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LBL MANUAL FOR THE EQ CHEMICAL SIMULATION PROGRAMS

Pat Iqbal

January 1979

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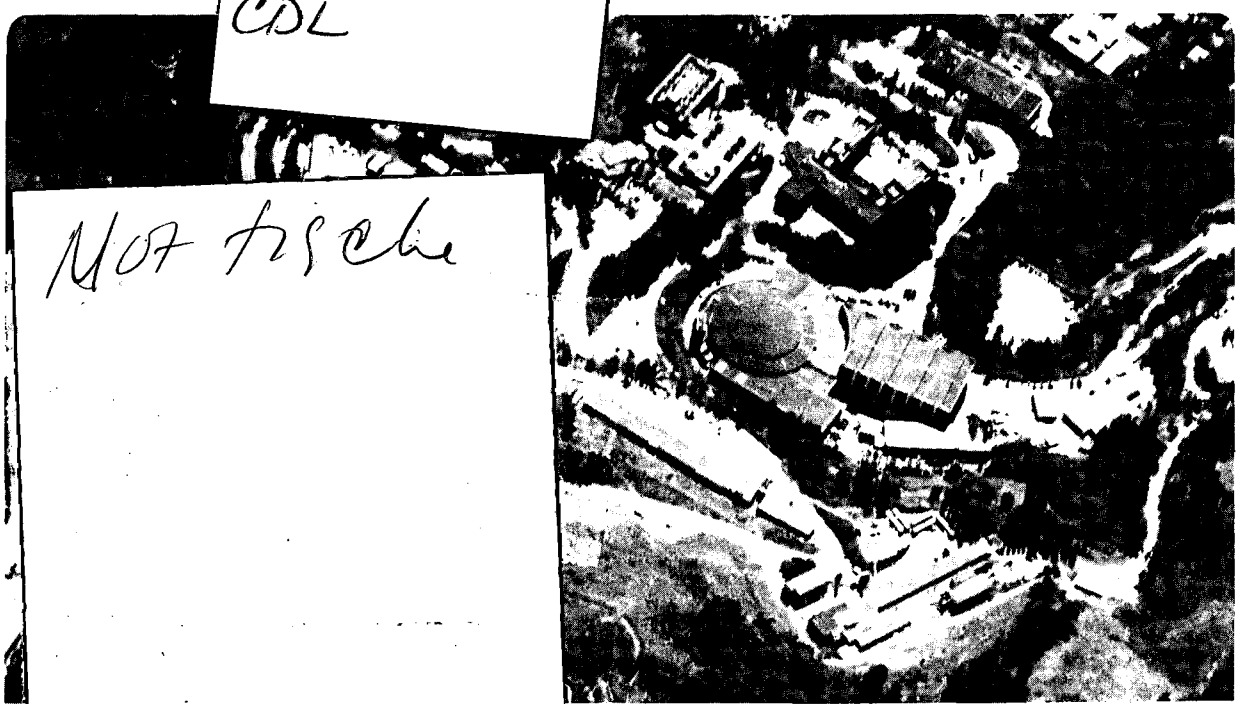

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LBL MANUAL FOR THE EQ CHEMICAL SIMULATION PROGRAMS

PAT IQBAL

JANUARY, 1979

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*                  P R O G R A M   M A N U A L              *
*                                                           *
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THIS MANUAL IS COMPOSED OF DOCUMENTATION PROVIDED BY THE AUTHOR OF THE SOURCE CODES, TOM WOLERY, TOGETHER WITH EXTRA INFORMATION ABOUT THE NEW DATA BASE FORMATS AND NEW INPUT FORMATS FOR THE LBL JANUARY 79 VERSION OF THESE PROGRAMS.

PAT IQBAL
LBL, CSAM
JANUARY, 1979

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1.1 EQF

GENERAL DESCRIPTION OF EQF PROGRAM

THIS ROUTINE READS A PRIMARY THERMODYNAMIC DATA FILE ON DEQXB AND CREATES A SIMILAR FILE (WRITTEN ON DEQXL) IN WHICH PARAMETERS SUCH AS LOG K VALUES, PRESS, ADH, BDH, ETC. ARE REPLACED BY POLYNOMIAL FIT COEFFICIENTS FOR THESE QUANTITIES VERSUS TEMPERATURE IN DEG C. IF IOPT=1 THEN INDIVIDUAL SETS OF FITS MAY BE MADE. THE IMSL EXTERNAL RLFOTW IS USED TO PERFORM THE FITS.

DESCRIPTION OF INPUT VARIABLES FOR EQF

NRST=NUMBER OF REACTIONS WITHIN THE AQUEOUS PHASE
NMT =NUMBER OF PURE MINERALS
NGT =NUMBER OF GASES
NXT =NUMBER OF SOLID SOLUTIONS

1/79

EQF INPUT FORMATS

DATA ENTRY FORM

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30 ...	73	74	75	76	77	78	79	80
	NRST					NMT						NGT						NXT							(4I5)												

1.2 EQS

GENERAL DESCRIPTION OF EQS PROGRAM

EQS READS THE INPUT FILES DATA1 AND DATA2. DATA1 = DEQCE, DATA2 = DEQCDL AND DEQXL (X=SSC OR 500). IT WRITES ON DEQCDS SHORT FORMAT REACTION COEFFICIENTS AND ON DEQXS CORRESPONDING POLYNOMIAL COEFFICIENTS FOR LOG K VALUES. IN ADDITION, ALL REACTIONS ARE CHECKED FOR CHARGE AND MASS BALANCE TO FIND POSSIBLE ERRORS IN THE REACTION COEFFICIENTS OR THE COMPOSITIONAL DATA. SUCH ERRORS ARE FLAGGED ON THE OUTPUT AND SHOULD THEN BE CORRECTED BY THE USER.

T.J. WOLERY

* *

ADDENDUM

THIS VERSION WAS RECEIVED AT LBL AT THE END OF NOVEMBER 1978, AND MODIFICATIONS TO THE DATA BASE (EQDAT02) FORMAT WERE MADE FOR ENHANCED LEGIBILITY AND EASIER UPDATE. THE RESULTING MAIN CHANGES IN EQS WERE TO ROUTINE INDATS, ALTHOUGH CHANGES TO ARRAY SIZES OCCUR THROUGHOUT. NOTE THAT AQUEOUS SPECIES NAMES WERE EXPANDED TO TWENTY CHARACTERS.

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JANUARY, 1979

* *

1.3 EQ3

GENERAL DESCRIPTION OF EQ3 PROGRAM

THIS PROGRAM COMPUTES THE FULL OR PARTIAL EQUILIBRIUM DISTRIBUTION OF SPECIES IN AN AQUEOUS SOLUTION AT A SPECIFIED TEMPERATURE AND A PRESSURE WHICH DEPENDS UPON THE TEMPERATURE AND THE DATA FILE WHICH IS USED (TAPE7=DATA2). ALL ION ASSOCIATION REACTIONS ARE PRESUMED TO BE IN EQUILIBRIUM. THE USER SPECIFIES WHICH OXIDATION-REDUCTION (CROSS-LINK) REACTIONS ARE PRESUMED TO BE IN EQUILIBRIUM. REDOX COUPLING IS ACHIEVED BY SPECIFYING A PH PARAMETER AND ONE OF THE FOLLOWING IOPT1 CONDITIONS

= 0 F O2 (G,AQ)
= 1 F O2 (AQ), CONC O2 (AQ), OR ACT O2 (AQ)
= 2 EH, IN VOLTS
= 3 CONC TOT SO4-- OR ACT SO4-- PLUS
CONC TOT HS- OR ACT HS-
= 4 F H2 (AQ), CONC H2 (AQ), OR ACT H2 (AQ)
= 5 P E-

IF EQ3 OUTPUT IS TO BE USED TO INITIALIZE A PATH ROUTINE, THEN A FULL EQUILIBRIUM MODEL MUST BE COMPUTED. THIS MAY BE ACCOMPLISHED BY SETTING JFLAG EQUAL TO 7 OR 8 FOR ALL AUXILIARY BASIS SPECIES, EXCEPT FOR THOSE WHICH ARE USED IN DEFINING THE FUGACITY OF O2 (G,AQ) THROUGH ONE OF THE IOPT1 OPTIONS. ALTERNATIVELY, THE BALANCE CONSTRAINTS FROM A PARTIAL EQUILIBRIUM MODEL MAY BE FED INTO PROGRAM EQ4 OR EQ5 AND EQUILIBRATED AT THE SAME OR DIFFERENT CONDITIONS OF PRESSURE AND TEMPERATURE.

NOTE THAT O2 (G,AQ) (NS=NSB) IS A FICTIVE AQUEOUS SPECIES USED TO DENOTE THE OXYGEN FUGACITY IN THE AQUEOUS PHASE. ALL REDOX REACTIONS ARE HANDLED DIRECTLY THROUGH THIS PARAMETER. IF IOPT1 IS NOT 0, THEN THIS FUGACITY IS COMPUTED DIRECTLY OR ITERATIVELY IN THE PROGRAM.

AQUEOUS SPECIES ARE SUBDIVIDED INTO

NS=1,NSB STRICT BASIS SPECIES
NS=NSB+1,NSQ AUXILIARY BASIS SPECIES
NS=NSQ+1,NST STRICT DERIVED SPECIES

AN EQ3 PROBLEM IS DEFINED BY THE CHOICE OF IOPT1 AND THE JFLAG CONTROL ARRAY. EACH BASIS SPECIES (NS=1,NSQ) IS ASSIGNED A JFLAG INDEX WHICH SPECIFIES THE TYPE OF ASSIGNED CONSTRAINT

= 0 TOTAL CONC
= 1 LOG ACTIVITY
= 2 LOG FREE CONC
= 3 PPM TOTAL CONC
= 4 CC STP/CC SOLN
= 5 FUGACITY
= 6 TITRATION ALKALINITY
= 7 DEPENDENT VARIABLE (NOT UNDER MASS BALANCE CONSTRAINT)
= 8 ELIMINATED VARIABLE (UNDER MASS BALANCE CONSTRAINT)
= 9 MINERAL ACTIVITY PRODUCT

TABLE OF RECOMMENDED JFLAG VALUES

1	H2O	0									FIXED	INDEX=1
2	NA+	0	1		3					9	FIXED	INDEX=2
3	K+	0	1		3					9	FIXED	INDEX=3
4	CA++	0	1		3					9	FIXED	INDEX=4
5	MG++	0	1		3					9	FIXED	INDEX=5
6	AL+++	0	1		3					9		
7	SIO2 (AQ)	0	1		3					9		
8	-----	0										
9	ZN++	0	1		3					9		
10	PB++	0	1		3					9		
11	AG+	0	1		3					9		
12	-----	0										
13	H+		1							9	FIXED	INDEX=13
14	CO3--	0	1		3		5	6		9	FIXED	INDEX=14
15	NH4+	0	1		3		5			9	FIXED	INDEX=15
16	CL-	0	1		3					9	FIXED	INDEX=16
17	SO4--	0	1		3					9	FIXED	INDEX=17
18	-----	0										
19	HG++	0	1		3					9		
20	AS(OH)4-	0	1		3					9		
21	MN++	0	1		3					9		
22	FE++	0	1		3					9		
23	CU+	0	1		3					9		
24	AU+	0	1		3					9		
25	O2 (G,AQ)						5				GENERAL	INDEX=NSB
26	O2 (AQ)		1	2		4	5		7		GENERAL	INDEX=NSB+1
27	H2 (AQ)		1	2		4	5		7		GENERAL	INDEX=NSB+2
28	N2 (AQ)		1	2		4	5		7	8	GENERAL	INDEX=NSB+3
29	CH4 (AQ)		1	2		4			7		GENERAL	INDEX=NSB+4
30	-----	0									GENERAL	INDEX=
31	HS-	0	1		3				7	8 9	GENERAL	INDEX=NSB+6
32	HS2++	0	1		3					8 9		
33	AS(OH)3---	0	1		3					8 9		
34	MN+++	0	1		3					8 9		
35	FE+++	0	1		3					8 9		
36	CU++	0	1		3					8 9		
37	AU+++	0	1		3					8 9		
38	-----	0										
39	NO3-	0	1		3				7	8 9		
40	OH-	0									GENERAL	INDEX=NSQ

VALUES OF THE CONSTRAINING PARAMETERS ARE INPUT IN THE ISP ARRAY. WATER (NS=1) AND OH- (NS=NSQ) ARE TREATED IN A PRE-PROGRAMMED MANNER, AND ZEROES MAY BE READ IN FOR THEIR JFLAG AND ISP VALUES. IF IOPT1 IS NOT ZERO, THEN JFLAG AND ISP INPUT FOR O2 (G,AQ) IS SIMPLY IGNORED.

TWO TREATMENTS ARE AVAILABLE FOR SOLID SOLUTIONS. (1) THE PROGRAM PROCESSES HYPOTHETICAL SOLID SOLUTION PHASES TO SEE IF THERE ARE ALLOWABLE COMPOSITIONS WHICH ARE IN EQUILIBRIUM WITH THE FINAL AQUEOUS PHASE MODEL. THE SATURATION STATE FOR A HYPOTHETICAL SOLID SOLUTION PHASE MAY BE SATURATED, UNDERSATURATED, SUPERSATURATED, OR UNDEFINED. THESE STATES ARE EVALUATED IN SUBROUTINE HYPSATX. (2) THE PROGRAM PROCESSES INPUT SOLID SOLUTION COMPOSITIONS AND EVALUATES THE SATURATION STATES OF THE END-MEMBERS DIRECTLY. THIS OPTION MUST BE EMPLOYED IF THE JFLAG=9 OPTION IS USED TO FORM AN ACTIVITY PRODUCT CONSTRAINT USING A

SOLID-SOLUTION END-MEMBER. CONTROL SWITCH IOPT4 SPECIFIES SOLID-SOLUTION TREATMENT.

