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X C D F O R

A FORTRAN IV PROGRAM FOR CALCULATING EQUILIBRIA ON T-X_{CO_2} SECTIONS

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Contents

I. General

The FORTRAN-IV program, XCDFOR, was written to calculate the position of mineral reaction curves on isobaric plots of the mole fraction of CO_2 in a CO_2- H_2O fluid against temperature. Mixed volatile reactions as well as simple dehydration or decarbonation reactions can be located. A number of options are provided in the program and these are described in detail below. For most applications the options are not necessary and the program is used in a standard mode with the following input data cards:

1. A mandatory option card, this card to be left blank if no options are used.

2. A reaction definition card for each reaction to be calculated. The following information is required on each card:

Columns 2 through 39 inclusive:		identification of the reaction
41 through 48	:	the constant, A
49 through 56	:	the constant, B
57 through 64	:	the constant, C

where A, B, C are constants in an equation of the form,

$$\log(f_{CO_2}^{\,n} \cdot f_{H_2O}^{m}) = \frac{A}{T} + B + \frac{C(P-2000)}{T}$$

Columns 65 through 70: The number of moles of CO_2 from the reaction stoichiometry (equivalent to the exponent n in the equilibrium equation). This number must be positive, i.e., the reaction must be written with CO_2 on the right-hand side. If CO_2 is not involved in the reaction, these columns are left blank.

Columns 71 through 76: The number of moles of H_2O from the reaction stoichiometry (equivalent to m in the equilibrium equation). It must be a positive number if both CO_2 and H_2O are involved on the same side of the reaction, or negative if CO_2 and H_2O are on opposite sides of the reaction. These columns are left blank if H_2O is not a component in the reaction.

Columns 77 through 80: Any positive number punched in these columns will result in a graphical display of the reaction curves.

Any number of reactions can be calculated by inserting a series of reaction definition cards. After the last such card, a data card with any negative number in columns 65 through 70 must be included to terminate the calculations.

The use of the above cards as data causes calculations to start at 730°C and proceed downwards at 5°C intervals until either the minimum temperature of 325°C is reached, or until no more useful results can be obtained. For each reaction, this series of calculations is first performed for a total gas pressure of 500 bars and then repeated for 1000 bars, 2000 bars, and 3000 bars.

Execution of the program requires approximately 8000 words of fast-memory (core) storage, a FORTRAN-IV compiler, a card reader, and a 130-position line printer.

For adaption to a 120-position line printer, only PRINT command 76, and print FORMATS 65 and 71 need to be modified, for example by removal of the redundant temperature column on the right side of the output.

II. Fugacity Coefficients

The method used in the program for determining equilibrium gas compositions is that described by Skippen (1971). The method requires fugacity coefficients for CO_2 and H_2O over the pressure and temperature range used in the program. At present, the required data are not available for CO_2-H_2O mixtures and it is necessary to use fugacity coefficients for the pure gases at the temperature and total presure of the calculations. Fugacity coefficients tabulated by Burnham, Holloway and Davis (1969) for H_2O and tabulated for CO_2 by Skippen (1971) have been used. By curve-fitting techniques, a sixth degree power series was derived and the resulting fugacity coefficients derived from the built-in coefficients for H_2O fall within 0.1 to 0.5% of the values given by Burnham et al. The method used by Skippen (1971) to derive fugacity coefficients for CO_2 is subject to considerable uncertainty and little accuracy can be claimed for the primary data. The "reconstituted" coefficients from the program are in close agreement with the original values and wherever there is a noticable, difference, the computer-generated coefficients line up into a smoother curve than the original data. A listing of fugacity coefficients is possible through the option card, as described below.

In anticipation of better fugacity coefficient data from P-V-T measurements of CO_2-H_2O mixtures, two options have been provided for in the input data. Under input option 1, the user may substitute his own coefficients for a polynomial expression to fit the fugacity coefficient data. Under the second input option, the user may specify a list of fugacity coefficients without the necessity of fitting a polynomial expression to the fugacity coefficient data.

III. Input

The input data supplied by the user consist of

1. An option card . (mandatory)

2. A pressure specification card. (optional)
   To be used if pressures other than the standard series of 500, 1000, 2000, and 3000 bars are used.

3. Fugacity coefficient deck. (optional)
   If the user wishes, he may substitute for the built-in fugacity coefficients, either a deck containing coefficients for a polynomial expression or a deck of fugacity coefficients.

4. A set of reaction definition cards. (mandatory)

5. A termination card. (mandatory)
   A negative number should be punched in the field defined by columns 65 through 70 of the termination card.

1. The option card

The program may be run in the standard mode by leaving the option card blank. Overall plotting of the output may be achieved by punching the numeral 1 in column 56 of the option card.

The standard mode provides the following:

a) Automatic generation of a table of fugacity coefficients for H_2O and CO_2 at the four standard pressures in the temperature interval, 325° C-730°C. The table is not printed out unless called for under option 8 below.

b) Calculation of equilibrium gas ratios for the standard pressures, 500, 1000, 2000 and 3000 bars, over the applicable part of the standard temperature interval, 325^{o}C-730^{o}C.

c) Organization of the printed output in such a way that it is suitable for a vertical format of 42 lines per sheet.

The option card allows the following modifications:

1. Column 8	Blank or 0 for default. Punch 1 for input option 1 (alternative set of polynomial coefficients for fugacity coefficient data). Punch 2 for input option 2 (alternative set of fugacity coefficients punched directly on cards).
2. Column 16	Degree of power series for polynomial expression under input option 1.
3. Columns 21-24	Redefinition of upper temperature limit.

4. Columns 29-32	Redefinition of lower temperature limit.
5. Column 40	Modification of the standard series of pressures. Indicate the number of pressures to be calculated by punching 1 to 4.
6. Columns 47-48	Modification of standard temperature interval (i.e. std. value of $5^{o}C$). Indicate the desired interval by punching 1 to 20.
7. Column 56	Punch any number for overall plotting.
8. Columns 61-64	Punch any number for listing of fugacity coefficients.
9. Columns 71-72	Punch the number of lines per output page.

1.1. Input options

There are three input options: 0, 1, and 2. Input option 0 is part of the standard mode; to implement it, nothing need be punched in column 8 of the option card. In this option, the program provides its own fugacity coefficients.

Input option 1

The user may substitute his own equation coefficients for the calculation of fugacity coefficients by first punching the numeral 1 in column 8 of the option card, and then presenting his own set of coefficients for a polynomial fit to fugacity coefficients immediately following the pressure definition card, or, if no pressure definition card is present, after the option card.

The equation in which these coefficients will be used to derive fugacity coefficients, is built into the program. It is a power series of potentially nine terms, that is, a series of the degree 8. However, unless the user specifies otherwise by punching the numeral representing the degree in column 16 of the option card, the standard assumption is that the degree should be 6, and consequently the program will attempt to read 7 coefficients for each gas species and for each pressure specified or assumed by default.

A detailed description of the set of polynomial coefficient cards is given later in the section on user-supplied coefficients.

Input option 2

In case the user wants to provide his own fugacity coefficients directly, he must first punch the numeral 2 in column 8 of the option card, and then present a deck of cards containing the necessary fugacity coefficients for the two gas species at the specified pressures.

A detailed description of this deck is given under the heading 'User-specified Coefficients'.

1.2. Specifying the degree of the equation called upon to calculate fugacity coefficients.

Column 16 of the option card may be used to specify the degree of the power-series from which the fugacity coefficients will be derived after the user has supplied his own equation coefficients. Consequently, this option is only applicable under input option 1. Under the other input options, column 16 of the option card will be ignored.

The lowest permissible degree is 3, the highest 8. Illegal values are automatically replaced: by 6 if specified too low, by 8 if too high.

1.3. Specifying the upper temperature limit.

Columns 21-24 of the option card represent an I4-field to specify an alternative maximum temperature (right-justified). The default value is 730°C; this is the maximum of the range within which the built-in fugacity coefficients apply. User-specified maxima above this temperature will automatically be reduced to 730°C unless the user first modifies the safe-guard-statement XCDFR 25: MAXPRO = 730.

1.4. Specifying the lower temperature limit

The I4-field defined by columns 29-32 of the option card is available for re-definition of the minimum temperature. The default value of 325°C is the program minimum below which the program-generated fugacity coefficients do not apply. Statement XCDFR 26, MINPRO = 325, safeguards against minima which are specified too low through the option under discussion; therefore, if the user wants to have calculations done for temperatures below 325°C, he must first modify this statement and supply his own coefficients.

The following restrictions should be borne in mind:

1. The program will automatically re-adjust the minimum temperature if it is more than 405° lower than the maximum temperature.

2. Automatic adjustment will ensue if the minimum temperature is less than 80° lower than the maximum temperature.

3. The same will happen if the range between minimum and maximum is less than 20 times the specified interval, or if it is greater than 81 times the specified interval.

