APPENDIX A

Data Input Guide for HYDROBIOGEOCHEM

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UNITS OF MEASURE: The unit of mass and length used for the data input should be kilogram (kg) and decimeter (dm), respectively. Any units of time may be used as long as the same unit is used consistently throughout all data sets. All total analytical concentrations and all initial conditions should be specified in units of moles of chemical per unit total volume of media (mol/dm^3). All source/sink concentrations should be specified in units of moles of chemical per volume of liquid (mol/dm^3). All boundary condition concentrations should be specified in units of moles of chemical per mass of phase in which the chemical exists (mol/kg).

NOTE: All data sets except for Data Set 1 must be preceded by a data set name.

DATA SET 1: TITLE

Two lines are used per problem

Line 1: FORMAT(I5,7A10)

1. NPROB = Problem number.

2. TITLE = Array for the title of the problem. It may contain up to 70 characters from column 6 to column 75.

Line 2: Free format input contains 5 integers as follows:

1. IITR = Integer indicating if iteration table of convergence information to be printed:
   0 = no.
   1 = transport iteration table be printed.
   2 = both transport and chemical iteration tables printed.

2. INTER = Integer indicating if concentration field is to be printed for each hydrological-chemical interaction:
   1 = yes
   0 = no.

3. ICOND = Integer indicating if the condition number of the Jacobian matrix in biogeochemical computations is to be printed:
   1 = yes.
   0 = no.

4. NHGCI = Integer indicating if biogeochemical information is to be printed:
0 = no.
> 0 = print every NHGCI inter-hydro-geochem iterations.

5. IGEOM = Integer signifying if the geometric data are to be printed:
0 = no.
1 = yes.

DATA SET 2: BASIC INTEGER PARAMETERS

Free format input contains 23 integers as follows:

1. NNP = Number of nodal points.

2. NEL = Number of elements.

3. NMAT = Number of material types.

4. NCM = Number of elements with material property correction.

5. NTI = Number of time steps or time increments.

6. KSS = Steady-state simulation control:
0 = Steady-state solution desired.
± 1 = No steady-state solution desired.

NOTE: The combination of KSS and NTI will determine the type of simulation run:
If KSS = 0 and NTI = 0, a steady state simulation will be performed.
If KSS = 0 and NTI > 0, a transient simulation using the steady state solution as initial conditions will be performed.
If KSS = 1 and NTI > 0, a transient simulation using user supplied initial conditions will be performed. The program will equilibrate the user supplied initial conditions before the transient simulation is run.
If KSS = -1 and NTI > 0, a transient simulation using user supplied initial conditions will be performed. The user supplied initial conditions will **not** be equilibrated. The user is cautioned against using this option.

7. NMPPM = Number of material properties per material: must be 4 in the current program.

8. KVI = Velocity input control:
- 1 = Velocity and moisture content defined by Data Set 16.
1 = Steady-state velocity and moisture content read from Logical Unit 11.
2 = Transient velocity and moisture content read from Logical Unit 11.

9. ILUMP = Mass matrix lumping control:
   0 = No lump.
   1 = Lump.

10. IMID = Mid-difference control:
   0 = No mid-difference.
   1 = Mid-difference, and W in Data Set 3 should be 1.

11. IWET = Weighting function control:
   0 = Galerkin weighting.
   1 = Upstream weighting.

12. IOPTIM = Optimization factor computing indictor:
   1 = Optimization factor is to be computed.
   0 = Optimization factor is set to 1.0, 0.0, or -1.0.

13. NITER = Number of iterations allowed between hydrological-chemical iterations.

14. NDTCHG = Number of times to reset the time-step size to the initial value.

15. NPITER = Number of iterations allowed for solving the linear matrix equation with pointwise iteration.

16. IPNTS = Method to be used to solve the matrix equations:
   0 = standard-banded Gaussian direct elimination procedure.
   1 = pointwise iteration method.
   2 = preconditioned conjugate gradient method, with polynomial as preconditioner.
   3 = preconditioned conjugate gradient method, with incomplete Cholesky decomposition as preconditioner.
   4 = preconditioned conjugate gradient method, with modified incomplete Cholesky decomposition as preconditioner.
   5 = preconditioned conjugate gradient method, with symmetric successive over-relaxation as preconditioner

17. KSTR = Auxiliary storage output control:
   0 = No storage.
   1 = Output stored in Logical Unit 12.

18. NSTR = Number of logical records to be read from Logical Unit 13 for restarting the calculation:
   0 = No restart.

19. LGRN = Is the Lagrangian-Eulerian approach to be used:
1 = Yes.
0 = No.

20. IQUAD = Indicator for quadrature integration:
11 = nodal quadrature for both surface integration and volume integration.
12 = nodal and Gaussian quadrature for surface and volume integration, respectively.
21 = Gaussian and nodal quadrature for surface and volume integration, respectively.
22 = Gaussian quadrature for both surface and volume integration.

21. IDETQ = Option for velocity for the Lagrangian step.
1 = average velocity approach.
2 = single velocity approach.

22. IOPTRS = Option for operator splitting.
0 = do not use operator splitting (use fully implicit scheme).
1 = use operator splitting.

23. IAIEF = Option for adaptive implicit-explicit handling of the reaction term in the transport equations.
0 = no. (reaction term on RHS of transport equation).
1 = yes. (reaction term adaptively adjusted to LHS or RHS depending on sign).