ELECTRICAL BALANCE IS ACHIEVED BY ADJUSTING THE TOTAL CONCENTRATION OF A MAJOR ION (NANION), USUALLY CL-. HENCE, JFLAG(NANION) MUST BE EQUAL TO 0 OR 3 ON INPUT, OR THE SYSTEM WILL TRY TO FIND ANOTHER MAJOR ION TO SERVE AS THE NANION. IF A SUITABLE NANION CAN NOT BE FOUND, THEN THE COMPUTATION IS TERMINATED. THE ACTIVITY OF WATER IS COMPUTED FROM THE EQUIVALENT STOICHIOMETRIC IONIC STRENGTH OF A SODIUM CHLORIDE SOLUTION (XISTEQ). THIS IS DEFINED AS THE TOTAL CONCENTRATION OF THE IACTION, WHICH IS EITHER CL- OR NA+. IN THIS VERSION, JFLAG(IACTION) MUST BE 0 OR 3 ON INPUT AND ISP(IACTION) MUST BE GREATER THAN ZERO. THE PROGRAM CHOOSES THE IACTION. IF BOTH NA+ AND CL- ARE SUITABLE, THE ION WITH THE GREATER ISP VALUE IS CHOSEN. IF NEITHER IS SUITABLE, IACTION IS SET TO ZERO AND THE ACTIVITY OF WATER IS ASSUMED TO BE UNITY.

IF EQ3 IS NOT BEING USED TO INITIALIZE ANOTHER PROGRAM, SUCH AS EQ5, BUT ONLY TO DETERMINE ESTIMATES OF ACTIVITIES AND SATURATION STATES, SET TOLSAT TO A VALUE IN ACCORD WITH THE UNCERTAINTY OF THE LOG K VALUES FOR THE MINERAL DISSOLUTION REACTIONS (I.E., AROUND 0.5-1.0). OTHER TOLERANCES (TOL, TOLEB, TOLXI) SHOULD BE ON THE ORDER OF 1.E-5-1.E-3.

IF THE 7 OR 9 JFLAG OPTIONS ARE BEING USED, IT IS RECOMMENDED THAT IOPT2 BE SET TO 1 FOR EXTRA PRINT-OUT AND FOR CHECKING OF THE MASS BALANCE AND MASS ACTION CONSTRAINTS.

MORE DETAILED COMMENTS REGARDING INPUTS AND OPTIONS MAY BE FOUND IN THE INPUT SECTION AND THROUGHOUT THE PROGRAM AND ITS SUBPROGRAMS.

THE BASIC STRUCTURE OF THIS PROGRAM CONSISTS OF THREE NESTED ITERATION LOOPS. THE INNER LOOP COMPUTES THE DISTRIBUTION OF SPECIES IN TERMS OF LOG CONC VALUES. THE MIDDLE LOOP ADJUSTS THE TOTAL CONCENTRATION OF A MAJOR ION (NANION) TO ACHIEVE AN ELECTRICALLY BALANCED SOLUTION. THE OUTER LOOP ADJUSTS THE IONIC STRENGTH TO THE VALUE WHICH IS CONSISTENT WITH THE DISTRIBUTION OF SPECIES.

THE INNER LOOP EMPLOYS A MONOTONE SEQUENCE ALGORITHM WHICH IS PARTLY DESCRIBED IN

WOLERY, T.J., AND WALTERS, L.J., JR., 1975, CALCULATION OF EQUILIBRIUM DISTRIBUTIONS OF CHEMICAL SPECIES BY MEANS OF MONOTONE SEQUENCES, MATHEMATICAL GEOLOGY, V.7, P.99-115.

IN THIS METHOD, EACH UNKNOWN IS SIMULTANEOUSLY APPROACHED FROM ABOVE AND BELOW, THUS YIELDING STRICTLY DEFINED ERROR BOUNDS.

THE MIDDLE AND OUTER LOOPS EACH SOLVE FOR THE ZERO OF A DEVIATION FUNCTION BY FITTING THE PARAMETER TO BE ADJUSTED AS A FUNCTION OF THE DEVIATION FUNCTION TO A POLYNOMIAL OF UP TO FOURTH ORDER AND COMPUTING THE VALUE AT ZERO AS THE NEXT ESTIMATE OF THE ADJUSTED PARAMETER. IOPT9 IS THE MAXIMUM NUMBER OF POINTS USED IN THE FITTING. IF IOPT9 = 2, THIS METHOD REDUCES TO THE SECANT METHOD.

THE FOLLOWING CONVENTIONS ARE EMPLOYED IN THIS PROGRAM

```
CONC H2O = 1.0    ACT H2O = G H2O
CONC O2 (G,AQ) = 0.0    G O2 (G,AQ) = 1.0
CONCLG O2 (G,AQ) = ACTLG O2 (G,AQ) = LOG FUGACITY O2 (G,AQ)
```

FOR NEUTRAL AQUEOUS COMPLEXES, Z = A MULTIPLE OF TEN. THE MULTIPLE IS A SWITCH WHICH DESIGNATES HOW THE ACTIVITY COEFFICIENT OF THE NEUTRAL SPECIES IS TO BE COMPUTED.

TROUBLE-SHOOTING NOTES.....

IF BOTH ULG AND SLG FOR CARBONATE DIVERGE TO MINUS INFINITY UNDER THE TITRATION ALKALINITY OPTION, THEN NON-CARBONATE ALKALINITY PROBABLY EXCEEDS THE INPUT VALUE OF TITRATION ALKALINITY AND THE PROBLEM IS ILL-POSED.

IF THE OXYGEN FUGACITY IS EXTREMELY LOW, THEN THE FERRIC IRON MASS ACTION RELATIONS MAY NOT BE SATISFIED. THIS PROBLEM IS CAUSED BY LOSS OF SIGNIFICANT DIGITS DURING ARITHMETIC OPERATIONS. TOL SHOULD BE TIGHTENED TO A VALUE OF ABOUT 1.E-10. THIS HAS SUFFICED TO SOLVE A TEST PROBLEM WITH FO2 = 1.E-100.

AFTER THE CORRECT DISTRIBUTION OF SPECIES HAS BEEN COMPUTED, THE COMPOSITION OF THE SOLUTION IS THEN COMPUTED IN TERMS OF THE MOLES OF THE ELEMENTS RELATIVE TO 1000 GRAMS OF H2O SPECIES. THE SATURATION STATES OF ALL RELEVANT MINERALS AND SOLID SOLUTION COMPONENTS ARE DETERMINED AND PRINTED. OPTIONAL PUNCHED OUTPUT OR DISK FILE STORAGE IS DESIGNED TO INTERFACE WITH COMPANION PROGRAMS.

THE DISK FILES DATA1 AND DATA2 ARE TAKEN FROM LOGICAL RECORDS OF TAPE FILE EQDAT02 OR ITS EQUIVALENT. EQDAT02 CONTAINS TEMPERATURE-DEPENDENT DATA IN BOTH GRID FORM AND AS POWER- SERIES COEFFICIENTS. ONLY THE LATTER ARE READ AND USED BY EQ3.

EQ3 WILL PROCESS MULTIPLE INPUT SETS IN A SINGLE RUN.

THIS VERSION CLEANED UP BY VCC TIDY ON 4 SEPTEMBER 1976. THIS PROGRAM IS WRITTEN FOR THE CDC 6400 COMPUTER AND CONFORMS TO THE FORTRAN EXTENDED REFERENCE MANUAL FOR CDC 6400/6500/ 6600/6700/7600 COMPUTERS (IT SHOULD BE COMPILED BY AN FTN COMPILER).

THIS PROGRAM WAS WRITTEN BY T.J. WOLERY, DEPT. OF GEOLOGICAL SCIENCES, NORTHWESTERN UNIVERSITY, EVANSTON, ILLINOIS 60201. KINDLY NOTIFY THE AUTHOR OF ANY BUGS YOU ENCOUNTER AND OF ANY CORRECTIONS OR MODIFICATIONS YOU MAY MAKE.

THIS IS THE EXPERIMENTAL VERSION OF 6 MARCH 1977.

T.J. WOLERY

* *

ADDENDUM

THIS VERSION WAS RECEIVED AT LBL AT THE END OF NOVEMBER 1978, AND MODIFICATIONS TO THE DATA BASE (EQDAT02) FORMAT AND TO THE INPUT FORMAT WERE MADE FOR ENHANCED LEGIBILITY AND EASIER UPDATE. THE MAIN CHANGES WERE TO ROUTINES EQ3 AND INDATX, ALTHOUGH CHANGES NEEDED TO GENERALIZE REFERENCES TO DATA BASE ELEMENTS BY INDEX OCCUR THROUGHOUT AS DO CHANGES RELATED TO ALLOWING AQUEOUS SPECIES NAMES TO BE TWENTY CHARACTERS LONG, AND THOSE DESIGNATING CERTAIN ARRAYS AS LCM (LEVEL 2). ALSO SOME ARRAY SIZES WERE INCREASED.

PAT IQBAL
LBL, CSAM
JANUARY, 1979

DESCRIPTION OF INPUT VARIABLES FOR EQ3

TITLE = FIVE CARDS OF VERBAL DESCRIPTION OF AN AQUEOUS SOLUTION COMPOSITION

TEMPC = TEMPERATURE, DEGREES CENTIGRADE

RHO = DENSITY OF SOLUTION IN G/CM3
WFS = WEIGHT FRACTION OF H2O SPECIES OF SOLUTION
SCREW = INNER LOOP CONVERGENCE ADJUSTMENT PARAMETER
--- SEE COMMENTS IN THE INNER LOOP ---
EH = EH, OXIDATION-REDUCTION PARAMETER
PE = P E-

TOL = CONVERGENCE TOLERANCE FOR INNER ITERATION LOOP
TOLXI = CONVERGENCE TOLERANCE FOR IONIC STRENGTH ITERATION
TOLEB = CONVERGENCE TOLERANCE FOR ELECTRICAL BALANCE ITERATION

NCONV = LIMIT ON NUMBER OF ITERATIONS FOR INNER LOOP
MCONV = LIMIT ON NUMBER OF ITERATIONS THROUGH ELECTRICAL BALANCE AND IONIC STRENGTH LOOPS

IOPT1 = OPTION SWITCH FOR REDOX COUPLING
= 0 F O2 (G,AQ) SPECIFIED
= 1 O2 (AQ) PARAMETER SPECIFIED
= 2 EH SPECIFIED IN VOLTS
= 3 SULFATE-BISULFIDE SPECIFIED
= 4 H2 (AQ) PARAMETER SPECIFIED
= 5 P E- SPECIFIED
IOPT2 = OPTION SWITCH
= 0 DEFAULTS TO = 2
= 1 PRINTS OUT RESULTS OF INNER LOOP EVERY ITERATION AND CHECKS BALANCE AND MASS ACTION CONSTRAINTS
= 2 CHECKS BALANCE AND MASS ACTION CONSTRAINTS (DEFAULT)
IOPT3 = OPTION SWITCH FOR PRODUCING INTERFACING OUTPUT
= 0 DOES NOTHING
= 1 WRITES INTERFACING OUTPUT ON A DISK FILE (TAPE8)
IOPT4 = OPTION SWITCH FOR SOLID SOLUTIONS
= 0 IGNORES ALL SOLID SOLUTIONS
= 1 PROCESSES HYPOTHETICAL SOLID SOLUTIONS
= 2 READS IN SOLID SOLUTION COMPOSITIONS AND PROCESSES BOTH INPUT AND HYPOTHETICAL SOLID SOLUTIONS.
IOPT5 = OPTION SWITCH
= 0 DOES NOTHING
= 1 PRINTS OUT THE LOG K VALUES
IOPT9 = OPTION SWITCH
= 2,5 = MAXIMUM NO. OF POINTS USED IN FIND ROUTINE. DEFAULT = 3. IF IOPT9 = 2 THE METHOD REDUCES TO THE SECANT METHOD.

IKEXP = OPTION SWITCH FOR ACTIVITY COEFFICIENTS OF NEUTRAL AQUEOUS COMPLEXES -- DO NOT USE IF MAKING A DECK FOR EQ4/5

= 0 DOES NOTHING
= 1 SETS Z TO 0. (FOR ALL NEUTRAL SPECIES)
= 2 SETS Z TO 10.
= 3 SETS Z TO 20.
= 4 SETS Z TO 30.
= 5 SETS Z TO 40.
= 6 SETS Z TO 50.