In all these cases it is only the minimum temperature that is reset. In most cases, therefore, where statement XCDFR 26 is modified, the preceding statement should also be adjusted.

1.5. Specifying alternative pressures

Column 40 of the option card may be used to modify the standard series of four pressures (500, 1000, 2000, 3000 bars), or to specify a smaller number of pressures for which calculations are to be done.

The desired number of different pressures should be punched in column 40; the minimum is 1, the maximum 4. Illegal values are replaced by the default value 4.

Any numerical punch in column 40, other than 0, renders use of a pressure specification card mandatory. This card is described below.

1.6. Modifying the standard temperature interval

Column 48 (or columns 47-48) of the option card may be used to specify the temperature interval for the calculation of successive equilibrium gas ratios. The program accepts any value from 1 to 20; if a higher integer is punched, the value will be reset to 20°C. The default value is 5°C.

1.7. Calling for overall plotting

Column 56 controls the overall plotting facility. Any numeral punched in this column or in one of the three preceding columns will result in the production of line-printer diagrams for every reaction, regardless of any positive or negative values which may appear in the last field of the reaction-definition cards.

1.8. Calling for coefficient listing(s)

Any numeral punched in column 64 or in one of the three preceding columns of the option card will produce, under any input option, a listing of the relevant fugacity coefficients. Under input options 0 and 1, this listing is preceded by a listing of the equation coefficients.

1.9. Changing the vertical output format

Columns 71-72 of the option card may be used to specify a number of lines per output page other than the standard number of 42. Where 11-inch high printer forms are in use, the appearance of the diagrams can be improved by specifying 60 to 62 lines per page through this option.

2. The pressure specification card

This card becomes mandatory where any numeral other than 0 has been punched in column 40 of the option card. It is compatible with the use of input option 0 provided the pressures specified in it are identical with the pressures forming the first part of the standard series and appear in the same order. In all other cases, input option 1 or input option 2 must be used to adjust fugacity coefficient data to the new pressure(s).

The format of the pressure specification card is (4(4X, I4)) and consequently the first-specified pressure must be punched right-justified in the field defined by columns 5-8, and so on.

If the program is run under either input option 1 or 2, the user-supplied coefficients must be presented in an arrangement corresponding to the order in which the pressures are given in the pressure-specification card.

3. User-supplied coefficients

If the user has chosen input option 1, he must now provide polynomial coefficients to replace those from which the program would normally have derived the fugacity coefficients.

Under input option 2, the user may not replace the built-in in polynomial coefficients; the program will look directly for user-supplied fugacity coefficients, and ignore the polynomial coefficients.

Both types of coefficients must be presented as a set of cards immediately following the pressure specification card, or, if the latter is not present, immediately following the option card.

Polynomial coefficients

One set of polynomial coefficients is needed for each pressure and for each gas species; this implies that the number of sets of coefficients is twice the number of pressures. All the coefficients pertaining to H_2O fugacity calculations must be given before those for carbon dioxide can be given. The very first set of equation coefficients must, therefore, refer to the fugacity calculations for water at the first-specified (or lowest standard) pressure; the second set must refer to the fugacity calculations for water at the second-specified (or second-lowest standard) pressure, and so on.

Each individual set of equation coefficients must be arranged in order of ascending powers of the terms of the power series. The computer will attempt to read one more coefficient than the number indicated by the degree of the power series.

As the reading format of the coefficient cards is (5(1X, E14.8)), the last digit of each E-field should be in one of the columns 15, 30, 45, 60, or 75 of the card. Certain compilers impose more stringent requirements in this respect than others.

Each card, under the above format, may contain up to five coefficients. Therefore, specification of a degree higher than 4 will require the use of card pairs. This is probably the most common case; therefore, normally, the number of cards in the entire polynomial coefficient deck will equal four times the number of pressures.

If the number of terms in the power series is not the same for each gas species at every required pressure, the user should specify the highest degree required in any of the equations. If this degree is 6, he need not take any action in this respect; otherwise, he must punch a numeral in column 16 of the option card. Furthermore, if a card pair is needed for the equation coefficients of this highest degree, then card pairs must be presented throughout, even though any or all second cards of the other pairs may have to be left blank. All defaulted coefficients will be interpreted as having the value 0, and thus will not affect the outcome of the calculation of fugacity coefficients.

Fugacity coefficients

Under input option 2, the fugacity coefficients must be read in directly. Coefficients must be given for the maximum temperature as well as for the minimum temperature; the user can provide as many values for intervening integer Centigrade temperatures as he thinks useful for his purpose. The program will perform linear interpolation to derive coefficients at intervals of 1^{o}C. There is no provision for extrapolation; therefore, the user must make sure that his deck contains cards for the minimum as well as for the maximum temperature. If these fugacity coefficients are missing, the program will attempt to reset minimum and/or maximum temperature until the above-mentioned condition is satisfied for each gas species at every specified pressure. Should this effort fail, then the program will print a diagnostic message and proceed to run the reaction input with its own coefficients.

The fugacity coefficient cards need not be presented in any particular order. For any given temperature, the last-read coefficients will overwrite any prior values. Thus it is possible to rectify faulty coefficients, after detection, by simply adding a card with corrected coefficients at the end of the deck.

The very last card of this deck must be left blank. Not more than 999 cards can be read in. The 999th card, if present, does not have to be a blank card.

Each card must contain the temperature to which it refers, punched as a right-justified integer in the field defined by columns 5-8. The next value in this card, punched in the F8-field immediately following the temperature field, will be understood to represent the fugacity coefficient for water at the first-specified (or lowest standard) pressure; the following value will be understood to represent the fugacity coefficient of water at the second-specified pressure, or, if only one pressure is specified, as the fugacity coefficient of carbon dioxide at that pressure.

After all (1 to 4) coefficients for water have been given, the next value is understood to be the first coefficient of CO_2. Thus, if there is only one pressure, the effective format of the card is (4X, I4, 2F8.4), although it is specified in the program as (4X, I4, 8F8.4).

4. Reaction definition cards

Depending upon the combination of options chosen, the first reaction definition card follows either the option card, or the pressure specification card, or the set of equation coefficient cards, or the card terminating the deck of fugacity coefficient cards. This effectively means that, aside from the termination card, the reaction definition cards form the last section of the user-supplied input. There is no limit to their number.

Of each reaction definition card, the first half is available for identification of the reaction. This information is used exclusively in page headings and diagram headings. It is recommended that the first and the 40th column be left blank. The remaining information to be punched on these cards has been previously described, beginning on page 3.

5. The termination card

This card should contain a negative number in the field defined by columns 65 through 70. This will notify the program that no more reaction definition cards are to be read and that the routine "EXIT" should be called.

IV. Output

The output of XCDFOR is entirely in the form of print. Standard line width is 130 real printing positions. Only two format specifications, however, require a width of more than 120 columns - see section I.

There are five types of output:

1. A listing of coefficients for a polynomial expression for fugacity coefficients (optional, called by punching a numeral in column 64 of the option card).

2. A listing of fugacity coefficients over the chosen temperature range (at 1^o intervals, in descending order) for both H_2O and CO_2 for each of the maximum four pressures chosen or accepted by default. This listing is optional (it, too, is called by punching a numeral in column 64 of the option card).

3. Tables of equilibrium gas composition data, listing maximum temperatures, if within the program temperature range, mole fractions CO_2, and pressures and fugacities for the gas species involved in the reaction.

4. Diagrams representing the equilibrium curves for all pressures represented by the tabulated output just described (diagrams optional, called by either a numerical punch in column 56 of the option card, or a numerical punch in column 80 of the reaction specification card, or both).

5. Two types of diagnostic output: the first to warn the user that an omission or error was found in his deck of fugacity coefficients (under input option 2); the second type to indicate that no suitable values of equilibrium compositions could be derived from the data provided. The latter case may happen where the maximum temperature of an equilibrium curve is found to be beneath the minimum temperature the program is required to handle; in such cases, no diagram, of course, can be shown either. There may also be cases where printed values can be tabulated, but no diagram can be shown because the values in question would, after rounding, coincide with the vertical boundaries of the diagram.

   It is appropriate here to mention the two rescue routines which may take temporary control of program execution after printing a diagnostic message of the first kind. Where the error is serious enough to preclude usage of the user-supplied fugacity coefficients altogether, the program will attempt to process the reaction data with the help of its own "reconstituted" fugacity coefficients. Where minor errors are found in this input deck, the program will utilize the usable portion of the fugacity coefficients and adapt its minimum and maximum temperature accordingly.

V. The plot

The plotting subroutine can be called by punching a numeral in column 56 of the option card, or, if desired for certain reactions only, by punching a numeral in column 80 of the reaction definition cards. If the latter method is chosen, the plotting facility can later be suppressed again by rendering that number negative.