NOTE: NTI can be computed by NTI = I1 + 1 + I2 + 1, where

I1 = Largest integer not exceeding Log(DELMAX/DELT)/LOG(1+CHNG).

I2 = Largest integer not exceeding (RTIME-DELT*((1+CHNG)**(I1+1)-1)/CHNG)/DELMAX.

RTIME = Real simulation time.

(DELMAX, DELT, and CHNG are defined in Data Set 3).

If IPNTS is .GE.2 (i.e. if a preconditioned conjugate gradient method (PCG) is to be used), a second line is needed for the following 4 parameters:

1. IEIGEN = Signal of parameter estimation for GG in the polynomial PCG method:
0 = not requested.
1 = requested.

2. GG = The upper bound on the maximum eigenvalue of the coefficient matrix used in the polynomial PCG method.

3. ALPHA = Weighting factor for computing the diagonal element of the diagonal matrix used in the modified incomplete Cholesky PCG method.

4. OMEGA = Relaxation parameter used in the SSOR PCG method.

DATA SET 3: BASIC REAL PARAMETERS

Free-field format input contains 10 real numbers as follows:

1. DELT = Initial time-step size (T).

2. CHNG = Percent change in the time-step size in each of the subsequent time increments, (dimensionless in decimal fraction).

3. DELMAX = Maximum allowable time-step size (T).

4. TMAX = Maximum simulation time (T).

5. W = Time-derivative weighting factor for all terms except the velocity terms:
   0.5 = Crank-Nicolson central.
   1.0 = Backward difference and mid-difference.

6. WV = Time integration factor for the velocity terms:
   0.0 = Forward difference (explicit).
   0.5 = Central difference.
   1.0 = Backward difference (completely implicit).

7. OME = Relaxation parameter for solving the nonlinear equation:
   0.0 - 1.0 = Under-relaxation.
   1.0 = Exact relaxation.
   1.0 - 2.0 = Over-relaxation.

8. OMI = Relaxation parameter for pointwise solving the matrix equation:
   0.0 - 1.0 = Under-relaxation.
   1.0 = Exact relaxation.
   1.0-2.0 = Over-relaxation.

9. TOLA = Error tolerance for solving the nonlinear equations. Half of its value is used as the tolerance for solving the linearized matrix equation with pointwise iteration.

10. APHAG = Upstream weighting factor if IOPTIM = 0:
Values are between 0.0 and 1.50 when the advection form of the equation is used. If APHAG > 1.34D0, the program will choose appropriate values of weighting factor. When the conservative form of the equations is used or when IOPTIM = 1, this value is not used by the program.

DATA SET 4: PRINTER OUTPUT, DISK STORAGE CONTROL, AND TIMES FOR RESETTING STEP SIZE

The number of lines here depends on the number of time increments, NTI, and the number of times to reset the time step, NDTCHG. The number of lines is [(NTI/80+1)*2] + NLINE: (NTI/80+1) lines for printer output control, (NTI/80+1) lines for storage control, and NLINE lines for time-step-size resetting control, which depends on NDTCHG. NLINE lines are required to enter NDTCHG real numbers with free format.

Line 1 to Line [(NTI/80+1)]: FORMAT(80I1)

KPR0	KPR(1)	KPR(2)	. . .	KPR(NTI)
1	2	3	. . .	80

KPR0 = Printer control for initial and steady state conditions.
KPR(I) = Printer control for the I-th time step:

0 = Print nothing.
1 = Print chemical component data from within biogeochemical subroutine.
2 = Print above plus chemical component species data.
3 = Print above plus product species data.
4 = Print above plus stoichiometric coefficients and reaction data.
5 = Print above plus mass flow rates (FLOW, FRATE, and TFLOW).
6 = Print above plus velocities.

(Note: summary concentration values at each node are printed when a convergent solution is reached for each time step. Options 1 through 4 provide more detailed output on the chemical speciation in the system from within the biogeochemical portion of the program every NHGCI iterations. NHGCI is specified in Data Set 1).

Line [(NTI/80+1)+1] to Line [(NTI/80+1)*2]: FORMAT(80I1)

KDSK0	KDSK(1)	KDSK(2)	. . .	KDSK(NTI)
1	2	3	. . .	80

KDSK0 = Auxiliary storage control for steady-state and initial conditions.
KDSK(I) = Auxiliary storage control for the I-th time-step, the same allowable values as for KDSKO;
0 = No storage.
1 = Store on Logical Unit 12.

Line greater than line (NTI/80+1)*2: Free-field format input contains NDTCHG real numbers:

1. TDTCH(1) = The first time at which the time-step size is reset to its initial value.
2. TDTCH(2) = The second time at which the time-step size is reset to its initial value.
N. TDTCH(N) = The N-th time at which the time-step size is reset to its initial value.

DATA SET 5: PRINTOUT INDICATOR

The number of lines in this data set depends on NCPRT. Normally two lines are sufficient.

Line 1: Free-field format input containing one integer.

1. NCPRT = Number of nodes at which detailed biogeochemical information will be printed.

Line 2: Free-field format input contains NCPRT integers.

1. IWRK(1) = Global node number of the first node where detailed chemical information will be printed.

2. IWRK(2) = Global node number of the second node where detailed chemical information will be printed.

N. IWRK(N) = Global node number of the N-th node where detailed chemical information will be printed.

NOTE: IWRK(I), for $1 \leq I \leq$ NCPRT is used to temporarily store the node numbers where detailed chemical information is to be printed. These node numbers are then used to set NODEP(NP) =1 or 0. When NODEP(NP) = 1, detailed chemical information will be printed for the NP-th node. When NODEP(NP)= 0, detailed chemical information will not be printed for the NP-th node.