NANION NAME = NAME OF SPECIES WHOSE CONCENTRATION IS TO BE ADJUSTED TO ACHIEVE ELECTRICAL BALANCE

NXRST = NO. OF AQUEOUS REACTIONS TO BE SUPPRESSED BY CARD INPUT
NXMNT = NO. OF MINERALS TO BE SUPPRESSED BY CARD INPUT
NXGST = NO. OF GAS SPECIES TO BE SUPPRESSED BY CARD INPUT
NXXXT = NO. OF SOLID SOLUTIONS TO BE SUPPRESSED BY CARD INPUT

JCOUNT = NUMBER OF JFLAG VALUES TO BE SPECIFIED.
THOSE NOT SPECIFIED DEFAULT TO 0

JFLAG = CONTROL PARAMETER SPECIFYING TYPE OF CONSTRAINT ON BASIS AND AUXILIARY SOLUTION SPECIES, AND EQUALS 0 THROUGH 9

= 0 TOTAL CONC (DEFAULT)
= 1 LOG ACTIVITY (-PH, FOR EXAMPLE)
= 2 LOG FREE CONC
= 3 PPM TOTAL CONC
= 4 CC STP/CC SOLN (FOR DISSOLVED GASES)
= 5 FUGACITY
--RESTRICTED USE--
-F CO2 FOR CO3--
-F O2 FOR O2 (G,AQ)
-F O2 FOR O2 (AQ)
-F N2 FOR NH4+
-F N2 FOR N2 (AQ)
= 6 TITRATION ALKALINITY (CO3-- ONLY)
= 7 DEPENDENT SPECIES
-AUXILIARY VARIABLES ONLY
-COMPUTES AUXILIARY SPECIES FROM CORRESPONDING STRICT BASIS SPECIES THROUGH CROSS-LINK REACTION
-DEPENDENT SPECIES ARE NOT INCLUDED IN A MASS BALANCE CONSTRAINT ON THE CORRESPONDING STRICT BASIS VARIABLE
= 8 ELIMINATED SPECIES
-AUXILIARY SPECIES ONLY
-TREATS AUXILIARY SPECIES AND ALL OF ITS DERIVED SPECIES AS ALL DERIVED SPECIES OF THE CORRESPONDING STRICT BASIS VARIABLE
-ELIMINATED SPECIES ARE INCLUDED IN A MASS BALANCE CONSTRAINT ON THE CORRESPONDING STRICT BASIS VARIABLE
-EXAMPLE..IF JFLAG(SO4--)=0 AND JFLAG(HS-)=7, THEN
ISP(SO4--)=CONC TOT SO4--
BUT IF JFLAG(HS-)=8,
ISP(SO4--)=CONC TOT SO4-- + CONC TOT HS-
IF JFLAG(SO4--) IS NOT 0, THEN THE 7 AND 8 OPTIONS FOR HS- PRODUCE THE EQUIVALENT RESULT

```
= 9   MINERAL ACTIVITY PRODUCT
      --SPECIAL CODING--
         -FOR A PURE MINERAL PHASE, ENTER NM INDEX AS
          AS A FLOATING POINT NUMBER
         -FOR A SOLID-SOLUTION END-MEMBER, WHERE NX = SOLID-
          SOLUTION PHASE, IK = COMPONENT INDEX, AND NEND(IK,NX)
          = THE CORRESPONDING PURE PHASE, ENTER
          50000 + 100*NX + IK AS A FLOATING POINT NUMBER
      --RESTRICTIONS--
         -LIMIT OF 7 SUCH CONSTRAINTS
         -NO MINERAL CAN BE USED MORE THAN ONCE
      --NOTE--
         -PHASE RULE VIOLATIONS CAN BE PROGRAMMED,
          BUT THE INNER LOOP WILL NOT CONVERGE
IF IOPT1 IS NOT 0, SET JFLAG(NSB)=5 AND ISP(NSB)=0.


 ICOUNT = NUMBER OF ISP VALUES TO BE SPECIFIED.
          THOSE NOT SPECIFIED DEFAULT TO 0.0

ISP = INITIAL SOLUTION PARAMETER FOR BASIS AND AUXILIARY SOLUTION
      SPECIES


SCOUNT = NUMBER OF SLGB VALUES TO BE SPECIFIED.
         THOSE NOT SPECIFIED DEFAULT TO 0.0

SLGB = INITIAL GUESS AT LOWER BOUND FOR LOG CONC OF EACH BASIS
AND AUXILIARY SOLUTION SPECIES


XCOUNT = NUMBER OF XBAR VALUES TO BE SPECIFIED.
         THOSE NOT SPECIFIED DEFAULT TO 0.0

XBAR=MOLE FRACTION OF END MEMBER IN A SOLID SOLUTION
```

EQ3 INPUT FORMAT

DATA ENTRY FORMS

	1–5	6–10	11–20	21–30	31–40	41–50	51–60	61–70	71–80	Format
	TITLE									(8A10)
	TITLE									"
	TITLE									"
	TITLE									"
	TITLE									"
	TEMPC		TEMPC							(5X,5E 15.6)
	RHO		RHO	WFS		SCREW		EH	PE	"
	TOL		TOL	TOLXI		TOLEB		TOLSAT		"
	CONV	NCONV	NCONV							(5X, 2I5)
	IOPT	IOPT1	IOPT2	IOPT3	IOPT4	IOPT5	IOPT6	IKEXP		(5X, 7I5)
	NAN	NANION	NAME							(5X, 2A10)
	SUPPR	NXRST	NXMNT	NXGST	NXXXT					(5X, 4I5)
IF NXRST>0	AQSP	AQSP (NAME) TO BE SUPPRESSED			AQSP (NAME) TO BE SUPPRESSED		AQSP (NAME) TO BE SUPPRESSED			(3(5X,2A10))
IF NXMNT>0	MINS	MIN (NAME) " " "			MIN " " " "		MIN " " " "			"
IF NXGST>0	GASES	GAS (NAME) " " "			GAS " " " "		GAS " " " "			"
IF NXXXT>0	SOLS	SOLID (NAME) " " "			SOLID " " " "		SOLID " " " "			"
	JFLAG	JCOUNT								(5X, I5)
IF JCOUNT>0	J 1	VALUE	NAME (aq. sp.)		VALUE	NAME (aq. sp.)		value	NAME (aq. sp.)	(5X,3(I5,2A10))
JCOUNT records	J 2	"	"		"	"		"	"	"
	ISP	ICOUNT								(5X, I5)
IF ICOUNT>0	I 1		ISP≠0	aq. sp. NAME			ISP ≠ 0	AQSP NAME		(5X, 2(E15.6,2A10))
	SLGB	SCOUNT								(5X, I5)
IF SCOUNT>0	SL 1		SLGB≠0	"	"		SLGB ≠ 0	"	"	"
IF IOPT4 ≥2	XBAR	XCOUNT								(5X, I5)
IF XCOUNT>0		XBAR	(1)	(2)	(3)	(4)		(5)	(6)	(6E13.6)

1.4 EQ6

GENERAL DESCRIPTION OF EQ6 PROGRAM

THIS PROGRAM COMPUTES THE PATH OF ONE OF SEVERAL EQUILIBRIUM OR PARTIAL EQUILIBRIUM REACTION MODELS WHICH DESCRIBES MASS TRANSFER BETWEEN A REACTANT SUBSYSTEM, AN EQUILIBRIUM SUBSYSTEM, AND A PHYSICALLY REMOVED SUBSYSTEM. (THIS PATH NEED NOT BE ISOTHERMAL, AND TEMPERATURE ALONE MAY BE VARIED IF NO REACTANTS ARE SPECIFIED). FOR THE CLOSED SYSTEM MODEL THE CONCEPT OF REACTION VESSEL ENCOMPASSES EITHER JUST THE EQUILIBRIUM SUBSYSTEM OR THE EQUILIBRIUM SUBSYSTEM PLUS THE REACTANT SUBSYSTEM. IN ALL CASES THE PRESSURE IS COMPUTED AS A DEPENDENT FUNCTION OF THE TEMPERATURE AND IS DETERMINED BY WHICH SUPPORTING DATA ARE USED IN THE RUN. NOTE...A GAS PHASE IS PRESENTLY NOT INLCUDED IN ANY OF THE CURRENT MODELS. THE EQUILIBRIUM SUBSYSTEM CONSISTS OF AN AQUEOUS PHASE IN INTERNAL EQUILIBRIUM PLUS ANY NUMBER OF OTHER PHASES IN REVERSIBLE EQUILIBRIUM WITH THAT PHASE.' A MODEL IS SPECIFIED BY THE CHOICE OF THE PARAMETERS MODEL AND MTYPE.

MODEL = 0 THE NEWTON-RAPHSON ROUTINE VERIFIES OR RECOMPUTES THE STARTING EQUILIBRIUM SUBSYSTEM, AND COMPUTATION TERMINATES WITHOUT COMPUTING A REACTION PATH MODEL.

MODEL = 1 REACTANTS ARE TITRATED FROM A REACTANT SUBSYSTEM INTO AN EQUILIBRIUM SUBSYSTEM. THE TOTAL SYSTEM CONSISTS SOLELY OF THE TWO ABOVE SUBSYSTEMS AND REMAINS CLOSED. THERE ARE TWO OPTIONS FOR MODEL=1. IF MTYPE=0 THE REACTION VESSEL IS CONCEPTUALIZED AS CONTAINING ONLY THE EQUILIBRIUM SUBSYSTEM AND ZI IS PROPORTIONAL TO REACTANT/WATER RATIO (REACTED REACTANTS/STARTING AQUEOUS SOLUTION). ALSO, THE THEORETICAL ROCK PRODUCED CONSISTS SOLELY OF PRODUCT MINERALS. THIS OPTION ACTUALLY PRODUCES A SEQUENCE OF EQUILIBRATED CLOSED SYSTEMS OF INCREASING REACTANT/WATER RATIO. IF MTYPE=1 THE REACTION VESSEL INCLUDES ALSO THE REACTANT SUBSYSTEM, AND ANY REACTANTS WHICH SATURATE WITH THE SOLUTION ARE CHANGED IN STATUS TO PRODUCT MINERALS. ANY SUBSEQUENT DISSOLUTION THEREFORE OCCURS REVERSIBLY. THE THEORETICAL ROCK CONSISTS OF PRODUCT MINERALS PLUS UNREACTED SOLID REACTANTS. (MODEL=1, MTYPE=1 WAS WHAT THE CLOSED SYSTEM OF OLD PATHI WAS INTENDED TO MODEL.)

MODEL = 2 THE ABOVE SYSTEM IS MODIFIED SUCH THAT ALL PRECIPITATED SOLID PHASES ARE PERIODICALLY TRANSFERRED INTO A PHYSICALLY REMOVED SUBSYSTEM (P.R.S.). THE TOTAL SYSTEM CONSISTS OF ALL THREE SUBSYSTEMS AND IS CLOSED, BUT THE SUBSYSTEM REACTANTS PLUS AQUEOUS PHASE IS OPEN. (THIS IS THE OPEN SYSTEM OF OLD PATHI). THE CONCEPT IS TO TRANSFER MINERAL MASSES TO THE P.R.S. SO THAT THEY NO LONGER INTERACT WITH THE FLUID. THE SIMULATION IS OF FLUID FLOWING THROUGH A REACTANT MEDIUM, LEAVING PRECIPITATED PHASES BEHIND. IN PRACTICE, SOME FRACTION OF EACH PRECIPITATE IS LEFT IN THE EQUILIBRIUM SUBSYSTEM. ALSO, THE USER MUST BE WILLING TO SACRIFICE SOME SMALL MASS (SPECIFIED BY ZKLOGU)

TO RE-DISSOLUTION. THE P.R.S. TRANSFERS ARE GOVERNED IN SEVERAL WAYS. ONE IS BY THE USER-SPECIFIED ARBITRARY DUMP INTERVAL (DLZIDMP), WHICH MAY BE SET TO A QUASI-INFINITE VALUE. OTHER MECHANISMS SENSE THE ONSET OF RE-DISSOLUTION (THE MAXIMUM CRITERION FOR SOLID PHASE SPECIES). THE MAXIMUM CRITERION IS NECESSARY AND SUFFICIENT WHEN THE PRECIPITATES ARE PURE MINERALS (OF FIXED COMPOSITION). IT IS NECESSARY BUT NOT SUFFICIENT FOR SOLID-SOLUTION END-MEMBER COMPONENTS. IF ATTEMPTING TO RUN AN OPEN SYSTEM MODEL WITH SOLID SOLUTIONS, CHOOSE AN APPROPRIATE VALUE FOR THE USER-SPECIFIED DUMP INTERVAL TO AID IN THE RESOLUTION OF THE MODEL.

THIS PROGRAM EMPLOYS A HIGHLY MODIFIED NEWTON-RAPHSON ROUTINE TO SOLVE FOR THE EQUILIBRIUM STATE OF THE EQUILIBRIUM SUBSYSTEM AT ANY POINT OF REACTION PROGRESS. THIS ROUTINE (SUBPROGRAM NEWTON) IS EQUIPPED TO EFFICIENTLY DETERMINE THE CORRECT PHASE/SPECIES ASSEMBLAGE WHICH SATISFIES THE ELEMENT MASS CONSTRAINTS AT EACH POINT. A SIXTH-ORDER FINITE-DIFFERENCE STEPPING-OUT ROUTINE IS USED TO COMPUTE STARTING ESTIMATES AT SUCCEEDING POINTS AND TO PROVIDE ESTIMATES OF FIRST, SECOND, ETC., DERIVATIVES OF THE PRINCIPAL VARIABLES. THE ACCURACY OF THE STEPPING-OUT ROUTINE IS CONSTRAINED TO THE FIRST ORDER BY THE SETSCREW PARAMETER *SCREW1*. AS SCREW1 IS DECREASED, THE ACCURACY OF THE STEPPING-OUT ROUTINE (OR PREDICTOR) IS INCREASED, BUT THE STEP-SIZE IS DECREASED. THE ACCURACY OF THE FINAL RESULTS AT A PARTICULAR STEP OF REACTION PROGRESS IS DETERMINED BY THE NEWTON-RAPHSON ROUTINE (WHICH ACTS AS A CORRECTOR) AND ITS TOLERANCE PARAMETERS *TOLNR* AND *TOLEB*.