In the diagram itself, a one-line caption identifies the reaction in the terms stated by the user in the first 40 columns of the reaction definition card, and adds the values of the pressure(s) for which equilibrium curves are shown.

In the diagram, points on the curve representing the lowest pressure are shown as dots; those on the curve for the next-higher pressure are shown as plus-signs; those on the next curve as asterisks, and those on the curve for the highest pressure as zeros. This technique allows representation of all four (or fewer) curves in one figure.

The positions of the points shown are defined by (vertically) the temperature for which the composition of the gas species has been determined, and (horizontally) the mole fraction of CO_2 in the gas phase. Along the vertical axes, temperatures are indicated at intervals five times the standard program interval (or five times the user-defined interval). If a curve maximum does not coincide with a multiple of the standard interval, the temperature of this maximum will be shown in the margin on the line which would be occupied by the next-higher multiple of the standard interval. This procedure may occasionally give rise to slight distortion of the plotted curve. The appearance of the odd temperature in the plot margin should draw the user's attention to the cause of this apparent distortion.

Whereas the vertical control of the curve points is based on temperature values which are always integers, horizontal control depends on equilibrium ratios which must first be rounded to the nearest multiple of 0.01. This permits only representation of those values which lie between 0.005 and 0.995; any equilibrium ratio outside this range would cause the curve point to coincide with one of the vertical boundaries of the plot. Tests in the plotting routine will prevent this from happening, unless the value in question represents the maximum of a reaction involving one gas species only.

If more curve points must be shown than can be accomodated on one page, the plotting routine will first determine whether it is necessary to print yet another page; this is deemed to be the case if there is at least one point left to be shown within the equilibrium composition range between 0.1 and 0.9. In such a case, printing on the next page will be resumed at such a temperature level that the sheet will be filled out as completely as possible; almost invariably this will entail a certain overlap of the two parts of the diagram. In no case will there be an omission of significant equilibrium points.

If further diagram printing on a fresh page is found to be unnecessary, the figure is completed by a horizontal line with a scale division in tenths to indicate the mole fraction of CO_2 represented by the horizontal direction in the graph.

References Cited

Burnham, C.W., Holloway, J.R., Davis, N.F. 1969. Thermodynamic properties of water to 1000°C and 10,000 bars. Geol. Soc. Am. Special Paper 132, 96 pp.

Skippen, G.B. 1971. Experimental data for reactions in siliceous marbles. Jour. Geol., 79, pp. 457-481.

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      DIMENSION FC(8),TEMPER(8),TEMP(406,8),FUCOEF(406,8)              XCDFOR 1
      COMMON FUCOEF                                                    XCDFOR 2
      COMMON/AAA/EQCOEF(2,4,9),WORD(3)                                 XCDFOR 3
      COMMON/BBB/IPRES(4),RENAME(10),SYMBOL(10),PLINE(101),IRA(83,4,3) XCDFOR 4
      EQUIVALENCE (TEMP,FUCOEF)                                        XCDFOR 5
C *** EXTERNAL ECONF (ONLY FOR SDS AND IBM COMPILERS)                   XCDFOR 6
      ECONF(TEMPK)=10.**(A/TEMPK+B)                                    XCDFOR 7
      CALL EOFSET(1065)
      DATA SYMBOL/ 1H., 1H+, 1H*, 1HO, 1H , 1HI, 1H-, 1H-, 1H
      DATA WORD/ 4H H2O, 4H CO2, 4H BAR/                               XCDFOR 9
      DATA IPRES/ 500, 1000, 2000, 3000/                               XCDFR 10
      DATA EQCOEF/6.017635,-.25121724,-1.2042535,-.50722465,-.56129643, XCDFR 11
     1 2.105797,-.57907187,1.7840157,-.063509832,.0078615211,.018139648,XCDFR 12
     2 .010330991, .0083421085, -.0047083335, .0086120867, .0086443766, XCDFR 13
     3  .00025322866,  -.16655348E-4,  -.00011004716,  -.22026544E-4,   XCDFR 14
     4  -.50544549E-4,  .16964035E-4,  -.52198619E-4,  -.24657175E-4,   XCDFR 15
     5-.46545618E-6,.16018889E-7,.34139617E-6,.21382778E-7,.15822439E-6,XCDFR 16
     6-.22837963E-7, .16420945E-6, .2885E-7, .410891E-9, -.58333335E-11,XCDFR 17
     7  -.54188497E-9,  -.79166667E-11,  -.24822086E-9,  .10416667E-10, XCDFR 18
     8  -.2612E-9,  -.125E-10,  -.14150667E-12, 0, .42941572E-12, 0,    XCDFR 19
     9  .19459203E-12, 0, .20869719E-12, 0, 0, 0, -.13577122E-15, 0,    XCDFR 20
     *  -.61359392E-16,  0,  -.67096305E-16,  17*0/                     XCDFR 21
C ***                                                                  XCDFR 22
C * SAFEGUARDS AND DEFAULT FACILITIES ARE BUILT IN HERE                XCDFR 23
C ***                                                                  XCDFR 24
      MAXPRO=730                                                       XCDFR 25
      MINPRO=325                                                       XCDFR 26
      IF(MINPRO.LT.MAXPRO-405) MINPRO=MAXPRO-405                       XCDFR 27
      READ 1,INPOPT,NDGREE,MAXTEM,MINTEM,NOPRES,INTVAL,IPLOT,NOCOEF,LP XCDFR 28
    1 FORMAT(10(4X,I4))                                                XCDFR 29
      IF(INTVAL.GT.20) INTVAL=20                                       XCDFR 30
      IF(INPOPT.LT.0) INPOPT=IABS(INPOPT)                              XCDFR 31
      IF(INPOPT.GT.2) INPOPT=2                                         XCDFR 32
      IF(LP.EQ.0) LP=42                                                XCDFR 33
      IF(NOPRES.EQ.0) GO TO 201                                        XCDFR 34
      READ 1,(IPRES(J),J=1,NOPRES)                                     XCDFR 35
  201 IF(INTVAL.LE.0) INTVAL=5                                         XCDFR 36
      MRANGE=INTVAL*81                                                 XCDFR 37
      IF(MINPRO.LT.MAXPRO-MRANGE) MINPRO=MAXPRO-MRANGE                 XCDFR 38
      MRANGE=20*INTVAL                                                 XCDFR 39
      IF(MINPRO.GT.MAXPRO-MRANGE) MINPRO=MAXPRO-MRANGE                 XCDFR 40
      IF(MAXPRO-MINPRO.GT.405) MINPRO=MAXPRO-405                       XCDFR 41
      IF(NDGREE.LT.3) NDGREE=6                                         XCDFR 42
      IF(NDGREE.GT.8) NDGREE=8                                         XCDFR 43
      IF(INPOPT.EQ.0) NDGREE=6                                         XCDFR 44
      IF(MAXTEM.LT.MINPRO) MAXTEM=MAXPRO                               XCDFR 45
      IF(MAXTEM.LT.MINPRO+80) MAXTEM=MINPRO+80                         XCDFR 46
      IF(MAXTEM.GT.MAXPRO) MAXTEM=MAXPRO                               XCDFR 47
      IF(MINTEM.LT.MINPRO) MINTEM=MINPRO                               XCDFR 48
      IF(MAXTEM-MINTEM.LT.80) MINTEM=MAXTEM-80                         XCDFR 49
      IF(NOPRES.LT.1) NOPRES=4                                         XCDFR 50
      IF(NOPRES.GT.4) NOPRES=4                                         XCDFR 51
      NP=NOPRES+NOPRES                                                 XCDFR 52
      LDGREE=NDGREE+1                                                  XCDFR 53
      MSTART=MAXTEM+1                                                  XCDFR 54
      KELMIN=MINTEM+273                                                XCDFR 55
      BOTTEM=KELMIN                                                    XCDFR 56
      IGRADE=MSTART-MINTEM                                             XCDFR 57
      ITEST=MAXTEM/INTVAL                                              XCDFR 58
      ITEST=ITEST*INTVAL                                               XCDFR 59
      IF(ITEST.EQ.MAXTEM) GO TO 202                                    XCDFR 60
      ITEST=ITEST+INTVAL                                               XCDFR 61
  202 IP=ITEST+INTVAL                                                  XCDFR 62
      IF(INPOPT-1)17,17,2                                              XCDFR 63
C ***                                                                  XCDFR 64
COEFFICIENTS READ IN UNDER INPUT OPTION 2 ARE HANDLED IN THIS SEGMENT  XCDFR 65
C ***                                                                  XCDFR 66
    2 DO 3 I=1,IGRADE                                                  XCDFR 67
      DO 3 J=1,NP                                                      XCDFR 68
      FUCOEF(I,J)=0                                                    XCDFR 69
    3 CONTINUE                                                         XCDFR 70
      DO 6 I=1,999                                                     XCDFR 71
      READ 4,IT,(FC(J),J=1,NP)                                         XCDFR 72
    4 FORMAT(4X,I4,8F8.4)                                              XCDFR 73
      IF(IT.GT.MAXTEM) GO TO 6                                         XCDFR 74
      IF(IT.EQ.0) GO TO 7                                              XCDFR 75
      IF(IT.LT.MINTEM) GO TO 6                                         XCDFR 76
      IT=MSTART-IT                                                     XCDFR 77
      DO 5 J=1,NP                                                      XCDFR 78
      FUCOEF(IT,J)=FC(J)                                               XCDFR 79
    5 CONTINUE                                                         XCDFR 80
    6 CONTINUE                                                         XCDFR 81
    7 INDEX=0                                                          XCDFR 82
C ***                                                                  XCDFR 83
CHECK-LOOP VERIFIES PRESENCE OF FUGACITY COEFFICIENTS AT MINIMUM AND   XCDFR 84
C * MAXIMUM TEMPERATURES SPECIFIED OF PROGRAM-DETERMINED               XCDFR 85
C ***                                                                  XCDFR 86
      DO 14 I=1,NP                                                     XCDFR 87
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      ITO=MSTART-MINTEM
      IF(FUCOEF(ITO,I).LE.0) GO TO 140
      ITO=1
      IF(FUCOEF(ITO,I).LE.0) GO TO 142
      MIS=0
      ITOP=1
C ***
C * START OF INTERPOLATION UNDER INPUT OPTION 2
C ***
      DO 13 IT=ITO,IGRADE
      IF(FUCOEF(IT,I).LE.0.) GO TO 9
      IF(MIS.GT.0) GO TO 10
      COEF=FUCOEF(IT,I)
      GO TO 12
    9 MIS=MIS+1
      GO TO 13
   10 STEPS=MIS+1
      STEPS=(FUCOEF(IT,I)-COEF)/STEPS
      COEF=FUCOEF(IT,I)
      K=ITOP
      DO 11 J=1,MIS
      L=K
      K=K+1
      FUCOEF(K,I)=FUCOEF(L,I)+STEPS
   11 CONTINUE
      MIS=0
   12 ITOP=IT
   13 CONTINUE
   14 CONTINUE
      IF(NOCOEF)520,520,500
C ***
C * THE FOLLOWING STATEMENTS EMBODY RESCUE ROUTINES TO ENSURE SUCCESS-
C * FUL EXECUTION EVEN IF USER FAILED TO PROVIDE FUGACITY COEFFICIENTS
C * AT THE EXACT MAXIMUM AND MINIMUM TEMPERATURES SPECIFIED OR PROVIDED
C ***
  140 ITO=ITO-1
      MINTEM=MINTEM+1
      IF(MAXTEM-MINTEM.LT.80) GO TO 15
      IF(FUCOEF(ITO,I).LE.0) GO TO 140
      KELMIN=MINTEM+273
      BOTTEM=KELMIN
      IGRADE=MSTART-MINTEM
      GO TO 7
  142 INDEX=INDEX+1
      MAXTEM=MAXTEM-1
      IF(MAXTEM-MINTEM.LT.80) GO TO 15
      ITO=ITO+1
      IF(FUCOEF(ITO,I).LE.0) GO TO 142
      MSTART=MAXTEM+1
      IGRADE=MSTART-MINTEM
      ITEST=MAXTEM/INTVAL
      ITEST=ITEST*INTVAL
      IF(ITEST.EQ.MAXTEM) GO TO 141
      ITEST=ITEST+INTVAL
  141 IP=ITEST+INTVAL
      DO 143 I=1,IGRADE
      K=I+INDEX
      DO 143 J=1,NP
      FUCOEF(I,J)=FUCOEF(K,J)
  143 CONTINUE
      GO TO 7
   15 PRINT 16
   16 FORMAT(49H SORRY, CANNOT FIND YOUR FUGACITY COEFFICIENTS.
     1 49H WILL NOW RUN YOUR DATA WITH MY OWB COEFFICIENTS.  /)
      INPOPT=0
      NDGREE=6
      MAXPRO=730
      MINPRO=325
      MAXTEM=0
      MINTEM=0
      INTVAL=5
      IPLOT=1
      NOCOEF=1
      GO TO 201
C ***
C * END OF RESCUE ROUTINES, START OF CALCULATION OF FUGACITY
COEFFICIENTS UNDER INPUT OPTION 0 OR 1
C ***
   17 T=MSTART
      DO 18 N=1,IGRADE
      T=T-1.
      TEMP(N,1)=T
      DO 18 M=2,NDGREE
      L=M-1
      TEMP(N,M)=TEMP(N,L)*T
   18 CONTINUE
      IF(NOCOEF.EQ.0) GO TO 231
      PRINT 23
```