DATA SET 6: MATERIAL PROPERTIES

A total of NMAT lines are required for this data set.

Each line is free-field format input containing the following information:

1. PROP(1,I) = Longitudinal dispersivity (L).

2. PROP(2,I) = Lateral dispersivity (L).

3. PROP(3,I) = Effective molecular diffusion coefficient of the I-th medium (L**2/T).

4. PROP(4,I) = Bulk density of medium I (M/L**3).

***** NOTE: Data Sets 7 and 8 are not needed if Logical Unit 11 is used as input (i.e., if KVI > 0 in Data Set 2).**

DATA SET 7: NODAL POINT COORDINATES

Typically, a total of 2*NNP lines are required: NNP lines each for the x- and z-coordinates. However, if a group of nodes appear in regular pattern, automatic generation can be used.

Line 1 to Line NNP: Each line is free-field format input containing:

1. NI = Node number of the first node in the sequence.

2. NSEQ = NSEQ subsequent nodes to be automatically generated.

3. NAD = Increment of the node number for each of the NSEQ subsequent nodes.

4. XNI = x-coordinate of node NI (L).

5. XAD = Increment of the x-coordinate for each of the NSEQ subsequent nodes (L).

6. XRD = Percent increase of the increment over its preceding increment (decimal fraction):
   0 = All increments, XAD's, are the same.
   > 0 = The first increment is XAD*(1+XRD), the second increment is XAD*(1+XRD)**2, the third increment is XAD*(1+XRD)**3, and so on.

NOTE: A line containing six zeros separated by spaces or commas must be used to signal the end of the x-coordinate data.

Line (NNP+1) to Line 2*NNP contain the same information as described above but for the z-coordinate.

NOTE: A line containing six zeros separated by spaces or commas must be used to signal the end of the z-coordinate data.

DATA SET 8: ELEMENT INCIDENCES

Typically, a total of NEL lines are needed, one for each element. However, only one line is needed if a group of elements appears in a regular pattern.

Free-field format input for each line contains the following information:

1. MI = Global element number.

2. IE(MI,1) = Global node number of the first node of element MI.

3. IE(MI,2) = Global node number of the second node of element MI.

4. IE(MI,3) = Global node number of the third node of element MI.

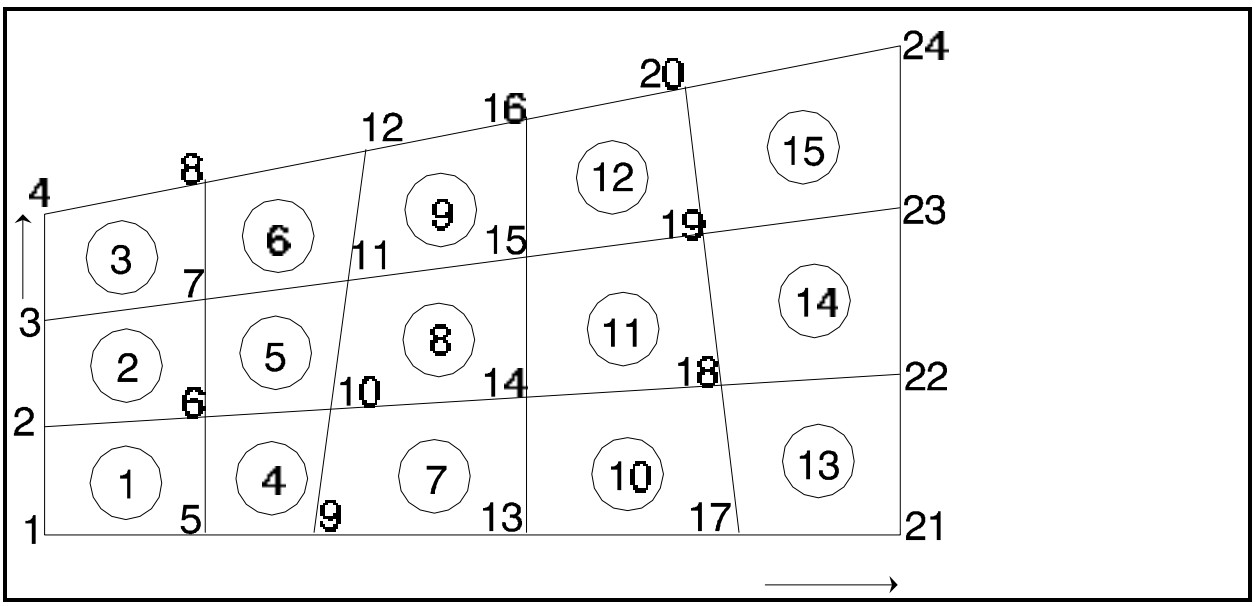
5. IE(MI,4) = Global node number of the fourth node of element MI.