THE EQ6 INPUT DECK IS DIVIDED INTO TWO PARTS, THE TOP HALF-DECK AND THE BOTTOM HALF-DECK. IN THIS REGARD, NOTE THE FOLLOWING. TO INITIALLY MODEL AN AQUEOUS SOLUTION USING VARIOUS INPUT DATA FOR PH, TOTAL CONCENTRATIONS, EQUILIBRIUM CONSTRAINTS, ETC., YOU MUST FIRST USE PROGRAM EQ3, WHICH PRODUCES THE BOTTOM HALF-DECK OF THE FULL EQ6 INPUT DECK. USERS DO NOT PUNCH UP BOTTOM HALF-DECKS (ALTHOUGH THEY MAY OF COURSE MODIFY THEM). BOTTOM HALF-DECKS ARE NORMALLY PUNCHED UP BY MACHINES. INSTRUCTIONS FOR INPUT DECKS ARE DISCUSSED IN SUBROUTINE READZ. A PICK-UP DECK, A FULL DECK TO RE-START A RUN AT SOME VALUE OF REACTION PROGRESS GREATER THAN ZERO, CAN BE WRITTEN BY SUBROUTINE ESCRITZ. SEE THAT ROUTINE FOR AN EXPLANATION OF THE OPTIONS.

***** W A R N I N G *****

IT IS THE USERS RESPONSIBILITY TO DETERMINE WHICH, IF ANY, OF THE ABOVE MODELS ARE APPLICABLE TO HIS PARTICULAR PROBLEM. SEE HELGESON ET AL. (1969) FOR EXAMPLES OF REASONABLE APPLICATIONS. IT IS ALSO THE USERS RESPONSIBILITY TO CHECK THE SUPPORTING DATA FILES TO INSURE THAT CORRECT AND NECESSARY DATA ARE PRESENT. USERS SHOULD NOTE THAT COMPARISON OF THEORETICAL PREDICTIONS WITH REAL DATA (EXPERIMENTAL OR FIELD) MAY PERMIT USERS TO MODIFY THE THEORETICAL RUNS TO BETTER FIT REALITY.

A REACTION PATH IS DESCRIBED IN THIS PROGRAM BY THE FOLLOWING PRINCIPAL VARIABLES OR DESCRIPTORS, WHICH ARE TREATED IN LOGARITHMIC FORM.

THE MASSES OF A BASIS SET OF AQUEOUS SPECIES (MOSS)
THE FUGACITY OF OXYGEN IN THE AQUEOUS PHASE (FO2)
THE EQUIVALENT STOICHIOMETRIC IONIC STRENGTH (XISTEQ)
THE IONIC STRENGTH (XI)
THE MASSES OF ANY PURE MINERALS PRESENT (MOMN)
THE MASSES OF ANY SOLID-SOLUTION END-MEMBERS PRESENT (MOMX)

THE CHIEF REDOX PARAMETER USED IN THE PROGRAM IS THE FUGACITY OF OXYGEN IN THE AQUEOUS PHASE. A FICTIVE AQUEOUS SPECIES, O2 (G,AQ), IS ASSOCIATED WITH THIS VARIABLE, AND IS NOT TO BE CONFUSED WITH O2 (AQ), THE SPECIES DISSOLVED OXYGEN. O2 (G,AQ) IS MASSLESS, ODORLESS, AND TASTELESS.

THE ACTIVITY OF WATER AND SEVERAL BULK SOLUTION PROPERTIES MAY BE COMPUTED AS FUNCTIONS OF THE EQUIVALENT STOICHIOMETRIC IONIC STRENGTH OF A SODIUM CHLORIDE SOLUTION. THIS IS DEFINED AS THE TOTAL DISSOLVED CONCENTRATION OF THE IACTION, WHICH IS EITHER NA+ OR CL-. NOTE THAT THIS TREATMENT IMPLIES THAT THE AQUEOUS PHASE IS EITHER VERY DILUTE OR IS BASICALLY A SODIUM CHLORIDE SOLUTION. THE LOG ACTIVITY OF WATER IS STORED AS THE FIRST ELEMENT IN THE ARRAY GLG, WHICH CONTAINS LOGARITHMS OF THE ACTIVITY COEFFICIENTS OF AQUEOUS SPECIES.

A REACTION PATH IS INITIALIZED BY COMPUTING A MODEL FOR THE EQUILIBRIUM SUBSYSTEM. EITHER OF PROGRAMS EQ3 AND EQ6 IS SUITABLE FOR THE PURPOSE (WHICH ONE DEPENDS ON THE SITUATION). THE INITIAL MODEL IS VERIFIED BY CALLING THE NEWTON-RAPHSON SUBROUTINE, WHICH IS CAPABLE OF REDUCING RESIDUALS, EQUILIBRATING PARTIAL EQUILIBRIUM STARTING SYSTEMS, AND ALTERING TEMPERATURE AND PRESSURE CONDITIONS. THIS STARTING CALL MAY FAIL BECAUSE STARTING ESTIMATES WERE POOR IF THE USER MAKES A LARGE INITIAL JUMP ON ZI OR MAKES A LARGE CHANGE IN TEMPERATURE/PRESSURE. RARELY, THE STARTING CALL MAY FAIL BECAUSE NEWTON WAS UNABLE DETERMINE THE CORRECT PHASE ASSEMBLAGE OR TO SUPPLY GOOD ENOUGH STARTING ESTIMATES UPON ALTERING THE ASSUMED PHASE ASSEMBLAGE. SEE COMMENTS IN SUBROUTINE NEWTON ON POSSIBLE COURSES OF ACTION. IF THE PRINCIPAL DESCRIPTORS (BASIS VARIABLES) ARE HIGHLY SENSITIVE TO THE DEFINITION OF THE IMPOSED MASS CONSTRAINTS WITHIN SOME REGION OF REACTION PROGRESS, THEN NEWTON WILL EXPERIENCE DIFFICULTY IN CONVERGING ON A STARTING CALL WITHIN SUCH A REGION UNLESS THE STARTING ESTIMATES ARE VERY, VERY GOOD. AN EXAMPLE OF SUCH A CRITICAL REGION IS THAT IN WHICH THE OXYGEN FUGACITY DROPS 30 TO OVER 70 ORDERS OF MAGNITUDE IN THE REDUCTION OF OXYGENATED SEA WATER BY REACTION WITH BASALT OR PERIDOTITE.

A REACTION PATH BEGINS AT ZI=0. NO REACTANT MASS IS DESTROYED AT THIS POINT. HOWEVER, THE INITIAL VALUE OF ZI MAY BE GREATER THAN ZERO IF THE RUN IS A PICK-UP RUN OR AN INITIAL JUMP USING THE NEWTON-RAPHSON CAPABILITY IS DESIRED. NOTE THAT ZI IS A STRICTLY INCREASING FUNCTION. IF ONE OR MORE REACTANTS IS A MINERAL THEN UNIT CHANGE IN ZI IS USUALLY EQUATED WITH THE DISSOLUTION OF ONE MOLE OF ONE OF THESE. FOR A SPECIAL REACTANT, IT IS CONVENIENT TO ARBITRARILY CHOOSE 100 G AS ONE MOLE. IF THE TEMPERATURE IS CHANGED WITH REACTION PROGRESS BUT THERE ARE NO REACTANTS, IT IS CONVENIENT TO EQUATE UNIT CHANGE IN ZI WITH UNIT CHANGE IN TEMPERATURE (DEG C). SOME OF THE PROGRAM DEFAULTS ASSUME THESE CONVENTIONS.

A SET OF ZERO OR MORE REACTANTS IS SPECIFIED, ALONG WITH A CORRESPONDING SET OF RELATIVE REACTION RATE COEFFICIENTS WHICH RELATE THE RATES OF INPUT TO THE EQUILIBRIUM SUBSYSTEM TO THE REACTION PROGRESS

VARIABLE, ZI. ALTHOUGH PROVISION IS MADE IN THE PROGRAMMING FOR SECOND AND THIRD ORDER RATE COEFFICIENTS, IT IS RECOMMENDED THAT THEY NOT ORDINARILY BE USED. EACH REACTANT FALLS INTO ONE OF THE FOLLOWING CATEGORIES...

1. SPECIAL REACTANTS
2. AQUEOUS SPECIES
3. STOICHIOMETRIC MINERALS (FIXED COMPOSITIONS)
4. SOLID SOLUTIONS
5. GAS SPECIES

A SPECIAL REACTANT MAY BE ANY SPECIES OR PHASE WHOSE COMPOSITION IS PROVIDED BY THE USER. POSSIBLE EXAMPLES INCLUDE ROCKS OF KNOWN ELEMENTAL COMPOSITION BUT UNCERTAIN MINERALOGY, A GLASS, ANOTHER AQUEOUS PHASE, OR A MINERAL WHICH IS NOT IN THE DATA SET. TO MODEL EVAPORATION, DECLARE WATER TO BE THE REACTANT AND CHOOSE A NEGATIVE RATE CONSTANT. REACTANTS MAY BE EXHAUSTED OR, IF THEY ARE PURE OR SOLID-SOLUTION MINERALS, REACH STATES OF SATURATION WITH THE EQUILIBRIUM SUBSYSTEM. IF THE LATTER, THEY NORMALLY REMAIN FORMALLY IN THE REACTANT SUBSYSTEM AND CONTINUE TO BE TITRATED INTO THE EQUILIBRIUM SUBSYSTEM. HOWEVER, UNDER MODEL=1 AND MTYPE=1 THEY ARE TRANSFERRED TO PRODUCT MINERAL STATUS AND RE-DISSOLVE REVERSIBLY IF AT ALL. (NOTE THAT THEIR DISSOLUTION PSEUDO-KINETICS ARE THEN CONTROLLED BY EQUILIBRIUM AND NOT BY THE USER-SPECIFIED RELATIVE RATE CONSTANTS.)

THE REACTION PATH TERMINATES NORMALLY WHEN ONE OR MORE OF THE FOLLOWING CONDITIONS HAVE BEEN MET...

1. A SPECIFIED LIMIT ON REACTION PROGRESS IS ACHIEVED (ZISTOP)
2. EXECUTION APPROACHES THE COMPUTING LIMIT
   (USE OF THIS FEATURE REQUIRES ADAPTATION TO EACH LOCAL INSTALLATION WHERE THE PROGRAM IS TO BE RUN, A PICK-UP DECK IS THEN WRITTEN AUTOMATICALLY BY SUBROUTINE ESCRITZ.)
3. EACH REACTANT IS EXHAUSTED OR SATURATED

THE ERROR IS MEASURED BY COMPUTING RESIDUAL FUNCTIONS (BETA) ON THE CONSTRAINTS AND DEFINITIONS WHICH APPLY TO THE SYSTEM DESCRIPTORS. SEVERAL SPECIAL RESIDUAL FUNCTIONS ARE EMPLOYED.....

BETARMS = ROOT MEAN SQUARE RESIDUAL
BETAMAX = GREATEST ABSOLUTE VALUE OF ANY RESIDUAL
ALPHA = ARRAY OF ABSOLUTE MASS BALANCE RESIDUALS
(CORRESPONDING BETA VALUES ARE RELATIVE)
ALPHMAX = MAGNITUDE OF GREATEST ABSOLUTE MASS IMBALANCE
BETAMAC = MAGNITUDE OF GREATEST MASS ACTION RESIDUAL
BETACHB = CHARGE IMBALANCE PER KG H2O
BETA(KSB) = ABSOLUTE CHARGE IMBALANCE

THE LAST NEWTON-RAPHSON CORRECTION TERMS (DEL) BOUND THE FIRST-ORDER ERROR IN THE BASIS VARIABLES THEMSELVES. DELMAX IS THE LARGEST MAGNITUDE OF ANY ELEMENT OF DEL. BOTH BETAMAX AND DELMAX ARE USED IN DETERMINING CONVERGENCE IN SUBROUTINE NEWTON.

OTHER BOOKKEEPING IS HANDLED THROUGH THE FOLLOWING.....

KCT = NO. OF ELEMENTS IN THE SYSTEM
KSB = KCT+1, KCOL INDEX OF THE CHARGE BALANCE RELATION
KXISTEQ = KCT+2, KCOL INDEX OF THE EQUIVALENT STOICHIOMETRIC

IONIC STRENGTH RELATION
KXI = KCT+3, KCOL INDEX OF THE IONIC STRENGTH RELATION
KM1 = KXI+1, KCOL INDEX OF THE FIRST PURE MINERAL IN THE SYSTEM
KMT = KCOL INDEX OF THE LAST PURE MINERAL PRESENT IN THE SYSTEM, = KXI IF NONE ARE PRESENT
KX1 = KMT+1, KCOL INDEX OF THE FIRST SOLID-SOLUTION END-MEMBER PRESENT IN THE SYSTEM
KXT = KCOL INDEX OF THE LAST SOLID-SOLUTION COMPONENT PRESENT PRESENT IN THE SYSTEM, = KMT IF NONE ARE PRESENT
KDIM = NO. OF DESCRIPTORS USED = DIMENSION OF THE JACOBIAN MATRIX.