```
 23 FORMAT(1H1,30X,45HEQUATION COEFFICIENTS USED IN CALCULATION OF        XCDF 176
   1 21HFUGACITY COEFFICIENTS,//)                                          XCDF 177
231 DO 29 N=1,2                                                            XCDF 178
    DO 27 M=1,NOPRES                                                       XCDF 179
    IF(INPOPT.NE.1) GO TO 25                                               XCDF 180
    READ  24,(EQCOEF(N,M,L),L=1,LDGREE)                                    XCDF 181
 24 FORMAT(5(1X, E14.8)/4(1X,E14.8))                                       XCDF 182
 25 IF(NOCOEF.EQ.0) GO TO 27                                               XCDF 183
    PRINT 26,WORD(N),IPRES(M),WORD(3),(EQCOEF(N,M,L),L=1,LDGREE)           XCDF 184
 26 FORMAT(1H0,A4,I5,A4,7(2X,E14.8)/14X,2(2X,E14.8)/)                      XCDF 185
 27 CONTINUE                                                               XCDF 186
    IF(NOCOEF.EQ.0) GO TO 29                                               XCDF 187
    PRINT 28                                                               XCDF 188
 28 FORMAT(1H0,/)                                                          XCDF 189
 29 CONTINUE                                                               XCDF 190
    LINES=LP                                                               XCDF 191
    DO 52 IT=1,IGRADE                                                      XCDF 192
    DO 30 I=1,NDGREE                                                       XCDF 193
    TEMPER(I)=TEMP(IT,I)                                                   XCDF 194
 30 CONTINUE                                                               XCDF 195
    DO 32 N=1,NOPRES                                                       XCDF 196
    NG=N                                                                   XCDF 197
    DO 32 I=1,2                                                            XCDF 198
    FUCOEF(IT,NG)=EQCOEF(I,N,1)                                            XCDF 199
    DO 31 L=2,LDGREE                                                       XCDF 200
    K=L-1                                                                  XCDF 201
    FUCOEF(IT,NG)=FUCOEF(IT,NG)+EQCOEF(I,N,L)*TEMPER(K)                    XCDF 202
 31 CONTINUE                                                               XCDF 203
    NG=NG+NOPRES                                                           XCDF 204
 32 CONTINUE                                                               XCDF 205
    IF(NOCOEF.EQ.0) GO TO 52                                               XCDF 206
    IF(LINES.LT.LP) GO TO 42                                               XCDF 207
    GO TO (320,322,324,326),NOPRES                                         XCDF 208
320 PRINT 321,IPRES(1),WORD(3)                                             XCDF 209
321 FORMAT(25H1FUGACITY COEFFICIENTS AT,I5,A4)                             XCDF 210
    GO TO 328                                                              XCDF 211
322 PRINT 323,IPRES(1),IPRES(2),WORD(3)                                    XCDF 212
323 FORMAT(1H1,2X,24HFUGACITY COEFFICIENTS AT,I5,4H AND,I5,A4)             XCDF 213
    GO TO 328                                                              XCDF 214
324 PRINT 325,(IPRES(J),J=1,3),WORD(3)                                     XCDF 215
325 FORMAT(1H1,7X,38HFUGACITY COEFFICIENTS AT THE PRESSURES,               XCDF 216
   1 2(I5,1H,),4H AND,I5,A4)                                               XCDF 217
    GO TO 328                                                              XCDF 218
326 PRINT 327,(IPRES(J),J=1,4),WORD(3)                                     XCDF 219
327 FORMAT(1H1,12X,38HFUGACITY COEFFICIENTS AT THE PRESSURES,              XCDF 220
   1 2(I5,1H,),4H AND,I5,A4)                                               XCDF 221
328 GO TO(33,35,37,39),NOPRES                                              XCDF 222
 33 PRINT 34                                                               XCDF 223
 34 FORMAT(1H0,12X,5HWATER,6X,14HCARBON DIOXIDE,/,6H  TEMP,/-              XCDF 224
    GO TO 41                                                               XCDF 225
 35 PRINT 36                                                               XCDF 226
 36 FORMAT(1H0,17X,5HWATER,10X,14HCARBON DIOXIDE,/,6H  TEMP,               XCDF 227
   1 47X,4HTEMP,/)                                                         XCDFA227
    GO TO 41                                                               XCDF 228
 37 PRINT 38                                                               XCDF 229
 38 FORMAT(1H0,19X,5HWATER,30X,14HCARBON DIOXIDE/6H  TEMP,                 XCDF 230
   1 33X,4HTEMP,37X,4HTEMP/)                                               XCDF 231
    GO TO 41                                                               XCDF 232
 39 PRINT 40                                                               XCDF 233
 40 FORMAT(1H0,23X,5HWATER,37X,14HCARBON DIOXIDE/6H  TEMP,40X,             XCDF 234
   1 4HTEMP,44X,4HTEMP/)                                                   XCDF 235
 41 LINES=6                                                                XCDF 236
 42 ITEMP=TEMPER(1)                                                        XCDF 237
    GO TO(43,45,47,49),NOPRES                                              XCDF 238
 43 PRINT 44,ITEMP,(FUCOEF(IT,NG),NG=1,2)                                  XCDF 239
 44 FORMAT(I6,4X,F8.4,8X,F8.4)                                             XCDF 240
    GO TO 51                                                               XCDF 241
 45 PRINT 46,ITEMP,(FUCOEF(IT,NG),NG=1,4),ITEMP                            XCDF 242
 46 FORMAT(I6,4X,2F8.4,3X,2F9.4,3X,I6)                                     XCDF 243
    GO TO 51                                                               XCDF 244
 47 PRINT 48,ITEMP,(FUCOEF(IT,NG),NG=1,3),ITEMP,(FUCOEF(IT,NG),NG=4,6)XCDF 245
   1,ITEMP                                                                 XCDF 246
 48 FORMAT(I6,3X,3F8.4,3X,I6,3X,3F9.4,3X,I6)                               XCDF 247
    GO TO 51                                                               XCDF 248
 49 PRINT 50,ITEMP,(FUCOEF(IT,NG),NG=1,4),ITEMP,(FUCOEF(IT,NG),NG=5,8)XCDF 249
   1,ITEMP                                                                 XCDF 250
 50 FORMAT(I6,3X,4F8.4,3X,I6,3X,4F9.4,3X,I6)                               XCDF 251
 51 LINES=LINES+1                                                          XCDF 252
 52 CONTINUE                                                               XCDF 253
    GO TO 520                                                              XCDF 254
500 LINES=LP                                                               XCDF 255
    ITEMP=MSTART                                                           XCDF 256
    DO 512 IT=1,IGRADE                                                     XCDF 257
    ITEMP=ITEMP-1                                                          XCDF 258
    IF(LINES.LT.LP) GO TO 506                                              XCDF 259
    GO TO (530,532,534,536),NOPRES                                         XCDF 260
530 PRINT 321,IPRES(1),WORD(3)                                             XCDF 261
    GO TO 538                                                              XCDF 262
```