6. IE(MI,5) = Material type to be applied to element MI.

7. MODL = Number of elements in the direction of the most rapid increase in node numbers.

8. NLAY = Number of elements in the direction of the least rapid increase in node numbers.

IE(MI,1) to IE(MI,4) are numbered beginning with the lower left corner and progressing around the element in a counterclockwise direction. For a rectangular block of elements, it is only necessary to specify the first element, the width MODL and the length NLAY, where MODL and NLAY are measured in elements. Element numbering proceeds most rapidly along the MODL dimension and least rapidly along the NLAY dimension. Figure A.1 provides an example. The object is considered to be rectangular because it has width MODL = 3 on two opposite sides and length NLAY = 5 on the other two opposite sides. To generate definitions of elements 2 through 15 automatically, including both the incidence and material type, only one line is necessary. Although all elements of this example will be assumed to contain the same material type, MITYP = 1, this situation can easily be changed by using the material-correction option in Data Set 9.

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-------------------------------------------------------------
   1    1    5    6    2    1    3    5
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Fig. A.1

DATA SET 9: MATERIAL TYPE CORRECTION

This data set is required only if NCM > 0. Normally NCM lines are required, but if the elements with different material properties appear in regular patterns, automatic generation can be used.

Free-field format input for each line contains the following information:

1. MI = Global element number of the first element in the sequence.
2. NSEQ = NSEQ subsequent elements will be generated automatically.
3. MAD = Increment of element number for each of the NSEQ subsequent elements.
4. MITYP = Material type to be applied to element MI.
5. MTYPAD = Increment of the type of material for each of the NSEQ subsequent elements.

NOTE: A line containing five zeros separated by spaces or commas must be used to signal the end of this data set.

DATA SET 10: CHEMICAL COMPONENT INFORMATION

Line 1: Free-field format input contains eight integers.

1. NOHA = Number of mobile components
2. NOHS = Number of immobile components
3. NOKX = Number of kinetic aqueous complexed species
4. NOKY = Number of kinetic adsorbed species
5. NOKZ = Number of kinetic ion-exchanged species
6. NOKP = Number of kinetic precipitated species
7. NOMB = Number of aqueous phase microbial species
8. NOMA = Number of adsorbed phase microbial species

Line 2 and Line 3 are repeated (NOHA + NOHS) times, once for each component in the simulation.

Line 2 FORMAT(A10) contains the following information:

1. CNAM(I) = component name of the I-th component

Line 3 FORMAT(2I5) contains the following information:

1. IDNTC(I,1) = Chemical component number of the I-th transport component

2. INDTC(I,1) = indicator of the I-the transport component,
   0 = conservative component
   1 = nonconservative mobile component
   2 = immobile component
   3 = component whose activity is fixed.

DATA SET 11: INPUT FOR INITIAL OR PRE-INITIAL CONDITIONS

This data set is needed only if NSTR = 0. (NSTR is specified in Data Set 2). When this data set is needed, typically a total of NNP lines is required for each chemical component, one each for each node. However, if the initial or pre-initial conditions appear in a regular pattern, automatic generation may be used. The following set of lines should be repeated for each of the NOHA + NOHS components, the NOKX + NOKY + NOKZ + NOKP kinetic chemical product species, and the NOMB + NOMA microbial species. (NOHA, NOHS, NOKX, NOKY, NOKZ, NOKP, NOMB, NOMA are specified in Data Set 10).

Each line is free-field format input containing the following information:

1. NI = Global node number of the first node in the sequence.

2. NSEQ = NSEQ subsequent nodes will be generated automatically.

3. NAD = Increment of the node number for each of the NSEQ nodes.

4. RNI = Initial or pre-initial total concentration at node NI (moles/total dm^3).

5. RAD = Increment of initial or pre-initial total concentration for each of the NSEQ nodes (moles/total dm^3).

6. RRD = Percent increase of the increment over its preceding increment (decimal fraction):
   0 = All increments, RAD's, are the same.
   > 0 = The first increment is RAD*(1+RRD), the second increment is RAD*(1+RRD)**2, the third increment is RAD*(1+RRD)**3, and so on.

NOTE: A line with six zeros separated by spaces or commas must be used to signal the end of this data set for each species.

NOTE: All initial concentrations are in moles per volume of media (= total volume of the solid and liquid phases).

NOTE: If the INDTC for any chemical component is equal to 3, then the log10 of its activity should be entered for initial or pre-initial values. (INDTC is specified in Data Set 10).

NOTE ON INITIAL CONDITIONS: The initial conditions for a transient calculation may be obtained in three different ways: from batch input, auxiliary storage input, or steady-state calculation using time-invariant boundary conditions. In the latter case, a batch input of the pre-initial conditions is required as the zero-th order iterate of the steady state solution. Auxiliary storage input is necessary whenever the restarting facility is being used. That is, concentration distribution for NSTR different times have been generated and written on disk or magnetic tape. If NSTR > 0, these distributions will be read from Logical Unit 13, and NSTR-th distribution will be used as the initial condition for current calculation. If KSTR > zero, the concentration values will be written on a different device as they are read from Logical Unit 13 so that a complete record of calculations may be kept on one device, Logical Unit 12. If either the first (batch input) or the last (steady-state) option is used, then NSTR = 0. (NSTR is specified in Data Set 2).

NOTE ON AUXILIARY UNITS: Logical Unit 11 is used to input hydrodynamic variables to HYDROGEOCHEM if KVI > 0. Logical Unit 12 is used to store output of HYDROGEOCHEM if KSTR > 0. Logical Unit 13 is used to input initial condition if NSTR > 0. Proper identification

of these three units must be made if either of these options is used. The DSNAME for Logical Unit 13 of the current job should be the same as that for Logical Unit 12 of the previous job.