INDEX(KCOL) = STORAGE ARRAY WHICH CONTAINS INDICES OF THE PRINCIPAL BASIS VARIABLES USED TO DESCRIBE THE EQUILIBRIUM SUBSYSTEM
JSFLAG(NS) = CONTROL ARRAY WHICH SPECIFIES THE STATUS OF THE AQUEOUS SPECIES
JMFLAG(NM) = CONTROL ARRAY WHICH SPECIFIES THE STATUS OF THE PURE MINERAL PHASES
JKFLAG(IK,NX) = CONTROL ARRAY WHICH SPECIFIES THE STATUS OF SOLID-SOLUTION END-MEMBER COMPONENTS
JXFLAG(NX) = CONTROL ARRAY WHICH SPECIFIES THE STATUS OF THE SOLID-SOLUTION PHASES
JGFLAG(NG) = CONTROL ARRAY WHICH SPECIFIES THE STATUS OF THE GAS SPECIES
JREAC(NRC) = CONTROL ARRAY WHICH SPECIFIES THE STATUS OF THE REACTANTS

ZI(1) = LATEST VALUE OF REACTION PROGRESS
ZI(2) = PREVIOUS POINT OF REACTION PROGRESS
MTE(NC) = MOLES OF ELEMENT PRESENT IN THE EQUILIBRIUM SUBSYSTEM
MTEAQ(NC) = MOLES OF ELEMENT DISSOLVED IN THE AQUEOUS PHASE
LOSS(NS) = LOG OF MASS (IN MOLES) OF AQUEOUS SPECIES
LOMN(NM) = LOG OF MASS (IN MOLES) OF STOICHIOMETRIC MINERAL
LOTX(NX) = LOG OF MASS (IN MOLES) OF SOLID SOLUTION
LOMX(IK,NX) = LOG OF MASS (IN MOLES) OF SOLID-SOLUTION END-MEMBER
XI = TRUE IONIC STRENGTH
XISTEQ = EQUIVALENT STOICHIOMETRIC IONIC STRENGTH OF A SODIUM CHLORIDE SOLUTION
MOSS(NS) = MOLES OF AN AQUEOUS SPECIES
MOMN(NM) = MOLES OF A STOICHIOMETRIC MINERAL
MOTX(NX) = MOLES OF A SOLID SOLUTION
MOMX(IK,NX) = MOLES OF A SOLID-SOLUTION END-MEMBER
MPRMN(NM) = MOLES OF A STOICHIOMETRIC MINERAL TRANSFERRED TO THE PHYSICALLY REMOVED SUBSYSTEM
MPRMX(IK,NX) = MOLES OF A SOLID-SOLUTION END-MEMBER TRANSFERRED TO THE PHYSICALLY REMOVED SUBSYSTEM
XLKS(NRS) = LOG K FOR AN AQUEOUS REACTION
XLKM(NM) = LOG K FOR A MINERAL DISSOLUTION REACTION
XLKG(NG) = LOG K FOR A GAS SPECIES DESTRUCTION REACTION
GLG(NS) = LOG ACTIVITY COEFFICIENT FOR AN AQUEOUS SPECIES
LAMLG(IK,NX) = LOG ACTIVITY COEFFICIENT FOR A SOLID-SOLUTION END-MEMBER
XBAR(IK,NX) = MOLE FRACTION OF A SOLID-SOLUTION END-MEMBER
XBARLG(IK,NX) = LOG OF ABOVE

AFF(NM) = AFFINITY OF A MINERAL TO PRECIPITATE
AFFLCX(NX) = AFFINITY OF A SOLID-SOLUTION TO PRECIPITATE
FUGLG(NG) = FUGACITY OF A GAS

AA = THE JACOBIAN MATRIX (IDENTICAL TO PATH GRAND MATRIX)
GG = COPY OF THE JACOBIAN MATRIX
ZLG1(KCOL,1) = LOGARITHMIC BASIS VARIABLE AT THE LATEST SOLVED POINT
ZLG2(KCOL,2) = SAME AT THE PREVIOUSLY SOLVED POINT
F1(KCOL,J) = FINITE DIFFERENCES FOR THE J-TH ORDER AT THE LATEST SOLVED POINT
F2(KCOL,J) = SAME AT THE PREVIOUSLY SOLVED POINT
DXLG(KCOL,J) = FINITE-DIFFERENCE ESTIMATES OF THE J-TH ORDER DERIVATIVES AT THE LATEST SOLVED POINT

THE USER MAY INPUT UP TO SIX ACTUAL ROCK COMPOSITIONS (IN TERMS OF OXIDE PERCENTAGES OF MAJOR ELEMENTS) WHICH ARE TO BE COMPARED IN THE LEAST-SQUARES SENSE TO THE THEORETICAL ROCK AT EACH PRINT POINT. IOPT7 IS THE NUMBER OF SUCH ROCK COMPOSITIONS TO BE ENTERED.

ALL SOLID SOLUTIONS CURRENTLY IN THIS PROGRAM ARE *CONVENTIONAL* SOLID SOLUTIONS. IDEAL SOLUTIONS ARE INCLUDED IN THIS CATEGORY. THESE SOLID SOLUTIONS HAVE EXCESS FREE ENERGY AND ACTIVITY COEFFICENT FUNCTIONS WHICH ARE (MULTIVARIABLE) POLYNOMIALS OR POWER SERIES IN THE MOLE FRACTIONS OF THE END-MEMBERS. IMPORTANT THEOREM.....SUCH A SOLID SOLUTION IS PRESENT (HAS A POSITIVE MASS) IF AND ONLY IF ALL ELIGIBLE END-MEMBERS ARE PRESENT. ALL END-MEMBERS ARE ELIGIBLE EXCEPT THOSE THAT ARE SUPPRESSED OR REQUIRE AN ELEMENT WHICH IS NOT PRESENT. IF A SOLID-SOLUTION EXHIBITS A MISCIBILITY GAP (E.G., NA-K FELDSPAR), THEN EACH SIDE OF THE GAP MUST BE TREATED AS A SEPARATE SOLID-SOLUTION (E.G., POTASSIC ALBITE AND SODIC K-FELDSPAR). THESE ARE DISTINGUISHED BY SEPARATE INDICES AND DIFFERENT UPPER LIMITS (XBARLIM) ON THE MOLE FRACTIONS OF THE END-MEMBERS. *SITE-MIXING* MODELS (E.G., OATES, 1969) HAVE NOT YET BEEN INCORPORATED INTO THIS PROGRAM.

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T.J. WOLERY

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----- PROGRAM STATUS AS OF 12 OCTOBER 1978 -----

A SEPARATE WRITE-UP ON THE COMPUTATIONAL METHODS OF THIS PROGRAM IS GIVEN IN PART II OF THE AUTHOR≠S PH.D. THESIS (WOLERY, 1978). THIS INCLUDES THE NECESSARY MATHEMATICAL DERIVATIONS AND A DISCUSSION OF PROGRAM PHILOSOPHY. THIS INFORMATION WILL ALSO SOON BE AVAILABLE IN A UCRL DOCUMENT.

MOST OF THE BASIC FEATURES OF THE PROGRAM HAVE NOW BEEN DOCUMENTED. HOWEVER, NO GUARANTEES CAN BE MADE THAT USERS WILL NOT EXPERIENCE TROUBLES. FIRST, THIS PROGRAM CONTAINS MANY OPTIONS, AND IT IS EASY TO TRY TO RUN A COMBINATION WHICH IS SELF-INCONSISTENT OR UNREALISTIC. SECONDLY, THE SUCCESSFUL OPERATION OF THE PROGRAM DEPENDS TO SOME EXTENT ON THE VALUES OF CONTROL PARAMETERS (TOLERANCES, ETC.) WHICH ARE ADOPTED. CHOOSING VALUES OTHER THAN THE DEFAULTS MAY BE RISKY.

THE AUTHOR WOULD APPRECIATE COMMENTS CONCERNING THIS PROGRAM, ESPECIALLY ANY ERRORS THAT USERS MAY UNCOVER. SOME KNOWN PROBLEMS TO WHICH THE CURRENT VERSION MAY BE SUSCEPTIBLE ARE...

1. THERE IS PRESENTLY ALMOST NO USEFUL DATA ON SOLID SOLUTIONS TO USE WITH THIS PROGRAM. SITE-MIXING MODELS HAVE NOT YET BEEN INCORPORATED INTO THIS CODE. IT IS PRESENTLY RECOMMENDED THAT THE USER INPUT IOPT4=0 TO IGNORE SOLID SOLUTIONS. MUCH OF THE CODE FOR TREATING NON-IDEAL PHASES HAS NOT BEEN SUFFICIENTLY TESTED. DIFFICULTIES WITH SUCH HIGHLY NON-IDEAL SOLID SOLUTIONS WHICH EXHIBIT MISCIBILITY GAPS HAVE YET TO BE SATISFACORILY RESOLVED. USE SOLID SOLUTION AT YOUR PERIL.

2. THERE IS CURRENTLY NO PROVISION FOR A GAS PHASE, ALTHOUGH THE STRUCTURE OF THE PROGRAM WAS DEVELOPED WITH THE IDEA OF ADDING SUCH A PROVISION LATER. FUGACITIES RELATIVE TO THE AQUEOUS PHASE ARE NOW CALCULATED, HOWEVER.

3. EQ3 AND EQ6 CURRENTLY USE OLD STYLE ACTIVITY COEFFICIENT FUNCTIONS (HELGESON, 1969) WHICH ARE NOT SUITABLE FOR HIGH IONIC STRENGTH (I .GT. ABOUT 1) BRINES. IT IS ANTICIPATED THAT THESE WILL BE REPLACED SOMETIME IN THE FUTURE.

4. A PROBLEM MAY OCCUR IN SOME RUNS IN WHICH THE OXYGEN

FUGACITY MAKES A BIG JUMP IN THAT THE RESIDUAL FUNCTIONS MAY DECAY TO A LEVEL CONSISTENT WITH ROUND-OFF/TRUNCATION ERROR WHILE THE UNKNOWNS IN THE BASIS SET BECOME RANDOMLY INACCURATE. THIS PROBLEM HAS BEEN NOTICED IN AT LEAST ONE RUN ON A CDC MACHINE AND WOULD BE MORE OF A PROBLEM ON AN IBM. THE ONLY RECOMMENDED SOLUTIONS ARE TO GO TO DOUBLE-PRECISION OR TO SKIP OVER THE REGION OF REACTION PROGRESS IN WHICH THE JUMP OCCURS.

5. THE PROGRAM MAY HAVE TROUBLE CONVERGING IF THE MASS OF ONE OF THE AQUEOUS BASIS SPECIES IS VERY SMALL RELATIVE TO THAT OF A COMPLEX OR A SIMPLE SPECIES IN AN ALTERNATE OXIDATION STATE. THE CURRENT CHOICE OF BASIS ELEMENTS IS FIXED IN THE STRUCTURE OF THE DATA BASE. CODING TO PERMIT BASIS SWITCHING IS PLANNED FOR THE FUTURE. PROBLEMS OF THIS SORT ARE MOST LIKELY TO BE ENCOUNTERED WHEN MODELLING THE BEHAVIOR OF TRACE METALS WHICH COMPLEX EXTREMELY STRONGLY OR OCCUR IN DIFFERENT OXIDATION STATES OF WIDELY DIFFERING POTENTIAL.

THE FOLLOWING CHANGES HAVE BEEN MADE SINCE THE LAST WIDELY-CIRCULATED VERSION (EQ6.1240)...

1. THE INPUT FORMAT HAS BEEN CHANGED. SEE THE INSTRUCTIONAL COMMENTS IN SUBROUTINE READZ.

2. COMMON BLOCKS HAVE BEEN CLEANED UP AND REORGANIZED SINCE THE LAST VERSION. VARIABLES BEGINNING WITH L OR M ARE NOW IMPLICITLY REAL IN NEARLY ALL SUBPROGRAMS. A NUMBER OF FLAG ARRAYS THAT FORMERLY BEGAN WITH L OR M NOW BEGIN WITH J.

3. NEWTON#S PHASE SELECTION ALGORITHMS HAVE BEEN IMPROVED.

4. THE OPEN SYSTEM NOW APPEARS TO WORK REASONABLY WELL, BUT LOOK OVER THE OUTPUT CAREFULLY IF YOU SELECT THIS OPTION.

5. PHASE BOUNDARIES ARE NOW ACCURATELY LOCATED IF YOU SELECT IOPT13=2 (AUTOMATICALLY SELECTED IF MODEL=2). IF YOU SELECT IOPT13=1, THEN PRINTED ADVISORIES OF PHASE BOUNDARY LOCATIONS ARE GIVEN, BUT COMPUTATIONS OF THE STATE OF THE SYSTEM AT SUCH POINTS ARE NOT PERFORMED' I.E., THE BOUNDARIES ARE SKIPPED OVER, AS WITH IOPT13=0.