```
  532 PRINT 323,IPRES(1),IPRES(2),WORD(3)
      GO TO 538
  534 PRINT 325,(IPRES(J),J=1,3),WORD(3)
      GO TO 538
  536 PRINT 327,(IPRES(J),J=1,4),WORD(3)
  538 GO TO(501,502,503,504),NOPRES
  501 PRINT 34
      GO TO 505
  502 PRINT 36
      GO TO 505
  503 PRINT 38
      GO TO 505
  504 PRINT 40
  505 LINES=6
  506 GO TO (507,508,509,510),NOPRES
  507 PRINT 44,ITEMP,(FUCOEF(IT,NG),NG=1,2)
      GO TO 511
  508 PRINT 46,ITEMP,(FUCOEF(IT,NG),NG=1,4),ITEMP
      GO TO 511
  509 PRINT 48,ITEMP,(FUCOEF(IT,NG),NG=1,3),ITEMP,(FUCOEF(IT,NG),NG=4,6)
     1,ITEMP
      GO TO 511
  510 PRINT 50,ITEMP,(FUCOEF(IT,NG),NG=1,4),ITEMP,(FUCOEF(IT,NG),NG=5,8)
     1,ITEMP
  511 LINES=LINES+1
  512 CONTINUE
C ***
C * READ REACTION SPECIFICATION CARD AND CONVERT CONSTANTS A AND C
C * INTO ONE COMBINED CONSTANT A FOR EACH PRESSURE SEPARATELY
C ***
  520 READ 521,(RENAME(J),J=1,10),A,B,C,CDMOL,WAMOL,JPLOT
  521 FORMAT(10A4,3F8.0,2F6.0,I4)
      IF(CDMOL.LT.0.) GO TO 106
      DO 522 N=1,NOPRES
      PTOTAL=IPRES(N)
      EQCOEF(1,N,1)=A+C*(PTOTAL-2000.)
  522 CONTINUE
      KONVRA=A
      DO 104 N=1,NOPRES
      A=EQCOEF(1,N,1)
      NOTA=1
      IPAGE=1
      NP=N+NOPRES
      PTOTAL=IPRES(N)

      PL=PTOTAL*.0005
      SL=PL*.03
      PRINT 53,(RENAME(J),J=1,10),IPRES(N),WORD(3),IPAGE,KONVRA,
     1 B,C
   53 FORMAT(1H1,9H REACTION,10A4,22HAT A TOTAL PRESSURE OF,I5,A4,
     1 20X,4HPAGE,I2/51X,2HA=,I7,4H, B=,F7.3,4H, C=,F6.4)
   54 FORMAT(1H1,9H REACTION,10A4,22HAT A TOTAL PRESSURE OF,I5,A4,
     1 20X,4HPAGE,I2/)
      IPAGE=IPAGE+1
C ***
C * IF DIAGRAM REQUESTED, INITIALIZE PORTION OF STORAGE ARRAY
C ***
      IF(JPLOT.GT.0) GO TO 541
      IF(IPLOT.EQ.0) GO TO 543
  541 DO 542 K=1,83
      DO 542 J=1,3
      IRA(K,N,J)=0
  542 CONTINUE
C ***
CONTROLS THE MAIN FLOW ACCORDING TO THE TYPE OF THE REACTION
C ***
  543 IF(WAMOL)79,780,55
   55 NOTA=2
      IF(CDMOL)106,781,56
C ***
C * IF H2O AND CO2 ON SAME SIDE, START TO DETERMINE MAXIMUM TEMPERATURE
C ***
   56 INDEX=INTVAL
      PCD=CDMOL*PTOTAL/(CDMOL+WAMOL)
      PCDMIN=PCD
      PWA=PTOTAL-PCD
      PWAMIN=PWA
      ITSTEP=512
      LIMIT=9
      IF(IGRADE.GT.256) GO TO 57
      ITSTEP=256
      LIMIT=8
      IF(IGRADE.GT.128) GO TO 57
      ITSTEP=128
      LIMIT=7
   57 ITEMK=KELMIN
      TEMPK=ITEMK
      FCD=PCD*FUCOEF(IGRADE,NP)
      FWA=PWA*FUCOEF(IGRADE,N)
```