NOTE ON STEADY-STATE INPUT: A steady-state option may be used to provide either the final state of a system under study or the initial conditions for a transient state calculation. In former case KSS = 0 and NTI = 0, and in the latter case KSS = 0 and NTI > 0. If KSS $\neq$ 0, there will be no steady-state calculation.

DATA SET 12: INTEGER PARAMETERS FOR SOURCES AND BOUNDARY CONDITIONS

Free-field format input contains 13 integers as follows:

1. NSEL = Number of source/sink elements.
2. NSPR = Number of source/sink profiles.
3. NSDP = Number of data points in each source/sink profile.

4. NWNP = Number of well or point source/sink nodes.
5. NWPR = Number of well or point source/sink strength profiles.
6. NWDP = Number of data points in each of the NWPR profiles.

7. NDNP = Number of Dirichlet nodes.
8. NDPR = Number of Dirichlet profiles (should be $\geq$ 1 if NDNP $\geq$ 1).
9. NDDP = Number of data points in each of the NDPR profiles (should be $\geq$ 2).

10. NVNP = Number of variable-boundary nodes.
11. NVES = Number of variable-boundary sides.
12. NVPR = Number of incoming fluid concentration profiles to be applied to variable-boundary element sides.
13. NVDP = Number of data points in each of the NVPR profiles.

DATA SET 13: ELEMENT (DISTRIBUTED) AND WELL (POINT) SOURCE/SINK

(13.1) Element Source/Sink: Subdata sets (13.1a, b, c) are needed if and only if NSEL > 0. When NSEL > 0, subdata sets (b) and (c) should be repeated (NOHA + NOHS + NOKX + NOMB + 2) times. (NSEL is specified in Data Set 12. NOHA, NOHS, NOKX, and NOMB are specified in Data Set 10).

(13.1a) Global element number of compressed source/sink element number: Free-field format input contains the following information:

1. LES(1) = Global element number of the first distributed source/sink element.

2. LES(2) = Global element number of the second distributed source/sink element.

N. LES(N) = Global element number of the N-th distributed source/sink element.

(13.1b) Element source/sink profile: Number of lines depends on NSPR, NSDP, and NON. Each line contains a number of data points = 2*NSDP numerical numbers. Each line is free-field format input.

For K =1, NOHA + NOHS + NOKX + NOMB + 2

For I = 1, NSPR

1. TSOSF(1,I,K) = Time of first data point in I-th profile for K-th component (T).

2. SOSF(1,I,K) = Source/sink value of first data point in I-th profile for K-th component:
= concentration (moles/dm^3 liquid) if K $\leq$ (NOHA+NOHS+NOKX+NOMB),
= flow rate of liquid (L**3/T) if K = (NOHA+NOHS+NOKX+NOMB+1), and
= density of incoming liquid (kg/dm^3) if K = (NOHA+NOHS+NOKX+NOMB+2).

3. TSOSF(2,I,K) = Time of second data point in I-th profile for K-th component (T).

4. SOSF(2,I,K) = Source/sink value of second data point in I-th profile for K-th component:

2N-1. TSOSF(N,I,K) = Time of N-th data point in I-th profile for K-th component (T).

2N. SOSF(N,I,K) = Source/sink value of N-th data point in I-th profile for K-th component:

(13.1c) Source/sink profile type in each source/sink element: Typically, one line per element is needed. However, automatic generation can be used.

Each line is free-field format input containing the following:

1. MI = Compressed source/sink element number of first element in the sequence.

2. NSEQ = NSEQ source/sink elements will have profile type MITYP.

3. MAD = Increment of MI for each of the NSEQ elements.

4. MITYP = Source/sink profile type for element MI.

5. MTYPAD = Increment of source profile type in each of the NSEQ subsequent elements.

NOTE: A line containing five zeros separated by spaces or commas must be used to end this data set.

(13.2) Point source/sink: Subdata sets (13.2a, b, c) are needed if and only if NWNP > 0. When NWNP > 0, subdata sets (b) and (c) should be repeated (NOHA + NOHS + NOKX + NOMB + 2) times. (NWNP is specified in Data Set 12. NOHA, NOHS, NOKX, and NOMB are specified in Data Set 10).

(13.2a) Global node number of compressed point source/sink number: Free-field format input contains the following information:

1. NPW(1) =Global node number of the first source/sink node.

2. NPW(2) =Global node number of the second source/sink node.

N. NPW(N) =Global node number of the N-th source/sink node.

(13.2b) Point source/sink profile: Number of lines depends on NWPR, NWDP, and NOHA + NOHS + NOKX + NOMB. Each line contains a number of data points = 2*NWDP numerical numbers. Each line is free-field format input.

For K =1, NOHA + NOHS + NOKX + NOMB + 2

For I = 1, NWPR

1.TWSSF(1,I,K) = Time of first data point in I-th profile for K-th component (T).

2. WSSF(1,I,K) = Source/sink value of first data point in I-th profile for K-th component:
= concentration (moles/dm^3 liquid) if K ≤ (NOHA+NOHS+NOKX+NOMB),
= flow rate of liquid (L**3/T) if K = (NOHA+NOHS+NOKX+NOMB+1), and
= density of incoming liquid (kg/dm^3) if K = (NOHA+NOHS+NOKX+NOMB+2).

3. TWSSF(2,I,K) = Time of second data point in I-th profile for K-th component (T).

4. WSSF(2,I,K) = Source/sink value of second data point in I-th profile for K-th component.

2N-1.TWSSF(N,I,K) = Time of N-th data point in I-th profile for K-th component (T).

