnO(s) + H_2S$	600 K	$ZnS(s) + H_2O$	$ZnO(s) + H_2S$	600 K	$ZnS(s) + H_2O$
			$2S(\ell)$	850 K	$0.2\ S_2 + 0.2\ S_8$
8. Fe-Ba					
$0.25\ BaS(s) + H_2O$	500 K	$0.25\ BaSO_4(s) + H_2$	$0.25\ BaS(s) + H_2O$	500 K	$0.25\ BaSO_4(s) + H_2$
$0.25\ BaSO_4(s) + 0.5\ S$	1400 K	$0.25\ BaS(s) + 0.5\ SO_2$	$0.25\ BaSO_4(s) + 0.05\ S_2 + 0.05\ S_8$	1400 K	$0.25\ BaS(s) + 0.5\ SO_2$
$Fe_2O_3(s) + 2.5\ SO_2$	600 K	$2FeSO_4(s) + 0.5\ S(\ell)$	$Fe_2O_3(s) + 2.5\ SO_2$	400 K	$2FeSO_4(s) + 0.5\ S(\ell)$
$2FeSO_4(s)$	1000 K	$Fe_2O_3(s) + SO_2 + SO_3$	$2FeSO_4(s)$	1000 K	$Fe_2O_3(s) + SO_2 + SO_3$
SO_3	1300 K	$SO_2 + 0.5\ O_2$	SO_3	1300 K	$SO_2 + 0.5\ O_2$
			$0.5\ S(\ell)$	850 K	$0.05\ S_2 + 0.05\ S_8$

TABLE I. – Continued.

Reported (ref. 2)			Revised		
9. Fe-Ca					
$0.25\ CaS(s) + S(\ell) + H_2O$	500 K ⇌	$0.25\ CaSO_4(s) + H_2S$	$0.25\ CaS(s) + S(\ell) + H_2O$	500 K ⇌	$0.25\ CaSO_4(s) + H_2S$
$0.25\ CaSO_4(s) + 0.5\ S$	1400 K ⇌	$0.25\ CaS(s) + 0.5\ SO_2$	$0.25\ CaSO_4(s) + 0.25\ S_2$	1400 K ⇌	$0.25\ CaS(s) + 0.5\ SO_2$
$Fe_2O_3(s) + 2.5\ SO_2$	600 K ⇌	$2FeSO_4(s) + 0.5\ S(\ell)$	$Fe_2O_3(s) + 2.5\ SO_2$	400 K ⇌	$2FeSO_4(s) + 0.5\ S(\ell)$
$2FeSO_4(s)$	1000 K ⇌	$Fe_2O_3(s) + SO_2 + SO_3$	$2FeSO_4(s)$	1000 K ⇌	$Fe_2O_3(s) + SO_2 + SO_3$
$H_2S + 0.667\ Bi(s)$	500 K ⇌	$0.333\ Bi_2S_3(s) + H_2$	$H_2S + 0.67\ Bi(s)$	500 K ⇌	$0.33\ Bi_2S_3(s) + H_2$
$0.333\ Bi_2S_3(s)$	1000 K ⇌	$0.667\ Bi(\ell) + S$	$0.33\ Bi_2S_3(s)$	1000 K ⇌	$0.67\ Bi(\ell) + 0.5\ S_2$
SO_3	1300 K ⇌	$SO_2 + 0.5\ O_2$	SO_3	1300 K ⇌	$SO_2 + 0.5\ O_2$
			$0.25\ S_2$	718 K ⇌	$0.5\ S(\ell)$
10. Fe(A)					
$H_2O + 1.5\ S$	850 K ⇌	$H_2S + 0.5\ SO_2$	$H_2O + 0.55\ S_2 + 0.05\ S_8$	850 K ⇌	$H_2S + 0.5\ SO_2$
H_2S	1300 K ⇌	$H_2 + S$	H_2S	1300 K ⇌	$H_2 + 0.5\ S_2$
$Fe_2O_3(s) + 2.5\ SO_2$	400 K ⇌	$2FeSO_4(s) + 0.5\ S(\ell)$	$Fe_2O_3(s) + 2.5\ SO_2$	400 K ⇌	$2FeSO_4(s) + 0.5\ S(\ell)$
$2FeSO_4(s)$	940 K ⇌	$Fe_2O_3(s) + SO_2 + SO_3$	$2FeSO_4(s)$	1000 K ⇌	$Fe_2O_3(s) + SO_2 + SO_3$
SO_3	1300 K ⇌	$SO_2 + 0.5\ O_2$	SO_3	1300 K ⇌	$SO_2 + 0.5\ O_2$
			$0.5\ S(\ell)$	850 K ⇌	$0.05\ S_2 + 0.05\ S_8$
11. Fe(B)					
$4H_2O + 6S$	850 K ⇌	$4H_2S + 2SO_2$	$4H_2O + 0.6\ S_2 + 0.6\ S_8$	850 K ⇌	$4H_2S + 2SO_2$
$Fe_2O_3(s) + 4H_2S$	600 K ⇌	$2FeS_2(s) + 3H_2O + H_2$	$Fe_2O_3(s) + 4H_2S$	600 K ⇌	$2FeS_2(s) + 3H_2O + H_2$
$2FeS_2(s) + 4SO_2$	500 K ⇌	$2FeSO_4(s) + 6S(\ell)$	$2FeS_2(s) + 4SO_2$	500 K ⇌	$2FeSO_4(s) + 6S(\ell)$
$2FeSO_4$	1000 K ⇌	$Fe_2O_3(s) + SO_3 + SO_2$	$2FeSO_4(s)$	1000 K ⇌	$Fe_2O_3(s) + SO_3 + SO_2$
SO_3	1300 K ⇌	$SO_2 + 0.5\ O_2$	SO_3	1300 K ⇌	$SO_2 + 0.5\ O_2$
			$6S(\ell)$	850 K ⇌	$0.6\ S_2 + 0.6\ S_8$