6. THE NAMES OF MOST OF THE FLAG ARRAYS WERE CHANGED TO BEGIN WITH J' E.G., MFLAG IS NOW JMFLAG.

7. VARIABLES BEGINNING WITH >Q> ARE IMPLICITLY OF TYPE LOGICAL' THOSE BEGINNING WITH >L> OR >M> ARE IMPLICITLY REAL.

8. THE PROPOSED BASIS SWITCHING FEATURE TO PERMIT USER OR PROGRAM SELECTION OF THE SET OF AQUEOUS SPECIES WHICH SERVE AS BASIS ELEMENTS HAS NOT BEEN IMPLEMENTED ON THIS VERSION OF EQ6. THIS VERSION WILL HOWEVER READ EQ3 INPUT FOR SWITCHING INFORMATION AND TERMINATE WITH A WARNING MESSAGE IF SWITCHING IS INDICATED.

;;;;; NOTES TO NEW USERS ;;;;;

THIS PROGRAM HAS MANY OPTIONS AND IS NOT NECESSARILY EASY TO OPERATE. READ THE MANUAL OR BE PREPARED TO SUFFER THE CONSEQUENCES. READ IT SEVERAL TIMES BEFORE YOU TRY TO RUN THIS PROGRAM. THE RIGHT STRATEGY USING THE MANY OPTIONS THIS PROGRAM OFFERS MAY MAKE THE DIFFERENCE IN SOLVING YOUR PROBLEM.

THIS PROGRAM WAS WRITTEN BY THOMAS J. WOLERY, FORMERLY OF THE DEPARTMENT OF GEOLOGICAL SCIENCES, NORTHWESTERN UNIVERSITY, EVANSTON, ILL. 60201, NOW AT L-224, LAWRENCE LIVERMORE LABORATORY, P.O. BOX 808, LIVERMORE, CALIFORNIA 94550.

THIS PROGRAM WAS WRITTEN FOR THE CDC FTN4.6 COMPILER AND CDC 6400, 6600, AND 7600 COMPUTERS. CONVERSION OF THIS PROGRAM TO RUN ON A MACHINE WITH A SMALL WORD LENGTH (I.E., IBM) MAY BE VERY DIFFICULT. IF YOU ELECT TO GO AHEAD AND DO THIS, I RECOMMEND BUYING A LARGE SUPPLY OF CANDLES (BOTH FOR WORKING LATE INTO THE NIGHT AND ALSO FOR THEOLOGICAL GUIDANCE). NEARLY EVERY FLOATING POINT VARIABLE WILL HAVE TO BE MADE DOUBLE PRECISION. SOME DOUBLE PRECISION IS ALREADY USED IN SUBROUTINE SHIFT AND IN THE IMSL (INTERNATIONAL MATHEMATICAL AND STATISTICAL LIBRARY) ROUTINES WHICH THIS PROGRAM EMPLOYS.

```
APPROXIMATE FIELD LENGTH TO COMPILE(OPT=2).....
     MOST SUBPROGRAMS      60000B
     NEWTON               150000B

APPROXIMATE FIELD LENGTH REQUIRED TO RUN.....
     SCM      145000B
     LCM        3000B
```

NOTE THAT THIS ROUTINE DOES NOT CONTAIN AN INITIALIZING DISTRIBUTION-OF-SPECIES ROUTINE. YOU MUST FIRST USE THE COMPANION PROGRAM EQ3 TO DO THIS. EQ3 WRITES INTERFACING OUTPUT ON A FILE CALLED PICAT, WHICH IS USUALLY PUNCHED, AND THE USER THEN ADDS THIS TO THE EQ6 INPUT DECK. HOWEVER, IT MAY BE LEFT ON DISK AND READ BY EQ6 DIRECTLY.

DISK FILES USED BY EQ6.....

TAPE6 (DATA1) AND TAPE7 (DATA2) CONTAIN SELECTED FILES FROM A SUPPORTING DATA LIBRARY AND ARE USED TO INPUT COMPOSITIONAL AND THERMODYNAMIC DATA (CF. SUBROUTINE INDATZ). FOR PROGRAM EQ6...

```
DATA1 = DEQCE + DEQCDS (MERGE TWO FILES)
DATA2 = DEQSSCS (STEAM SATURATION CURVE), OR
      = DEQ500S (500 BARS)
```

TAPE8 (PICAT) IS AN OPTIONAL FILE WHICH MAY SUPPLEMENT INPUT (TAPE60) (CF. SUBROUTINE READZ) AND/OR OUTPUT (CF. SUBROUTINE ESCRITZ). THIS FILE IS USED TO INTERFACE EQ- SERIES PROGRAMS. THIS FILE IS REWOUND BEFORE READING AND SOMETIMES BEFORE WRITING.

OTHER UNITS MAY BE USED FOR SUPPLEMENTAL I/O, PLOTTING,

ETC. CHECK THE PROGRAM CARD.

THIS PROGRAM PRODUCES ITS OWN INTERFACING I/O FOR PICK-UP RUNS AND OTHER PURPOSES. THE USER SHOULD ACQUAINT HIMSELF WITH THIS FACILITY BY EXAMINING SUBPROGRAMS READZ AND ESCRITZ.

THIS VERSION USES SUBROUTINES FROM THE IMSL PROPRIETARY LIBRARY TO SOLVE LINEAR SYSTEMS IN THE MAIN PROGRAM AND ALSO IN SUBROUTINES HYPSATZ, NEWTON, SHIFT, AND RESCALE. SUBROUTINE LUDATF CREATES THE L-U DECOMPOSITION OF THE GIVEN MATRIX AND SETS THE FLAG VARIABLE *IER* TO ZERO IF THE COMPUTATION IS SUCCESSFUL. SUBROUTINE LUELMF SOLVES FOR A GIVEN RIGHT-HAND-SIDE VECTOR USING THE L-U DECOMPOSITION FROM LUDATF. SUBROUTINE LJREFF ITERATIVELY IMPROVES AN APPROXIMATE SOLUTION TO MACHINE ACCURACY GIVEN THE MATRIX, AN APPROXIMATE L-U DECOMPOSITION, AND THE RIGHT-HAND-SIDE VECTOR, AND RETURNS THE FLAG VARIABLE *IER* AS ZERO IF SUCCESSFUL. IF YOU CAN NOT FIND THESE ROUTINES IN YOUR INSTALLATIONS IMSL WRITE-UP, LOOK UNDER *LEQT2F*.

LOCAL EXTERNALS MAY BE USED TO EXAMINE THE NUMBER OF COMPUTING UNITS REMAINING. AT NUCC (NORTHWESTERN UNIV.) THE EXTERNAL *SECOND* RETURNS THE NUMBER OF EXHAUSTED COMPUTING UNITS AND MUST BE COMPARED WITH *CPLIM*, THE USER-DEFINED AND USER-INPUT VALUE OF THE COMPUTING LIMIT. AT BKY (LAWRENCE BERKELEY LABORATORY) THE EXTERNAL *STATUS* IS CALLED, AND THE PARAMETER IRAY(3), WHICH CONTAINS THE NUMBER OF REMAINING MILLI-COMPUTING UNITS, IS RETURNED DIRECTLY. THESE ROUTINES ARE EMPLOYED IN SUBPROGRAMS *EQ4* AND *SCRIPZ*. WHEN THE COMPUTING LIMIT IS APPROACHED THE PROGRAM TERMINATES NORMALLY AFTER WRITING INTERFACING I/O FOR A PICK-UP RUN BEGINNING AT THE LAST VALUE OF ZI. THIS FEATURE IS NOT CURRENTLY USED AT LLL (LAWRENCE LIVERMORE LABORATORY).

A WORD OF WARNING. THE EXTERNAL *SECOND* USED AT NUCC IS A STANDARD CDC NOS EXTERNAL WHICH RETURNS THE NUMBER OF CP SECONDS USED. AT NUCC THE JOB COMPUTING LIMIT IS DEFINED IN TERMS OF CP SECONDS. THIS EXTERNAL CAN NOT BE USED EVEN AT ANOTHER CDC INSTALLATION WHICH SUPPORTS IT IF THE JOB COMPUTING LIMIT IS DEFINED IN A DIFFERENT MANNER (E.G., BKY). BE VERY CAREFUL WHEN IMPLEMENTING THIS FEATURE AT NEW INSTALLATIONS.

****

T.J. WOLERY

* *

ADDENDUM

THIS VERSION WAS RECEIVED AT LBL AT THE END OF NOVEMBER 1978, AND MODIFICATIONS TO THE DATA BASE (EQDAT02) FORMAT AND TO THE INPUT FORMAT WERE MADE FOR ENHANCED LEGIBILITY AND EASIER UPDATE. THE MAIN CHANGES WERE TO ROUTINES EQ6, READZ, INDATZ, AND ESCRITZ, ALTHOUGH CHANGES NEEDED TO GENERALIZE REFERENCES TO DATA BASE ELEMENTS BY INDEX OCCUR THROUGHOUT AS DO CHANGES RELATED TO ALLOWING AQUEOUS SPECIES NAMES TO BE TWENTY CHARACTERS LONG, AND THOSE DESIGNATING CERTAIN ARRAYS AS LCM (LEVEL 2). ALSO SOME ARRAY SIZES WERE INCREASED.

PAT IQBAL
LBL, CSAM
JANUARY, 1979

* *

DESCRIPTION OF INPUT VARIABLES FOR EQ6

THE TOP HALF-DECK IS USER-PREPARED OR CREATED BY A PREVIOUS EQ6 RUN AS PART OF A PICK-UP RUN DECK.

```
TITLE = FIVE CARD IMAGES OF VERBAL DESCRIPTION FOR THIS RUN


JTEMP = TEMPERATURE TRACKING CODE
   = 0 POWER SERIES TRACKING
   = 1 FLUID MIXING TRACKING
TEMPC0 = INITIAL TEMPERATURE, DEG C
   (TEMPC AT ZI=0.)
TK1,TK2,TK3 = TEMPERATURE TRACKING COEFFICIENTS
   JTEMP=0  TEMPC=TEMPC0 + TK1*ZI + TK2*ZI**2 + TK3*ZI**3
   JTEMP=1  TEMPC= (TEMPC0*TK1 + ZI*TK2)/(ZI+TK1)
       TK1 = MASS OF FLUID IN MOLES, WHERE 1 MOLE
         HAS THE SAME DEFINITION AS FOR THE REACTANT FLUID
         AND UNIT CHANGE IN ZI MEANS ONE MOLE OF
         REACTANT FLUID HAS BEEN ADDED
         USUALLY THIS IS 1000 G, SO USUALLY TK1 = 1.0
       TK2 = TEMPERATURE OF THE REACTANT FLUID


ZISTART = STARTING VALUE OF REACTION PROGRESS FOR THIS RUN
ZISTOP = UPPER LIMIT FOR ZI FOR THIS RUN
   (TERMINATES THE RUN)
DELZIPR = PRINT INCREMENT IN TERMS OF ZI
DLZIDMP = FIXED P.R.S. TRANSFER INTERVAL FOR THE
   OPEN SYSTEM MODEL (MODEL=2)


TOLERANCE PARAMETERS (DEFAULT VALUES ARE HIGHLY RECOMMENDED)

   TOLX = SEARCH/FIND TOLERANCE = SATURATION TOLERANCE
   TOLNR = NEWTON-RAPHSON CONVERGENCE TOLERANCE
   TOLEB = CONVERGENCE TOLERANCE ON ELECTRICAL BALANCE


SETSCREW PARAMETERS (DEFAULT VALUES ARE HIGHLY RECOMMENDED)

   SCREW1 = MAXIMUM ESTIMATE OF ERROR IN LOGARTHMIC
      VARIABLE UPON STEPPING OUT, BOUNDS THE STEP SIZE
      (FUNCTIONS SIMILARLY TO EPS IN HERRICK PATHI, BUT
      CAN BE GREATER IN MANY CIRCUMSTANCES IF THE ACCURACY
      OF THE STEPPING-OUT NEED NOT BE TIGHT)
   SCREW2 = MAXIMUM MAGNITUDE OF NEWTON-RAPHSON CORRECTION TERM
      PER ITERATION
   SCREW3 = MAXIMUM INITIAL VALUE OF BETAMAX AT WHICH
      NEWTON WILL NOT TRY TO DECREASE THE STEP SIZE
```

SENSITIVITY PARAMETERS FOR LOG MASS OF SOLIDS (DEFAULT VALUES ARE HIGHLY RECOMMENDED)

ZKLOGU = A THRESHHOLD PARAMETER FOR THE LOGARITHMIC MASSES OF SOLID SPECIES. AT OR BELOW THIS LIMIT TAYLOR≠S SERIES ACCURACY IS NOT REQUIRED FOR A SOLID SPECIES LOG MASS, AND UNDER THE OPEN SYSTEM MODEL, THIS MUCH SOLID MASS MAY BE DESTROYED WITHOUT NEWTON CUTTING THE STEP SIZE. RECOMMENDED VALUES LIE IN THE RANGE OF -6.0 TO -10.0.

ZKLOGL = AMOUNT BY WHICH LOGARITHMIC MASS OF A SOLID IS DECREMENTED BY A TRANSFER TO THE P.R.S. UNDER MODEL=2. ZKLOGL=2. MEANS THAT 99< OF THE MASS IS TRANSFERRED, A VALUE OF 3. MEANS THAT 99.9< IS TRANSFERRED. IT IS RECOMMENDED THAT VALUES LIE IN THE RANGE OF 2.0 TO 4.0. ZKLOGU DETERMINES THE ACCURACY OF THE OPEN SYSTEM MODEL, BUT ZKLOGL ONLY AFFECTS THE COMPUTATIONAL BEHAVIOR OF THE RUN.