2N. WSSF(N,I,K) = Source/sink value of N-th data point in I-th profile for K-th

component.

(13.2c) Type of point source/sink nodes: Typically, one line per well node is needed. However, automatic generation may be used.

Each line is free-field format input containing the following:

1. NI = Compressed well node number of the first node in a sequence.

2. NSEQ = NSEQ subsequent well nodes will be generated automatically for the source profile type.

3. NIAD = Increment of compressed well node number for each of the NSEQ subsequent nodes.

4. NITYP = Type of well source/sink profile assigned to NI-th well node.

5. NITYPA = Increment of NITYP for each of the NSEQ subsequent nodes.

NOTE: A line containing five zeros separated by spaces or commas must be used to signal the end of this subdata set.

DATA SET 14: VARIABLE BOUNDARY CONDITIONS

This data set is required if and only if NVES > 0. Boundary conditions must be specified for all mobile components (i.e. those with INDTC(I,1) = 0 or 1), for all kinetic aqueous complexed chemical product species, and for all aqueous phase microbial species. (NVES is specified in Data Set 12; INDTC is specified in Data Set 10).

Four groups of lines are required for this data set: The first group is used to specify the incoming concentration profiles, the second group is used to assign the type of incoming concentration profile to each of the NVES boundary sides, the third group is used to read the global nodal number of NVNP in-flowing and out-flowing nodes, and the fourth group is used to specify the information of the NVES element sides. The first group and the second group should be repeated (NOHA + NOKX + NOMB) times, once for each of these species, followed by the third and fourth groups. For example: if there were three chemical components, the order of the groups would be a b a b a b c d, where the first, second, and third a and b would apply to the first, second, and third chemical components, respectively. The program checks INDTC(I,1) for each of the NOH components, and only reads a boundary condition if $\leq$ 1. (i.e. do not specify a boundary condition for fixed concentration or immobile components).

(a) Incoming concentration profiles: This subdata set is read in similarly to that of 13 (b).

For I = 1, NVPR

1.TCVBF(1,I,K) = Time of first data point in I-th incoming concentration versus time profile for K-th component (T).

2. CVBF(1,I,K) = Concentration of first data point in I-th incoming concentration versus time profile for K-th component: (moles/liter).

3. TCVBF(2,I,K) = Time of second data point in I-th incoming concentration versus time profile for K-th component (T).

4. CVBF(2,I,K) = Concentration of second data point in I-th incoming concentration versus time profile for K-th component: (moles/liter).

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2N-1. TCVBF(N,I,K) = Time of the N-th data point in I-th incoming concentration versus time profile for K-th component (T).

2N. CVBF(N,I,K) = Concentration of the N-th data point in I-th incoming concentration versus time profile for K-th component: (moles/liter).

(b) Incoming concentration profile type assigned to variable-boundary sides: This subdata set is read in similarly to that in 13 (c).

1. MI = Compressed variable-boundary side number of the first side in a sequence.
2. NSEQ = NSEQ subsequent sides will be generated automatically.
3. MIAD = Increment of the compressed variable-boundary element side number for each of the NSEQ subsequent sides.
4. MITYP = Type of incoming concentration profile assigned to side MI.
5. MTYPAD = Increment of the type of incoming concentration profile for each of the NSEQ subsequent sides.

NOTE: A line containing five zeros separated by spaces or commas is used to end the input of this subdata set.

(c) Global nodal number of NVNP variable-boundary condition nodes: Typically, NVNP lines are needed. However, automatic generation can be used.

Each line is free-field format input containing the following:

1. NI = Compressed variable-boundary node number of the first node in a sequence.

2. NSEQ = NSEQ subsequent nodes will be generated automatically.

3. NIAD = Increment of the compressed variable-boundary node number for each of the NSEQ subsequent sides.

4. NODE = Global node of the compressed node NI.

5. NODEAD = Increment of NODE for each of the NSEQ subsequent nodes.

NOTE: A line containing five zeros separated by spaces or commas is used to end the input of this subdata set.

(d) Specification of variable-boundary sides: Typically, NVES lines are required, one each for a variable-boundary element side. However, if a group of variable-boundary element sides appears in a regular pattern, automatic generation may be used.

Each line is free-field format input containing the following:

1. MI = Compressed variable boundary element-side number of the first element side in a sequence.

2. NSEQ = NSEQ subsequent variable-boundary element sides will be generated automatically.

3. M = Global element number to which the MI-th element side belongs.

4. IS1 = Compressed variable-boundary nodal number of the first node of element side MI.

5. IS2 = Compressed variable-boundary nodal number of the second node of element side MI.

6. MIAD = Increment of MI for each of the NSEQ subsequent variable-boundary element sides.

7. MAD = Increment of M for each of the NSEQ subsequent variable-boundary element sides.

8. IS1AD = Increment of IS1 for each of the NSEQ subsequent variable-boundary element sides.

9. IS2AD = Increment of IS2 for each of the NSEQ subsequent variable-boundary element sides.

NOTE: A line with nine zeros separated by spaces or commas is used to end the input of this subdata set.

DATA SET 15: DIRICHLET BOUNDARY CONDITIONS

This data set is required if and only if NDNP > 0. Boundary conditions must be specified for all mobile components (i.e. those with INDTC(I,1) = 0 or 1), for all kinetic aqueous complexed product species, and for all aqueous phase microbial species. (NDNP is specified in Data Set 12; INDTC is specified in Data Set 10).