TABLE I. - Concluded.

Reported (ref. 2)			Revised		
12. Cd(A)					
$H_2O + 1.5\ S$	850 K	$H_2S + 0.5\ SO_2$	$H_2O + 0.15\ S_2 + 0.15\ S_8$	850 K	$H_2S + 0.5\ SO_2$
$H_2S + Cd(s)$	500 K	$CdS(s) + H_2$	$H_2S + Cd(s)$	500 K	$CdS(s) + H_2$
$0.33\ CdO(s) + 0.67\ CdS(s) + 1.83\ SO_2$	500 K	$CdSO_4(s) + 1.5\ S(\ell)$	$0.33\ CdO(s) + 0.67\ CdS(s) + 1.83\ SO_2$	500 K	$CdSO_4(s) + 1.5\ S(\ell)$
$CdSO_4(\ell)$	1300 K	$CdO(s) + SO_2 + 0.5\ O_2$	$CdSO_4(s)$	1273 K	$CdO(s) + SO_2 + 0.5\ O_2$
$0.67\ CdO(s) + 0.33\ CdS(s)$	1300 K	$Cd + 0.33\ SO_2$	$0.67\ CdO(s) + 0.33\ CdS(s)$	1300 K	$Cd + 0.33\ SO_2$
			$1.5\ S(\ell)$	850 K	$0.15\ S_2 + 0.15\ S_8$
13. Cd(B)					
$H_2O + Cd(s)$	400 K	$CdO(s) + H_2$	$H_2O + Cd(s)$	400 K	$CdO(s) + H_2$
$1.33\ CdO(s) + 1.33\ SO_2$	500 K	$CdSO_4(s) + 0.33\ CdS(s)$	$1.33\ CdO(s) + 1.33\ SO_2$	500 K	$CdSO_4(s) + 0.33\ CdS(s)$
$CdSO_4(\ell)$	1300 K	$CdO(s) + SO_2 + 0.5\ O_2$	$CdSO_4(s)$	1273 K	$CdO(s) + SO_2 + 0.5\ O_2$
$0.67\ CdO(s) + 0.33\ CdS(s)$	1300 K	$Cd + 0.33\ SO_2$	$0.67\ CdO(s) + 0.33\ CdS(s)$	1300 K	$Cd + 0.33\ SO_2$

TABLE II. - CYCLE ANALYSES RESULTS

[Reported results are from ref. 2.]