DLZIMAX(1) = INITIAL STARTING STEP SIZE (NORD=0), THE STARTING STEP SIZE ITSELF MAY BE DECREASED BY THE PROGRAM

DLZILIM = ARBITRARY UPPER LIMIT ON STEP SIZE FOR ORDER GREATER THAN ONE (USUALLY NONE IS NEEDED, SO TAKE THE DEFAULT, WHICH IS QUASI-INFINITE).

IFILE = SUPPLEMENTARY INPUT FILE, 60=INPUT, 8=FICAT

MODEL = MODEL SWITCH (SEE MANUAL SECTION OF EQ6)
- = 0 COMPUTE STARTING SYSTEM ONLY, THEN QUIT
- = 1 COMPUTE A CLOSED SYSTEM MODEL
- = 2 COMPUTE AN OPEN SYSTEM MODEL

MTYPE = REACTION VESSEL DEFINITION FOR CLOSED SYSTEM (SEE MANUAL SECTION OF EQ6)
- = 0 COMPUTE A SEQUENCE OF CLOSED SYSTEMS IN THE FINAL STATE
- = 1 COMPUTE A TRUE SINGLE CLOSED SYSTEM

CPLIM = USER-DEFINED COMPUTING LIMIT (THIS PARAMETER IS INSTALLATION DEPENDENT AND NEED NOT BE USED EVERYWHERE. ITS PURPOSE IS TO PERMIT SENSING THE APPROACH OF THE JOB COMPUTING LIMIT BEFORE ABNORMAL TERMINATION OCCURS. IT IS NEEDED AT NORTHWESTERN UNIVERSITY, BUT NOT AT LAWRENCE BERKELEY LABORATORY.)

OPTION SWITCHES

IOPT2 = PRINT LEVEL
= 0 NORMAL, SHORT (DEFAULT)
= 1 NORMAL, LONG
= 2 EXTENDED, PRINT A COMPLETE LIST OF RESIDUAL FUNCTIONS PLUS VALUES AND DERIVATIVES OF BASIS ELEMENTS AT EACH PRINT POINT
= 3 EXTENDED, DEBUGGING LEVEL

IOPT3 = INTERFACING I/O
= 0 NOTHING WRITTEN
= 1 WRITES BOTTOM HALF-DECK ASSUMING ZI WILL BE REDEFINED
= 2 WRITES FULL DECK FOR PICK-UP RUN
= 3 WRITES A SEQUENCE OF BOTTOM HALF-DECKS FOR ZI VALUES AT WHICH SCRIPZ IS CALLED
IF NOT = 0 A FULL DECK FOR A PICK-UP RUN IS ALWAYS WRITTEN ON STOPPING. IF THE TIME LIMIT IS SENSED, IOPT3 IS RESET INTERNALLY TO 2.

IOPT4 = PERMIT SOLID SOLUTION PRODUCTS IF = 1

IOPT5 = PRINT ALL LOG K VALUES IF = 1

IOPT6 = PRINT ITERATION STEPS IN HYPSATZ IF = 1
(DEBUGGING PURPOSES ONLY)

IOPT7 = NO. OF INPUT OXIDE ROCK COMPOSITIONS FOR COMPARISON WITH THEORETICAL ROCK, = 0-6

IOPT8 = SUPPRESSES ALL SOLIDS IF = 1
(SEE ALSO IOPT12=3)

IOPT9 = MAX. NO. OF POINTS USED IN FIND ROUTINE
= 2-5 (2=SECANT METHOD, 3=DEFAULT)

IOPT10 = CONVERT PICK-UP DECK TO NEW BOTTOM HALF-DECK IF GREATER THAN 1. IF = 2 ALL SOLIDS ARE WIPED FROM THE SYSTEM PRIOR TO WRITING.

IOPT11 = PRINT BASIS VARIABLES AND DERIVATIVES AT EVERY POINT IF = 1 (MODEL=2 ONLY)
(DEBUGGING PURPOSES ONLY)

IOPT12 = TRANSFER MINERAL MASSES TO PHYSICALLY REMOVED SUBSYSTEM AFTER STARTING NEWTON CALL
= 0 DOES NOTHING, STARTING MINERALS ARE RETAINED
= 1 STARTING MINERALS REMAIN IN THE SYSTEM BUT WITH TRIVIAL MASSES (I.E., REMAIN IN THE MATRIX)
= 2 STARTING MINERALS ARE TOTALLY WIPED
= 3 ALL SOLIDS ARE SUPPRESSED AFTER THE STARTING CALL

IOPT13 = PREDICT PHASE BOUNDARIES
= -1 SUPPRESSES THE SEARCH FOR MINERAL MAXIMA WHICH IS NORMALLY ENABLED UNDER MODEL=2
= 0 DOES NOTHING
= 1 THE LOCATION OF PHASE BOUNDARIES IS ESTIMATED FROM

TAYLOR≠S SERIES AND PRINTED, THE STEP-SIZE IS UNCHANGE
= 2 THE STEP SIZE IS CONSTRAINED BY THE LOCATIONS OF THE PREDICTED PHASE BOUNDARIES

IOPT14 = TURN OFF POTENTIALLY UNSAFE OPTIMIZATION OF STARTIN ESTIMATES UPON ADDING A NEW PHASE TO THE MATRIX. IF NEWTON PERSISTS IN TRYING TO ADD A NEW PHASE AND THE ITERATION KEEPS DIVERGING, TRY THIS.
= 0 THE OPTIMIZATION IS PERFORMED
= 1 THE OPTIMIZATION IS SKIPPED

IOPT15, IOPT16 = NOT CURRENTLY USED

NART = NO. OF AQUEOUS SPECIES REACTANTS
NMRT = NO. OF FIXED-COMPOSITION MINERAL REACTANTS
NGRT = NO. OF GAS SPECIES REACTANTS
NXRT = NO. OF SOLID SOLUTION REACTANTS
NSRT = NO. OF SPECIAL REACTANTS

MOOR = STARTING REACTANT MASS IN MOLES
RK = REACTANT TRACKING COEFFICIENTS OR RELATIVE RATE CONSTANTS

RXBAR = MOLE FRACTIONS FOR SOLID SOLUTION REACTANTS
VREAC = MOLAR VOLUME OF THE SPECIAL REACTANT IF A SOLID, OTHERWISE ZERO
NUM = NUMBER OF COMPONENTS IN CESR
CESR = ELEMENTAL COMPOSITION ARRAY OF SPECIAL REACTANT

NROCK = TWO CARD IMAGES OF VERBAL DESCRIPTION OF ACTUAL ROCK COMPOSITIONS (OXIDE S) INPUT FOR COMPARISON WITH THE THEORETICALLY GENERATED ROCK

OXIDE = OXIDE PERCENTAGE FOR ACTUAL ROCK

* *

THE BOTTOM HALF-DECK IS ALWAYS CREATED BY A PREVIOUS RUN OF EQ3 OR EQ6.
--------- USERS DO NOT PUNCH UP BOTTOM HALF-DECKS ----------

EQ6

DATA ENTRY FORMS

Condition	Card	Fields	Format
	TITLE		(8A10)
	TITLE		"
	TITLE		"
	TITLE		"
	TITLE		"
	TEMPS	ITEMP, TEMPCØ, TK1, TK2, TK3	(5X, I15, 4E15.9)
	ZI	ZISTART, ZISTOP, DLZIPR, DLZIDMP	(5X, 4E15.9)
	TOL	TOLX, TOLNR, TOLEB	"
	SCREW	SCREW1, SCREW2, SCREW3	"
	ZKLOG	ZLOGU, ZLOGL	"
	DLZI	DLZIMX(1), DLZILIM	"
	FILE	IFILE, MODEL, MTYPE, CPLIM	(5X, 3I5, E10.3)
	IOPTS	2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16	(5X, 15I5)
	REACS	NART, NMRT, NGRT, NXRT, NSRT	(5X, 5I5)
IF NART>0	REAQ	aq. sp. reactant name, MOOR, RK1, RK2, RK3	(5X, 2A10, 5E10.4, I5)
IF NMRT>0	REMIN	min " ", MOOR, RK1, RK2, RK3	"
IF NGRT>0	REGAS	gas " ", MOOR, RK1, RK2, RK3	"
IF NXRT>0	RESOL	SOLID " ", MOOR, RK1, RK2, RK3	"
		rxbar(1), rxbar(2), (3), (4), (5), (6)	(6E13.6) XX
IF NSRT>0	RESP	SPECIAL REACT ", MOOR, RK1, RK2, RK3, "VREAC, NUM	
	CESR	val el. name, val el. name, val el. name, val name, val name	(5X, 5(F10.5, A5))
		nrock(j) = verbal descrip of rock (8A10)	
		" " "	
IOPT7 of these		oxide (1), (2), (3), (4)	
		(5), (6), (7), (8)	(4E20.13)
		(9), (10), (11), (12)	

RL-2145-1

GENERAL DESCRIPTION OF DATA BASE EQDAT02

DEQREM, REMARKS FILE FOR THE EQDAT02 DATA FILE PACKAGE

DATE OF LAST REVISION = JANUARY, 1979

THIS EQDAT03 PACKAGE CONSISTS OF TEN FILES =10 LOGICAL RECORDS.....

1. DEQCE
   COMPOSITION DATA FOR ELEMENTS, AQUEOUS SPECIES, MINERALS, GASES, AND SOLID SOLUTIONS. ALSO INVARIANT PROPERTIES OF AQUEOUS SPECIES SUCH AS ELECTRICAL CHARGE.

2. DEQCOL
   COEFFICIENTS FOR DESTRUCTION/DISSOLUTION REACTIONS OF AQUEOUS SPECIES, MINERALS, AND GASES, WRITTEN IN TERMS OF AN EXPANDED BASIS SET OF AQUEOUS SPECIES.

3. DEQCOS
   COEFFICIENTS FOR DESTRUCTION/DISSOLUTION REACTIONS OF AQUEOUS SPECIES, MINERALS, AND GASES, WRITTEN IN TERMS OF A STRICT BASIS SET OF AQUEOUS SPECIES.
   (CREATED FROM DEQCOL BY UTILITY PROGRAM EQS)

DATA FOR THE 1 ATM.-STEAM SATURATION CURVE...

4. DEQSSCB
   TEMPERATURE-DEPENDENT DATA, INCLUDING LOG K VALUES FOR THE REACTIONS AS WRITTEN IN THE EXPANDED BASIS FORMAT, AT TEMPERATURES OF 0, 25, 60, 100, 150, 200, 250, AND 300 DEGREES CENTIGRADE. ALSO COEFFICIENTS FOR THE EXCESS GIBBS ENERGY FUNCTIONS OF SOLID SOLUTIONS. THIS FILE IS MEANT TO BE READ ONLY BY THE UTILITY PROGRAM EQF, NEVER BY THE MAIN WORKING PROGRAMS EQ3 OR EQ6.

5. DEQSSCL
   POLYNOMIAL COEFFICIENTS FOR ALL TEMPERATURE-DEPENDENT DATA (INCLUDING LOG K FUNCTIONS FOR REACTIONS WRITTEN IN THE EXPANDED BASIS FORMAT) PLUS COEFFICIENTS FOR THE EXCESS GIBBS ENERGY FUNCTIONS OF SOLID SOLUTIONS.
   (CREATED FROM DEQSSCB BY UTILITY PROGRAM EQF)

6. DEQSSCS
   POLYNOMIAL COEFFICIENTS FOR ALL TEMPERATURE-DEPENDENT DATA (INCLUDING LOG K FUNCTIONS FOR REACTIONS WRITTEN IN THE STRICT BASIS FORMAT) PLUS COEFFICIENTS FOR THE EXCESS GIBBS ENERGY FUNCTIONS OF SOLID SOLUTIONS.
   (CREATED FROM DEQSSCL BY UTILITY PROGRAM EQS)

DATA AT A CONSTANT PRESSURE OF 500 BARS...

7. DEQ500B
   ANALOG OF DEQSSCE

8. DEQ500L
   ANALOG OF DEQSSCL

9. DEQ500S
   ANALOG OF DEQSSCS

SOURCE INFORMATION.....

10. DEQREM
    REMARKS CONCERNING THE STRUCTURE OF THE DATA FILE PACKAGE, ITS APPLICATION, AND THE SOURCE OF THE DATA. (YOU ARE READING IT NOW.)

DATA FILE CONSTRUCTION FOR SUPPORTED PROGRAMS.....
DATA1 AND DATA2 ARE DISK FILES WHICH ARE CREATED AT THE START OF A JOB. THESE ARE READ BY THE INDAT- SUBROUTINES. INCLUDING DEQREM IS OPTIONAL--IF INCLUDED IT WILL BE PRINTED AS PART OF EITHER PROGRAM≠S OUTPUT.