Subdata sets (a) and (b) should be repeated (NOHA + NOKX + NOMB) times, once for each of these species, followed by the third group. For example: if there were three chemical components, the order of the groups would be a b a b a b c, where the first, second and third a and b would apply to the first, second and third chemical components respectively. (The program checks INDTC(I,1) for each of the NOH components, and only reads a boundary condition if $\leq$ 1).

(a) Dirichlet concentration profile: This subdata set is read in similarly to that in 13 (b).

For I = 1, NDPR

1. TCDBF(1,I,K) =Time of first data point in I-th Dirichlet concentration versus time profile for K-th component (T).

2. CDBF(1,I,K) = Concentration of first data point in the I-th Dirichlet concentration versus time profile for K-th component: (moles/kg).

3. TCDBF(2,I,K) =Time of second data point in the I-th Dirichlet concentration versus time profile for K-th component (T).

4. CDBF(2,I,K) = Concentration of second data point in the I-th Dirichlet concentration versus time profile for K-th component: (moles/kg).

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2N-1. TCDBF(N,I,K) =Time of the N-th data point in the I-th Dirichlet concentration versus time profile for K-th component (T).

2N. CDBF(N,I,K) = Concentration of the N-th data point in the I-th Dirichlet concentration versus time profile for K-th component: (moles/kg).

(b) Type of Dirichlet node: This subdata set is read in similarly to that of Data Set 14 (b).

Each line is free field format input containing five intergers:

1. NI = Compressed Dirichlet node number of the first node in the sequence.
2. NSEQ = NSEQ subsequent Dirichlet nodes will be generated automatically.
3. NAD = Increment of compressed Dirichlet node number for each of the NSEQ nodes.
4. NITYP = Type of Dirichlet concentration profile for node NI and the NSEQ subsequent nodes.
5. NTYPAD = Increment of NITYP for each of the NSEQ subsequent nodes.

NOTE: A line with five zeros separated by spaces or commas must be used to signal the end of this subdata set.

(c) Dirichlet nodes: This subdata set is read in similarly to that of Data Set 14 (c).

Each line is free-field format input containing five integers:

1. NI = Compressed Dirichlet boundary node number of the first node in a sequence.
2. NSEQ = NSEQ subsequent nodes will be generated automatically.
3. NIAD = Increment of the compressed Dirichlet boundary node number for each of the NSEQ subsequent sides.
4. NODE = Global node of the compressed node NI.
5. NODEAD= Increment of NODE for each of the NSEQ subsequent nodes.

NOTE: A line containing five zeros separated by spaces or commas is used to end the input of this subdata set.

DATA SET 16: VELOCITY, MOISTURE CONTENT, AND LIQUID DENSITY

If KVI > 0, the velocity and moisture data is not needed because they will be read via Logical Unit 11. (KVI is specified in Data Set 2).

(a) Velocity field: Normally, one line per node is needed. However, automatic generation can be used.

Each line is free-field format input containing seven variables:

1. NI = Node number of the first node in the sequence.
2. NSEQ = NSEQ subsequent nodes will be automatically generated.
3. NAD = Increment of node number in each of the NSEQ subsequent nodes.
4. VXNI = x-velocity component of node NI (L/T).
5. VZNI = z-velocity component of node NI (L/T).
6. VXAD = Increment of x-velocity for each of the NSEQ subsequent nodes (L/T).
7. VZAD = Increment of z-velocity for each of the NSEQ subsequent nodes (L/T).

NOTE: A line with seven zeros separated by spaces or commas signals the end of this subdata set.

(b) Moisture content field: Typically, one line per element is needed. However, automatic generation can be used.

Each line is free-field format input containing five variables:

1. NI = Element number of the first element in the sequence.
2. NSEQ = NSEQ subsequent elements will have the moisture content automatically generated.
3. NAD = Increment of element number for each of the NSEQ subsequent elements.
4. THNI = Moisture content of element NI (decimal point).
5. THNIAD = Increment of moisture content for each of the NSEQ subsequent elements (decimal point).

NOTE: A line with five zeros separated by spaces or commas signals the end of this subdata set.

(c) Liquid density field: Typically, one line per node is needed. However, automatic generation can be used.

Each line is free-field format input containing six variables:

1. NI = Node number of the first node in the sequence.

2. NSEQ = NSEQ subsequent nodes will have liquid density automatically generated.

3. NAD = Increment of the node number for each of the NSEQ subsequent nodes.

4. RHOLNI = Liquid density at node NI (M/L^3).

5. RHOLAD = Incremental increase of the liquid density for each of the NSEQ subsequent nodes (M/L^3).

6. RHOLRD = Percent increase of the increment over its preceding increment (decimal fraction).

NOTE: A line containing six zeros separated by spaces or commas must be used to signal the end of the this subdata set.

DATA SET 17: NUMBER OF COMPONENTS AND PRODUCT SPECIES

One line (FREE FORMAT) contains 6 variables as follows:

1. NONA = Number of aqueous components.
2. NONS = Number of adsorbent components.
3. NOMX = Number of complexed species.
4. NOMY = Number of adsorbed species.
5. NOMZ = Number of ion-exchanged species.
6. NOMP = Number of species subject to precipitation/dissolution.