Process	1		3		5		7		8		10		11	
	Mg(A)		Zn-Ba		Zn(A)		Zn(B)		Fe-Ba		Fe(A)		Fe(B)	
	Reported	Revised	Reported	Revised	Reported	Revised	Reported	Revised	Reported	Revised	Reported	Revised	Reported	Revised
Number of reactions	3	4	4	5	4	5	5	6	5	6	5	6	5	6
Temperature of water splitting step, K	500	600	500	500	850	850	850	850	500	500	850	850	850	850
Maximum temperature in process, K	1400	1400	1400	1400	1300	1300	1300	1300	1400	1400	1300	1300	1300	1300
Maximum ΔG, kcal	6.31	6.31	2.61	2.46	6.31	6.31	6.31	6.31	1.92	2.46	6.31	6.31	2.27	4.47
Maximum molar recycle ratio[a]	3.59	8.10	4.43	11.89	3.59	3.59	3.59	3.89	4.43	11.89	3.59	3.59	5.52	6.16
Work of separation, kcal[b]	14.48	16.85	9.09	6.91	19.64	19.09	25.65	24.58	11.80	10.40	22.22	22.58	34.88	30.73
Heat required after matching, kcal	116.40	116.37	107.04	108.34	105.43	104.77	117.93	117.57	133.49	138.45	134.51	137.40	167.31	167.34
η_1(HHV)[c]	0.59	0.50	0.69	0.71	0.51	0.52	0.44	0.45	0.63	0.66	0.48	0.48	0.37	0.38
η_2(HHV)[d]	0.41	0.37	0.53	0.46	0.34	0.30	0.28	0.26	0.46	0.34	0.25	0.24	0.23	0.20

[a] Moles of recycle per mole of hydrogen produced.

[b] At 100 percent equilibrium conversion, gases only.

[c] 30 Percent heat to work, 100 percent separation efficiency.

[d] 30 Percent heat to work, 50 percent separation efficiency.

TABLE III. - RESULTS FOR INDIVIDUAL STEPS IN THE CYCLES

Cycle	Step	Molar recycle ratio	Work of separation		ϵ	Cycle	Step	Molar recycle ratio	Work of separation		ϵ
			kcal	Percent					kcal	Percent	
1	1	8.10	3.76	22.3	0.198	8	1	11.89	3.49	33.6	0.078
	2		2.66	15.8	1		2	.10	.83	8.0	.462
	3	3.59	10.44	61.9	.218		3				1
	4				1		4		2.76	26.5	1
		11.69	16.86				5	.07	3.20	30.8	.935
							6		.12	1.1	1
3	1	11.89	3.49	50.5	0.078			12.06	10.40		
	2	.12	.83	12.0	.462						
	3				1	10	1	2.48	6.06	26.9	0.352
	4		2.47	35.8	1		2	3.59	10.44	46.2	.218
	5		.12	1.7	1		3				1
		12.01	6.91				4		2.76	12.2	1
							5	.07	3.20	14.2	.935
5	1	2.48	6.06	31.8	0.230		6		.12	.5	1
	2	3.59	10.44	54.7	.218			6.14	22.58		
	3				1						
	4		2.47	12.9	1	11	1	6.16	20.69	67.3	0.458
	5		.12	.6	1		2		2.68	8.7	1
		6.07	19.09				3				.417
							4		2.76	9.0	1
7	1	3.89	11.20	45.6	0.427		5	.07	3.20	10.4	.935
	2	3.59	10.44	42.5	.218		6		1.40	4.6	1
	3				1			6.23	30.73		
	4		2.47	10.0	1						
	5				1						
	6		.47	1.9	1						
		7.48	24.58								

TABLE IV. - COMPARISON OF EFFICIENCIES CALCULATED USING EQUILIBRIUM EXTENTS OF REACTION AND ASSUMING COMPLETE REACTION

Process	Equilibrium	Complete reaction	Equilibrium	Complete reaction
	η_1		η_2	
1. Mg(A)	0.50	0.70	0.37	0.52
3. Zn-Ba	.71	.80	.46	.50
5. Zn(A)	.52	.66	.30	.40
7. Zn(B)	.45	.62	.26	.38
8. Fe-Ba	.66	.72	.34	.37
10. Fe(A)	.48	.61	.24	.31
11. Fe(B)	.38	.53	.20	.28

TABLE V. - COMPARISON OF CALCULATED AND ESTIMATED EFFICIENCIES

Process	η_1	η_2	η_E
1. Mg(A)	0.50	0.37	0.51
3. Zn-Ba	.71	.46	.58
5. Zn(A)	.52	.30	.55
7. Zn(B)	.45	.26	.45
8. Fe-Ba	.66	.34	.47
10. Fe(A)	.48	.24	.42
11. Fe(B)	.38	.20	.30

FIGURE 1

FLOW DIAGRAM OF LINKED PROGRAMS