```
      ECTEST=FCD**CDMOL*FWA**WAMOL
      IF(ECTEST.LT.ECONF(TEMPK)) GO TO 102
      ITEMK=MAXTEM+273
      TEMPK=ITEMK
      FCD=PCD*FUCOEF(1,NP)
      FWA=PWA*FUCOEF(1,N)
      ECTEST=FCD**CDMOL*FWA**WAMOL
      IF(ECTEST.LT.ECONF(TEMPK)) GO TO 572
      PRINT 571,MAXTEM
  571 FORMAT(30H0 MAXIMUM TEMPERATURE IS ABOVE,I5,
     1 19H DEGREES CENTIGRADE,/////)
      IT=1
      GO TO 63
  572 ITEMK=MSTART+273
      INDEX=0
      IT=0
      L=0
   58 L=L+1
      IF(L.GT.LIMIT) GO TO 62
      ITSTEP=IABS(ITSTEP)/2
   59 ITEMK=ITEMK-ITSTEP
      IT=IT+ITSTEP
      IF(ITEMK.GE.KELMIN) GO TO 61
   60 L=L+1
      IF(L.GT.LIMIT) GO TO 62
      ITSTEP=-IABS(ITSTEP)/2
      GO TO 59
   61 TEMPK=ITEMK
      FCD=PCD*FUCOEF(IT,NP)
      FWA=PWA*FUCOEF(IT,N)
      ECTEST=FCD**CDMOL*FWA**WAMOL
      EC=ECONF(TEMPK)
      IF(ECTEST-EC)58,63,60
   62 IF(ECTEST.LE.EC) GO TO 63
      ITEMK=ITEMK+1
      TEMPK=TEMPK+1.
      IT=IT-1
   63 ITMAX=ITEMK-273
C ***
C IF DIAGRAM REQUESTED, STORE MAXIMUM TEMPERATURE AND CO2 FRACTION
C IF CURVE MAXIMUM ABOVE PROGRAM MAXIMUM, PROCEDURE IS MODIFIED
C ***
      IF(JPLOT.GT.0) GO TO 630
      IF(IPLOT.EQ.0) GO TO 632
  630 J=(IP-ITMAX)/INTVAL
      IRA(83,N,1)=ITMAX
      IRA(83,N,3)=INTVAL
      IF(INDEX)631,631,640
  631 IRA(J,N,1)=ITMAX
      IRA(J,N,2)=PCD*100./PTOTAL+.5
      IRA(J,N,3)=0
      IRA(83,N,2)=1
  632 IF(INDEX)633,633,640
  633 PRINT 64,ITMAX,PCD,PWA,FCD,FWA
   64 FORMAT(21H0 MAXIMUM TEMPERATURE,I5/6H  PCO2,F8.2/6H  PH2O,F8.2/
     1 6H  FCO2,F8.2/6H  FH2O,F8.2/)
      ITEST=ITMAX/INTVAL
      ITEST=ITEST*INTVAL
      IF(ITEST.EQ.ITMAX) GO TO 641
      INDEX=ITEST-ITMAX+INTVAL
  640 IT=IT-INDEX
      ITMAX=ITMAX+INDEX
  641 ITSTEP=(ITMAX-MINTEM)/INTVAL
      IF(ITSTEP.LT.1) GO TO 107
      INDEX=3
      NOUSE=0
      PRINT 65
   65 FORMAT(56H0 -------------- CARBON-DIOXIDE POOR GASES -------------
     1 15X,56H--------------- CARBON-DIOXIDE RICH GASES --------------//
     2 6H  TEMP,5X,4HFCO2,6X,4HFH2O,6X,4HPCO2,6X,4HPH2O,6X,4HXCO2,6X,
     3   4HTEMP,8X,4HFCO2,6X,4HFH2O,6X,4HPCO2,6X,4HPH2O,6X,4HXCO2,6X,
     4   4HTEMP/)
      LINES=14
C ***
C * TRACE BOTH BRANCHES OF EQUILIBRIUM CURVE FROM MAXIMUM TEMPERATURE
C * DOWNWARD UNTIL BOTH VALUES OF X-CO2 OUT OF RANGE
C ***
      DO 78 I=1,ITSTEP
      IF(NOUSE.GT.2) GO TO 104
      ITMAX=ITMAX-INTVAL
      TEMPK=ITMAX+273
      IT=IT+INTVAL
   66 EC=ECONF(TEMPK)
      PCD=PCDMIN*.5
      PSTEP=PCD
      GO TO 69
   67 PCD=PCD+PSTEP
      GO TO 69
```

```
 68 PCD=PCD-PSTEP
 69 PSTEP=PSTEP*.5
    PWA=PTOTAL-PCD
    FWA=PWA*FUCOEF(IT,N)
    FCD=PCD*FUCOEF(IT,NP)
    IF(PSTEP.LT.SL)  GO TO 70
    ECTEST=FCD**CDMOL*FWA**WAMOL
    IF(ECTEST-EC)67,70,68
 70 PCDMIN=PCD
    PCDLO=PCD
    XCDLO=PCD/PTOTAL
    FCDLO=FCD
    PWALO=PWA
    FWALO=FWA
    IF(NOUSE.EQ.2) GO TO 71
    IF(PCD.LT.PL) NOUSE=NOUSE+2
 71 PWA=PWAMIN*.5
    PSTEP=PWA
    GO TO 74
 72 PWA=PWA+PSTEP
    GO TO 74
 73 PWA=PWA-PSTEP
 74 PSTEP=PSTEP*.5
    PCD=PTOTAL-PWA
    FWA=PWA*FUCOEF(IT,N)
    FCD=PCD*FUCOEF(IT,NP)
    IF(PSTEP.LT.SL)  GO TO 75
    ECTEST=FCD**CDMOL*FWA**WAMOL
    IF(EC-ECTEST)73,75,72
 75 XCD=PCD/PTOTAL
    PWAMIN=PWA
    IF(NOUSE.EQ.1) GO TO 751
    IF(PWAMIN.LT.PL) NOUSE=NOUSE+1
751 IF(LINES.LT.LP) GO TO 76
    PRINT 54,(RENAME(J),J=1,10),IPRES(N),WORD(3),IPAGE
    PRINT 65
    LINES=7
    IPAGE=IPAGE+1
 76 PRINT 77,ITMAX,FCDLO,FWALO,PCDLO,PWALO,XCDLO,ITMAX,FCD,FWA,PCD,PWA
   1,XCD,ITMAX
 77 FORMAT(I6,4F10.2,F10.5,3X,I6,3X,4F10.2,F10.5,3X,I6)
    LINES=LINES+1
C ***
C * IF DIAGRAM REQUESTED, STORE TEMPERATURE AND X-CO2 FOR PLOTTING
C ***
    IF(JPLOT.GT.0) GO TO 771
    IF(IPLOT.EQ.0) GO TO 78
771 J=(IP-ITMAX)/INTVAL
    IF(INDEX.GT.82) GO TO 78
    IF(INDEX-23)776,772,773
772 IF(XCDLO.GE..005) GO TO 775
    INDEX=INDEX+60
    GO TO 78
773 IF(XCD.LT..995) GO TO 774
    INDEX=INDEX+20
    GO TO 78
774 IRA(J,N,3)=XCD*100.+.5
    GO TO 779
775 IRA(J,N,2)=XCDLO*100.+.5
    GO TO 779
776 IF(XCD.LT..995) GO TO 777
    INDEX=INDEX+20
    GO TO 772
777 IF(XCDLO.GE..005) GO TO 778
    INDEX=INDEX+60
    GO TO 774
778 IRA(J,N,3)=XCD*100.+.5
    IRA(J,N,2)=XCDLO*100.+.5
779 IRA(J,N,1)=ITMAX
    IRA(83,N,2)=IRA(83,N,2)+1
 78 CONTINUE
C ***
CALCULATIONS DISCONTINUED BECAUSE MINIMUM TEMPERATURE ATTAINED
C ***
    GO TO 104
780 CALL ONEMOB(N,NOPRES,   INTVAL,CDMOL,IGRADE,KELMIN,MINTEM,BOTTEM,
   1 NOTA,A,B,PTOTAL,IP,IPLOT,JPLOT,PL,LP)
    GO TO 104
781 CALL ONEMOB(N, NOPRES,  INTVAL,WAMOL,IGRADE,KELMIN,MINTEM,BOTTEM,
   1 NOTA,A,B,PTOTAL,IP,IPLOT,JPLOT,PL,LP)
    GO TO 104
C ***
CO2 AND H2O ON DIFFERENT SIDES OF CHEMICAL EQUATION
C ***
 79 PRINT 80
 80 FORMAT(6HO TEMP,5X,4HXCO2,6X,4HPCO2,6X,4HFCO2,6X,4HPH2O,6X,
   1 4HFH2O/)
    LINES=5
```

```
      NOTA=0
      WMOLE=-WAMOL
      ITEST=MAXTEM/INTVAL
      ITMAX=ITEST*INTVAL+INTVAL
      INDEX=ITMAX-MAXTEM
      IT=1-INDEX
      INDEX=1
      ITSTEP=(ITMAX-MINTEM)/INTVAL
C ***
C * DETERMINE WHETHER CURVE SLOPES TO THE LEFT OR TO THE RIGHT
C ***
      IF(A.LE.0.) GO TO 83
      TEMPK=MAXTEM+273
      ECMIN=ECONF(TEMPK)
      FCD=FUCOEF(1,NP)
      FWA=FUCOEF(1,N)
      ECTMIN=FCD**CDMOL/FWA**WMOLE
      EC=ECONF(BOTTEM)
      EC=EC/ECMIN
      FCD=FUCOEF(IGRADE,NP)
      FWA=FUCOEF(IGRADE,N)
      ECTEST=FCD**CDMOL/FWA**WMOLE
      ECTEST=ECTEST/ECTMIN
      IF(ECTEST-EC)82,81,83
C ***
C * POINTER NOTA IS SET UP TO SIGNAL TYPE OF SLOPE+ NOTA=0 FOR REGULAR
CASE, NOTA=1 FOR REVERSED SLOPE, NOTA=2 FOR INTERMEDIATE CASE
C ***
   81 NOTA=NOTA+1
   82 NOTA=NOTA+1
   83 DO 101  I=1,ITSTEP
      PCD=0
      PSTEP=PTOTAL
      IT=IT+INTVAL
      ITMAX=ITMAX-INTVAL
      TEMPK=ITMAX+273
      EC=ECONF(TEMPK)
   84 PSTEP=PSTEP*.5
      IF(PSTEP.LT.SL)  GO TO 87
      PCD=PCD+PSTEP
   85 PWA=PTOTAL-PCD
      FCD=PCD*FUCOEF(IT,NP)
      FWA=PWA*FUCOEF(IT,N)
      ECTEST=FCD**CDMOL/FWA**WMOLE