EQ3.....
DATA1 = DEQCE
DATA2 = DEQCDL,DEQSSCL(,DEQREM) FOR SSC PRESSURES
= DEQCDL,DEQ500L(,DEQREM) FOR 500 BARS PRESSURE

EQ6.....
DATA1 = DEQCE AND DEQCDS
DATA2 = DEQSSCS (AND DEQREM) FOR SSC PRESSURES
= DEQ500S (AND DEQREM) FOR 500 BARS PRESSURE

DATA SOURCES

******WARNING******

ALL USERS SHOULD EXAMINE THE DATA FILE PRIOR TO RUNNING THE PROGRAMS TO INSURE THAT ADEQUATE SUPPORTING DATA ARE AVAILABLE. MOST MINERAL DATA ARE TAKEN FROM HELGESON, DELANEY, NESBITT, AND BIRD (1978, AMER. JOUR. SCI., IN PRESS). THE FREE ENERGIES AT 25 DEG C AND 1 ATM OF MINERALS WHICH HAVE A *W* SUFFIXED TO THEIR SOURCE INDICES WERE ESTIMATED BY T.J. WOLERY USING A MODIFIED TARDY- GARRELS METHOD. A *WW* SUFFIX INDICATES THAT T.J. WOLERY ALSO ESTIMATED THE VOLUME AT 25 DEG C AND 1 ATM. USING A MODIFIED TARDY- GARRELS METHOD AND THE REMAINING THERMODYNAMIC FUNCTIONS USING ALGORITHMS DISCUSSED BY HELGESON ET AL.

AQUEOUS SPECIES

6400 OLD PATHI DATA FILES (AS MODIFIED BY C. HERRICK, LASL)
8600 MISCELLANEOUS ADDITIONS AND MODIFICATIONS BY T.J. WOLERY
c0-- ANONYMOUS, PERSONAL COMMUNICATION
16-- SUPCRT DATA BANK (SUPCRT INDEX)

NOTE...NON-SUPCRT DATA FOR AQUEOUS REACTIONS FOR 500 BARS WERE DERIVED FROM STEAM SATURATION PRESSURE DATA USING THE DIELECTRIC CONSTANT APPROXIMATION DESCRIBED BY HELGESON (1969). THIS RESULTS IN ESSENTIALLY NO CORRECTION AT TEMPERATURES LESS THAN 100 DEG C, HENCE NO CORRECTIONS WERE COMPUTED FOR DATA AT 0, 25, AND 60 DEG C.

MINERALS

10--, 11--, 15-- SUPCRT DATA BANK (SUPCRT INDEX), INCLUDING THE SUPPLEMENTARY DATA PROVIDED BY T.J. WOLERY AS NOTED ABOVE
0000 FROM OLD PATHI FILES

GASES
13-- SUPCRT DATA BANK (SUPCRT INDEX)

SOLID SOLUTIONS
0000 NO DATA--IDEAL SOLUTION
9011 H.C. HELGESON (UNIV. OF CALIF., BERKELEY)
9012 R. BEANE (UNIV. OF ARIZONA)

LEAST-SQUARES POLYNOMIAL FITS ARE GENERATED FOR TWO TEMPERATURE RANGES....0-100 AND 100-300 DEG C. THE 100 DEG C DATA POINT, IF ANY, IS WEIGHTED SO AS TO MINIMIZE THE DISCONTINUITY IN THE TWO FITTED LOG K FUNCTIONS AT THE 100 DEG C TEMPERATURE. THE FUNCTIONS WERE SMOOTHED BY TAKING THE ORDER TO BE ONE LESS THAN THE POSSIBLE MAXIMUM IF MORE THAN THREE POINTS WERE AVAILABLE. IT IS POSSIBLE FOR A SPECIES TO BE SUPPRESSED BY LACK OF DATA IN ONE TEMPERATURE RANGE BUT NOT IN THE OTHER, WHICH MAY LEAD TO A TROUBLESOME DISCONTI- NUITY AT 100 DEG C. USERS ARE REMINDED THAT THE BASIC DATA FROM WHICH THE POLYNOMIAL FITS WERE DERIVED COVER ONLY THE TEMPERATURE INTERVAL (AT MOST) FROM 0 TO 300 DEG C. EXTRAPOLATION BEYOND 350 DEG C IS UNWISE.

UPDATING THE DATA BASE

A full description of the structure and contents of EQDAT02 can be found in DEQREM. In brief this structure is -

Record	Filename	Type		
1	DEQCE	Primary		
2	DEQCDL	Primary	-	read by EQSABS to produce DEQCDS
3	DEQCDS	Sec		
4	DEQSSCB	Primary	-	read by EQFABS to produce DEQSSCL
5	DEQSSCL	Sec	-	read by EQSABS to produce DEQSSCS
6	DEQSSCS	Sec		
7	DEQ500B	Primary	-	read by EQFABS tp produce DEQ500L
8	DEQ500L	Sec	-	read by EQSABS to produce DEQ500S
9	DEQ500S	Sec		
10	DEQREM	Primary		

PRIMARY RECORDS = RECORDS CREATED OR CHANGED BY THE USER
SECONDARY RECORDS = RECORDS CREATED BY PROGRAMS EQF OR EQS

IT IS EXPECTED THAT THE USER WILL UPDATE THE PRIMARY RECORDS HIMSELF WHENEVER NEW ELEMENTS MUST BE ADDED TO THE DATA BASE. THEN USE PROGRAMS EQF AND EQS TO PRODUCE NEW CORRESPONDING VERSIONS OF THE SECONDARY RECORDS.

THE RULES FOR ADDING NEW ELEMENTS TO THE DATA BASE ARE--

A. NO OLD ELEMENTS MAY BE MOVED OR DELETED.

B. NEW ELEMENTS ARE TO BE ADDED TO DEQCE AS FOLLOWS-

1. UPDATE THE TOTALS (NUMBERS AT THE TOP OF FILE DEQCE)
   NCT=TOTAL NUMBER OF BASIC ELEMENTS IN THE DATA BASE. MAX IS 30.
   NSC=TOTAL NUMBER OF BASIC SPECIES IN THE DATA BASE. MAX IS 60.
   NST=TOTAL NUMBER OF AQUEOUS SPECIES IN THE DATA BASE. MAX IS 250.
   NMT=TOTAL NUMBER OF MINERALS IN THE DATA BASE. MAX IS 150.
   NGT=TOTAL NUMBER OF GASES IN THE DATA BASE. MAX IS 10.
   NXT=TOTAL NUMBER OF SOLID SOLUTIONS IN THE DATA BASE. MAX IS 20.

2. IF ANY NEW BASIC ELEMENTS ARE TO BE ADDED, ADD AS MANY CARDS AS YOU NEED, WITH 24 NAMES/LINE, EACH A LEFT-JUSTIFIED 3-LETTER NAME FORMAT IS 24(A3). THEN FILL IN THEIR CORRESPONDING ATOMIC WEIGHTS AND ADD NEW CARDS IF NECESSARY, WITH 7 ATOMIC WEIGHTS PER LINE. FORMAT IS 7F10.5. THE MAXIMUM NUMBER OF NEW BASIC ELEMENTS YOU CAN ADD IS 6.

3. FOR EACH BASIC ELEMENT ADDED IN STEP 2, YOU MUST ADD A NEW CORRESPONDING STRICT BASIC SPECIE. THESE MUST BE ADDED IN THE SAME ORDER AS THE NEW BASIC ELEMENTS AND MUST BE ADDED IMMEDIATELY PRECEDING THE SPECIE LABELED NSB WHICH IS O2 (G,AQ).

4. ALL NEW AUXILIARY BASIC SPECIES MUST BE ADDED IMMEDIATELY PRECEDING THE SPECIE LABELED NSQ, WHICH IS OH-. THE MAXIMUM NUMBER OF NEW AUXILIARY BASIC SPECIES YOU CAN ADD IS 14.

5. ADD NEW NON-BASIC SPECIES AT THE END OF THE AQUEOUS SPECIES SECTION. THE MAXIMUM NUMBER OF NON-BASIC SPECIES YOU CAN ADD IS 90.

   ALL OF THE AQUEOUS SPECIES (STEPS 3 THROUGH 5) HAVE THE SAME FORMAT. FOR EACH NEW AQUEOUS SPECIE ADDED, THE FORMAT IS-
   A. LABEL OR INDEX, LEFT-JUSTIFIED SPECIE NAME, NUMBER OF COMPONENTS, MOLECULAR WEIGHT, CHARGE, TITRATION, AND AZERO ON THE FIRST CARD, IN FORMAT (A5,2A10,I5,4F10.5)
   B. COMPOSITION CARDS, EACH CONTAINING UP TO 5 PAIRS OF VALUE-BASIC ELEMENT NAME, IN THE FORMAT (5X,5(F10.0,A5))

6. TO ADD NEW MINERALS TO THE DATA BASE, JUST FILL IN ALL ENTRIES MARKED VACANT. THEN CONTINUE TO ADD AT THE END OF THE MINERAL SECTION. THE MAXIMUM NUMBER OF MINERALS YOU CAN HAVE IS 150. FOR EACH NEW MINERAL, THE FORMAT IS-
   A. LABEL OR INDEX, LEFT-JUSTIFIED MINERAL NAME, NUMBER OF COMPONENTS, MOLECULAR WEIGHT, AND VOLUME ON THE FIRST CARD, WITH THE FORMAT- (A5,2A10,I5,2F10.5)
   B. COMPOSITION CARDS, EACH CONTAINING UP TO 5 PAIRS OF VALUE-BASIC ELEMENT NAME, IN THE FORMAT (5X,5(F10.0,A5))

7. ADD ALL NEW GASES AT THE END OF THE GAS SECTION. THE MAXIMUM NUMBER OF NEW GASES YOU CAN ADD IS 2.
   FOR EACH NEW GAS, THE FORMAT IS-
   A. LABEL OR INDEX, LEFT-JUSTIFIED GAS NAME, NUMBER OF COMPONENTS, AND MOLECULAR WEIGHT ON THE FIRST CARD, IN THE FORMAT (A5,A10,10X,I5,F10.5)
   B. COMPOSITION CARDS, EACH CONTAINING UP TO 5 PAIRS OF VALUE-BASIC ELEMENT NAME, IN THE FORMAT (5X,5(F10.0,A5))

8. ADD ALL NEW SOLID SOLUTIONS AT THE END OF THE SOLID SOLUTION SECTION. THE MAXIMUM NUMBER OF NEW SOLID SOLUTIONS YOU CAN ADD IS 8. THE FORMAT FOR EACH NEW SOLID SOLUTION IS-
   A. LABEL OR INDEX, LEFT-JUSTIFIED SOLID-SOLUTION NAME, NUMBER OF COMPONENTS AND INDEX OF SOLID-SOLUTION LAW ON THE FIRST CARD, IN THE FORMAT (A5,2A10,I5,I5)
   B. COMPOSITION CARDS, EACH CONTAINING UP TO 2 PAIRS OF VALUE-MINERAL NAME, IN THE FORMAT (5X,2(F10.0,2A10))

C. WHENEVER YOU ADD NEW ELEMENTS TO THE COMPOSITION RECORD, DEQCE, (R1) OF THE DATA BASE, AS IN STEPS 1 THROUGH 8 ABOVE, YOU MUST CORRESPONDINGLY UPDATE RECORDS DEQCDL (R2), DEQSSCB (R4), AND DEQ500B (R7). THE STRUCTURE OF THESE IS SIMILAR TO THAT OF DEQCE AND YOU MUST OBSERVE THE SAME RULES OF ORDER (STEPS 4-8) AS FOR DEQCE.

   THE FORMATS FOR DEQSSCB AND DEQ500B HAVE NOT CHANGED.

   ALL THREE SECTIONS OF DEQCDL HAVE THE SAME FORMAT-
   FOR EACH NEW ELEMENT ADDED THE FORMAT IS-
   A. LABEL OR INDEX, LEFT-JUSTIFIED ELEMENT NAME AND NUMBER OF COMPONENTS ON THE FIRST CARD, IN THE FORMAT (A5,2A10,I5)
   B. COEFFICIENT CARDS, EACH CONTAINING UP TO 2 PAIRS OF VALUE-AQUEOUS SPECIE NAME, IN THE FORMAT (5X,2(F10.0,2A10))
   -EXCEPT THAT THE FIRST PAIR NEED NOT CONTAIN AN ELEMENT NAME, AS THE FIRST VALUE MUST BE THAT OF THE COEFFICIENT OF THE

-EQF-

INPUT	OUTPUT
DEQXB=DEQSSCB(R4)	DEQXL =DEQSSCL(R5)
DEQXB=DEQ500B(R7)	DEQXL =DEQ500L(R8)

-EQS-

INPUT	OUTPUT
DATA1=DEQCE(R1) DATA2=DEQCDL(R2)+DEQSSCL(R5)	DEQCDS(R3) DEQXS =DEQSSCS(R6)
DATA1=DEQCE(R1) DATA2=DEQCDL(R2)+DEQ500L(R8)	DEQCDS(R3) DEQXS =DEQ500S(R9)

-EQ3-

INPUT	
DATA1=DEQCE(R1) DATA2=DEQCDL(R2)+DEQSSCL(R5)	FOR SSC PRESSURES
DATA1=DEQCE(R1) DATA2=DEQCDL(R2)+DEQ500L(R8)	FOR 500 BARS PRESSURE

-EQ6-

INPUT	
DATA1=DEQCE(R1)+DEQCDS(R3) DATA2=DEQSSCS(R6)	FOR SSC PRESSURES
DATA1=DEQCE(R1)+DEQCDS(R3) DATA2=DEQ500S(R9)	FOR 500 BARS PRESSURE

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