      IF(ECTEST-EC)84,87,86
   86 PSTEP=PSTEP*.5
      IF(PSTEP.LT.SL ) GO TO 87
      PCD=PCD-PSTEP
      GO TO 85
   87 XCD=PCD/PTOTAL
      IF(NOTA-1)88,90,89
   88 IF(PWA.LT.PL) GO TO 101
   89 IF(LINES.LT.LP) GO TO 91
      PRINT 54,(RENAME(J),J=1,10),IPRES(N),WORD(3),IPAGE
      PRINT 80
      LINES=5
      IPAGE=IPAGE+1
      GO TO 91
   90 IF(PCD-PL )101,89,89
   91 PRINT 92,ITMAX,XCD,PCD,FCD,PWA,FWA
   92 FORMAT(I6,F10.5,4F10.2)
      LINES=LINES+1
      IF(NOTA-1)94,93,95
   93 IF(PWA-1.)104,95,95
   94 IF(PCD.LT.1.) GO TO 104
C ***
C * IF DIAGRAM REQUESTED, STORE VALUES TO BE PLOTTED LATER BY IGRAPH
C ***
   95 IF(JPLOT.GT.0) GO TO 951
      IF(IPLOT.EQ.0) GO TO 101
  951 IF(INDEX.GT.82) GO TO 101
      IF(NOTA-1)96,97,99
   96 IF(XCD-.005)100,99,98
   97 IF(XCD.GE..995) GO TO 100
      IF(XCD-.005)101,99,99
   98 IF(XCD.GE..995) GO TO 101
   99 J=(IP-ITMAX)/INTVAL
      IRA(J,N,1)=ITMAX
      IRA(J,N,2)=XCD*100.+.5
      IRA(J,N,3)=0
      IRA(83,N,2)=IRA(83,N,2)+1
      IF(IRA(83,N,2).GT.1) GO TO 101
      IRA(83,N,1)=ITMAX
      IRA(83,N,3)=INTVAL
      GO TO 101
  100 INDEX=83
  101 CONTINUE
      GO TO 104
```

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  102 PRINT 103,MINTEM
  103 FORMAT(52HO MAXIMUM TEMPERATURE IS BELOW THE SPECIFIED MINIMUM,
     1 15H TEMPERATURE OF,I4,19H DEGREES CENTIGRADE)
      GO TO 104
  107 ITMAX=ITMAX-INDEX
      PRINT 108, IPRES(N),ITMAX
  108 FORMAT(24H  OTHER CALCULATIONS FOR,I5,20H BAR SKIPPED BECAUSE,
     1 28H MAXIMUM TEMPERATURE IS ONLY,I4,19H DEGREES CENTIGRADE)
  104 CONTINUE
C ***
CONTROL HAS TO GO TO SUBROUTINE IGRAPH UNDER EITHER PLOTTING OPTION
C ***
      IF(JPLOT.GT.0) GO TO 105
      IF(IPLOT)105,520,105
  105 CALL IGRAPH(INTVAL,MINTEM,MAXTEM,IP,NOPRES,LP)
      GO TO 520
  106 CALL EXIT
      END
      SUBROUTINE ONEMOB(NC,NOPRES,INTVAL,FLMOL,IGRADE,KELMIN,MINTEM,
     1 BOTTEM,NOTA,A,B,PTOTAL,IP,IPLOT,JPLOT,PL,LP)
      DIMENSION FUCOEF(406,8)
      COMMON FUCOEF
      COMMON/AAA/EQCOEF(2,4,9),WORD(3)
      COMMON/BBB/IPRES(4),RENAME(10),SYMBOL(10),PLINE(101),IRA(83,4,3)
C ***
CHEMICAL EQUATION SHOWS ONLY ONE MOBILE COMPONENT
C ***
C *** IF THE EXTERNAL-DECLARATION OF XCDFCR 6 IS USED, THE FOLLOWING
C *** STATEMENT MUST BE REMOVED
      ECONF(TEMPK)=10.**(A/TEMPK+B)
      IPAGE=2
      N=NC
      LINES=5
      IF(NOTA.EQ.2) GO TO 2
      NO=NC+NOPRES
      GO TO 4
    1 FORMAT(35HO TEMP       XCO2        PCO2        FCO2/)
    2 NO=NC
    3 FORMAT(35HO TEMP       XH2O        PH2O        FH2O/)
    4 CMOLE=1./FLMOL
C ***
C * BEGIN CALCULATIONS BY DETERMINING MAXIMUM TEMPERATURE
C ***
      PCD=PTOTAL
      ITSTEP=512
      LIMIT=9
      IF(IGRADE.GT.256) GO TO 5
      ITSTEP=ITSTEP/2
      LIMIT=8
      IF(IGRADE.GT.128) GO TO 5
      ITSTEP=ITSTEP/2
      LIMIT=7
    5 ITEMK=KELMIN
      TEMPK=BOTTEM
      FCD=PCD*FUCOEF(IGRADE,NO)
      ECTEST=FCD**FLMOL
      IF(ECTEST.LT.ECONF(TEMPK)) GO TO 21
      ITEMK=ITEMK+IGRADE
      IT=0
      L=0
    6 L=L+1
      IF(L.GT.LIMIT) GO TO 10
      ITSTEP=IABS(ITSTEP/2)
    7 ITEMK=ITEMK-ITSTEP
      IT=IT+ITSTEP
      IF(ITEMK.LT.KELMIN) GO TO 8
      TEMPK=ITEMK
      FCD=PCD*FUCOEF(IT,NO)
      EC=ECONF(TEMPK)
      ECTEST=FCD**FLMOL
      IF(ECTEST-EC)6,10,8
    8 L=L+1
      IF(L.GT.LIMIT) GO TO 10
      ITSTEP=-IABS(ITSTEP/2)
      GO TO 7
    9 TEMPK=TEMPK-1.
      IT=IT+1
      IF(IT.GT.IGRADE) GO TO 21
   10 EC=ECONF(TEMPK)
      FCD=EC**CMOLE
      PCD=FCD/FUCOEF(IT,NO)
      IF(PCD.GT.PTOTAL) GO TO 9
      ITMAX=TEMPK-273.
      IF(NOTA.EQ.2) GO TO 11
      XCD=PCD/PTOTAL
      GO TO 12
   11 XCD=1.-PCD/PTOTAL
   12 IF(NOTA.EQ.2) GO TO 121
```

```
      PRINT 1
      GO TO 122
  121 PRINT 3
  122 PRINT 13,ITMAX,XCD,PCD,FCD
   13 FORMAT(I6,F10.5,2F10.2)
      LINES=LINES+1
C ***
C * STORE VALUES IF DIAGRAM REQUESTED
C ***
      INDEX=0
      IF(JPLOT.GT.0) GO TO 131
      IF(IPLOT.EQ.0) GO TO 132
  131 J=(IP-ITMAX)/INTVAL
      IRA(J,N,1)=ITMAX
      IRA(J,N,2)=XCD*100.+.5
      IF(IRA(J,N,2).LT.1) IRA(J,N,2)=101
      IRA(J,N,3)=0
      IRA(83,N,1)=ITMAX
      IRA(83,N,2)=1
      IRA(83,N,3)=INTVAL
C ***
C * PREPARE FOR SCANNING THE CURVE DOWNSLOPE AT INTERVALS SPECIFIED
C ***
  132 ITEST=ITMAX/INTVAL
      ITEST=ITEST*INTVAL
      IF(ITEST.EQ.ITMAX) GO TO 14
      INDEX=ITEST-ITMAX+INTVAL
      IT=IT-INDEX
      ITMAX=ITMAX+INDEX
   14 ITSTEP=(ITMAX-MINTEM)/INTVAL
      IF(ITSTEP.LT.1) GO TO 221
      INDEX=J
      DO 20 I=1,ITSTEP
      INDEX=INDEX+1
      ITMAX=ITMAX-INTVAL
      TEMPK=ITMAX+273
      IT=IT+INTVAL
      J=J+1
      EC=ECONF(TEMPK)
      FCD=EC**CMOLE
      PCD=FCD/FUCOEF(IT,NO)
      IF(NOTA.EQ.2) GO TO 15
      XCD=PCD/PTOTAL
      GO TO 16
   15 XCD=1.-PCD/PTOTAL
   16 IF(LINES.LT.LP) GO TO 188
      PRINT 17,(RENAME(K),K=1,10),IPRES(N),WORD(3),IPAGE
   17 FORMAT(10H1 REACTION,10A4,4X,22HAT A TOTAL PRESSURE OF,I5,A4,
     1 20X,4HPAGE,I2/)
      IF(NOTA.EQ.2) GO TO 18
      PRINT 1
      GO TO 187
   18 PRINT 3
  187 LINES=5
      IPAGE=IPAGE+1
  188 PRINT 13,ITMAX,XCD,PCD,FCD
      LINES=LINES+1
      IF(PCD.LT.PL) GO TO 23
      IF(INDEX.GT.82) GO TO 20
C ***
C * STORE VALUES IF DIAGRAM REQUESTED
C ***
      IF(JPLOT.GT.0) GO TO 191
      IF(IPLOT.EQ.0) GO TO 20
  191 IRA(J,N,1)=ITMAX
      IRA(J,N,2)=XCD*100.+.5
      IRA(J,N,3)=0
      IRA(83,N,2)=IRA(83,N,2)+1
      IF(NOTA-1)192,193,192
  192 IF(IRA(J,N,2)-100)20,194,194
  193 IF(IRA(J,N,2).GE.1) GO TO 20
  194 IRA(83,N,2)=IRA(83,N,2)-1
      IRA(J,N,1)=0
      IRA(J,N,2)=0
      INDEX=83
   20 CONTINUE
      GO TO 23
   21 PRINT 22,MINTEM
   22 FORMAT(30H0 MAXIMUM TEMPERATURE IS BELOW,I4,8H DEGREES ,
     1 10HCENTIGRADE)
      GO TO 23
  221 ITMAX=ITMAX-INDEX
      PRINT 222, IPRES(N),ITMAX
  222 FORMAT(25H FURTHER CALCULATIONS FOR,I5,20H BAR SKIPPED BECAUSE,
     1 28H MAXIMUM TEMPERATURE IS ONLY,I4,19H DEGREES CENTIGRADE)
   23 RETURN
      END
      SUBROUTINE IGRAPH(INTVAL,MINTEM,MAXTEM,IP,NOPRES,LP)
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      COMMON/BBB/IPRES(4),RENAME(10),SYMBOL(10),PLINE(101),IRA(83,4,3)
      GO TO (40,42,44,46), NOPRES
   40 PRINT 41,(RENAME(J),J=1,10),IPRES(1)
   41 FORMAT(1H1,15X,27HT/XCO2 DIAGRAM FOR REACTION,10A4,2HAT,I5,4H BAR)
C *************************
      GO TO 46
   42 PRINT 43,(RENAME(J),J=1,10),(IPRES(J),J=1,2)
   43 FORMAT(1H1,10X,27HT/XCO2 DIAGRAM FOR REACTION,10A4,2HAT,I5,4H AND,
     1 I5,4H BAR)
      GO TO 48
   44 PRINT 45,(RENAME(J),J=1,10),(IPRES(J),J=1,3)
   45 FORMAT(1H1,5X,27HT/XCO2 DIAGRAM FOR REACTION,10A4,2HAT,2(I5,1H,),
     1 4H AND,I5,4H BAR)
      GO TO 46
   46 PRINT 47,(RENAME(J),J=1,10),(IPRES(J),J=1,4)
   47 FORMAT(28HT/XCO2 DIAGRAM FOR REACTION,10A4,2HAT,3(I5,1H,),4H AND,
     1 I5,4H BAR)
   48 MAXTMP=MINTEM
      MINTMP=MAXTEM
      DO 3 J=1,NOPRES
      IF(IRA(83,J,2).EQ.0) GO TO 3
      MINTRY=IRA(83,J,1)-INTVAL*IRA(83,J,2)+INTVAL
      IF(MAXTMP.GE.IRA(83,J,1)) GO TO 2
      MAXTMP=IRA(83,J,1)
    2 IF(MINTRY.GE.MINTMP) GO TO 3
      MINTMP=MINTRY
    3 CONTINUE
      IF(MAXTMP.LT.MINTMP) GO TO 20
      ITEST=MAXTMP/INTVAL
      ITEST=ITEST*INTVAL
      IF(ITEST.EQ.MAXTMP) GO TO 4
      MLINE=ITEST+INTVAL
      GO TO 5
    4 MLINE=ITEST
    5 ITEST=MINTMP/INTVAL
      ITEST=ITEST*INTVAL
      IF(ITEST.EQ.MINTMP) GO TO 6
      MINTMP=ITEST+INTVAL
    6 NOLIN=(MLINE-MINTMP)/INTVAL
      IF(NOLIN.LT.1) GO TO 20
      J=(IP-MAXTMP)/INTVAL
      K=J+NOLIN
      IPAGE=0
      LPLOT=LP-2

      IF(NOLIN.LT.LPLOT) GO TO 64
      L=J+LPLOT
      DO 63 M=1,NOPRES
      IF(IRA(L,M,2).GE.10) GO TO 61
      IF(IRA(L,M,3).GE.10) GO TO 62
      GO TO 63
   61 IF(IRA(L,M,2).LE.90) GO TO 65
      IF(IRA(L,M,3).GE.10) GO TO 62
      GO TO 63
   62 IF(IRA(L,M,3).LE.90) GO TO 65
   63 CONTINUE
   64 IPAGE=IPAGE+1
   65 IPAGE=IPAGE+1
      LINES=1
      LPLOT=LPLOT-1
      IF(IPAGE.EQ.1) LINES=-1
      MLINE=MLINE+INTVAL
      DO 19 L=J,K
      MLINE=MLINE-INTVAL
      PLINE(1)=SYMBOL(9)
      PLINE(101)=SYMBOL(9)
      DO 7 M=2,100
      PLINE(M)=SYMBOL(5)
    7 CONTINUE
      DO 8 M=11,91,10
      PLINE(M)=SYMBOL(10)
    8 CONTINUE
      DO 10 M=1,NOPRES
      IF(IRA(L,M,2).EQ.0) GO TO 9
      IF(IRA(L,M,2).EQ.101) IRA(L,M,2)=0
      NL=IRA(L,M,2)+1
      PLINE(NL)=SYMBOL(M)
    9 IF(IRA(L,M,3).EQ.0) GO TO 10
      NL=IRA(L,M,3)+1
      PLINE(NL)=SYMBOL(M)
   10 CONTINUE
      MARGIN=MLINE-INTVAL
      INDEX=1
      DO 11 M=1,NOPRES
      NL=IRA(L,M,1)
      IF(NL.EQ.0) GO TO 11
      IF(NL.EQ.MLINE) GO TO 11
      IF(NL.GT.MARGIN) MARGIN=NL
      INDEX=0
```

```
 11 CONTINUE
    IF(INDEX.EQ.0) GO TO 12
    MARGIN=MLINE
    ITEST=MLINE/INTVAL
    ITEST=ITEST/5
    ITEST=ITEST*5*INTVAL
    IF(ITEST.NE.MARGIN) GO TO 16
 12 IF(LINES.LT.LPLOT) GO TO 14
    PRINT 15,MARGIN,(PLINE(I),I=1,101),MARGIN
121 IF(IPAGE.GT.1) GO TO 22
    PRINT 13
 13 FORMAT(1H1)
    LINES=1
    IPAGE=IPAGE+1
    LOLD=L
    L=K-LPLOT+1
    IF(L.GT.LOLD) L=LOLD
    MLINE=MLINE+(LOLD-L)*INTVAL
    GO TO 19
 14 PRINT 15,MARGIN,(PLINE(I),I=1,101),MARGIN
 15 FORMAT(I5,1X,101A1,I4)
    LINES=LINES+1
    GO TO 19
 16 IF(LINES.LT.LPLOT) GO TO 18
    PRINT 17,(PLINE(I),I=1,101)
 17 FORMAT(6X,101A1)
    GO TO 121
 18 PRINT 17,(PLINE(I),I=1,101)
    LINES=LINES+1
 19 CONTINUE
    GO TO 22
 20 PRINT 21,MINTEM,MAXTEM
 21 FORMAT(51H CANNOT BE SHOWN BECAUSE THERE ARE NO SUITABLE XCO2,
  1 23H-VALUES IN THE RANGE OF,I4,3H TO,I4,19H DEGREES CENTIGRADE)
    GO TO 27
 22 DO 23 M=2,100
    PLINE(M)=SYMBOL(7)
 23 CONTINUE
    DO 24 M=11,91,10
    PLINE(M)=SYMBOL(9)
 24 CONTINUE
    PRINT 17,(PLINE(I),I=1,101)
    PRINT 25
 25 FORMAT(8H XCO2=.0,7X,3H0.1,7X,3H0.2,7X,3H0.3,7X,3H0.4,7X,3H0.5,
  1                    7X,3H0.6,7X,3H0.7,7X,3H0.8,7X,3H0.9,7X,3H1.0)
    DO 26 I=1,4
    DO 26 J=1,3
    IRA(83,I,J)=0
 26 CONTINUE
 27 RETURN
    END
```