DATA SET 18: H^+, e^-, AND IONIC STRENGTH CORRECTION INFORMATION

One line (FREE FORMAT) contains the following five variables:

1. SICOR = User's specified ionic strength for computing activity coefficients. (This will be used as a constant ionic strength if the user sets ICOR = 1 below).

2. ICOR = Is Ionic strength used to correct activity coefficient ?
   0 = no,
   1 = constant ionic strength is used (value specified by the user above),
   2 = variable ionic strength is used (as calculated by the program).

3. LNH = Location of the component H^+ among component list (in Data Sets 23 and 24).

4. LNG = Location of the gas component among component list (in Data Sets 23 and 24).

5. LNE = Location of the component e^- among component list (in Data Sets 23 and 24).

DATA SET 19: TEMPERATURE, PRESSURE, AND EXPECTED pe AND pH

Two lines per problem are required.

Line 1 (FREE FORMAT) contains the following information:

1. TEMP = Absolute temperature in Kelvin.
2. PRESU = Pressure in ATM.

Line 2 (FREE FORMAT) contains the following information:

1. PEMN = Expected minimum pe.
2. PEMX = Expected maximum pe.
3. PHMN = Expected minimum pH.
4. PHMX = Expected maximum pH.

DATA SET 20: ADSORPTION INFORMATION

This data set is needed if and only if NONS .GT. 0. (NONS, the number of adsorbent components, is specified in Data Set 17). This set reads information for NSORB adsorbing sites.

Line 1 contains the following two variables:

1. NSORB = Number of adsorbing sites

2. IADS = Adsorption model index:
   0 = simple surface complexation,
   1 = constant capacitance model,
   2 = triple layer model.

Note: If IADS = 0, NONS = 1 x NSORB
If IADS = 1, NONS = 2 x NSORB
If IADS = 2, NONS = 3 x NSORB

Lines 2 to Record NSORB + 1:

Total number of lines in this subset is NSORB. Each record contains the following two variables.

1. LNOA(I) = Location of the exp(-e*psio/kt) component in the component list for the I-th adsorbing site. (Components are listed in Data Sets 23 and 24).

2. LNBA(I) = Location of the exp(-e*psib/kt) component in the component list for the I-th adsorbing site. (Components are listed in Data Sets 23 and 24).

Record NSORB+2 to Record NSORB+1+NMAT:
Total number of records in this subset is NMAT. Each record contains the following variables

1. CAP1M(1,I) = Capacitance between the surface and "o" plane, (Farady/L**2) for the first adsorbing site in material I,

2. CAP2M(1,I) = Capacitance between the "o" plane and "b" plane, (Farady/L**2) for the first adsorbing site in material I,

3. SREAM(1,I) = Surface area of the first adsorbing site in material I, (L**2/M of solid),

4. CAP1M(2,I) = Capacitance between the surface and "o" plane, (Farady/L**2) for the second adsorbing site in material I,

5. CAP2M(2,I) = Capacitance between the "o" plane and "b" plane, (Farady/L**2) for the second adsorbing site in material I,

6. SREAM(2,I) = Surface area of the second adsorbing site in material I, (L**2/M of solid),

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3J-2. CAP1M(J,I) = Capacitance between the surface and "o" plane, (Farady/L**2) for the J-th adsorbing site in material I,

3J-1. CAP2M(J,I) = Capacitance between the "o" plane and "b" plane, (Farady/L**2) for the J-th adsorbing site in material I,

3J. SREAM(J,I) = Surface area of the J-th adsorbing site in material I, (L**2/M of solid),

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3NSORB-2. CAP1M(NSORB,I) = Capacitance between the surface and "o" plane, (Farady/L**2) for the NSORB-th adsorbing site in material I,

3NSORB-1. CAP2M(NSORB,I) = Capacitance between the "o" plane and "b" plane, (Farady/L**2) for the NSORB-th adsorbing site in material I,

3NSROB. SREAM(NSORBI) = Surface area of the NSORB-th adsorbing site in material I, (L**2/M of solid).

DATA SET 21: ION-EXCHANGE INFORMATION

This data set is needed only if NOMZ .GT. 0. (NOMZ, the number of ion-exchanged species, is specified in Data Set 17). This set reads information of ion exchange information for NSITE exchange sites.

Record 1 contains the following variable

1. NSITE = Number of ion-exchange sites

Record 2 to Record NSITE + 1
Total number of records in this subset is NSITE. Each Record contains the following two variables for the I-th site

1. NOMZI(I) = Number of ion-exchanged species participating in reactions at the I-th exchanged site.

2. LNI(I) = Indicator for the "reference" ion-exchange species for the I-th site. It gives the location of this "reference" species on the ion-exchanged species list.

Record NSITE+2 to Record NSITE+1+NMAT
Total number of records in this subset is NMAT. Each record contains the following variables

1. CECM(1,I) = Ion-exchange capacity (equivalents per unit mass of solid) for the first site in material I.

2. CECM(2,I) = Ion-exchange capacity (equivalents per unit mass of solid) for the second site in material I.
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J. CECM(J,I) = Ion-exchange capacity (equivalents per unit mss of solid) for the J-th site in material I,
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NSITE. CECM(NSITE,I) = Ion-exchange capacity (equivalents per unit mass of solid) for the NSITE-th site in material I.

DATA SET 22: BASIC REAL AND INTEGER PARAMETERS

One line of unformatted input contain the following 6 variables.

1. OMEGAC = relaxation parameters for iteration:
   0 ~ 1 = under-relaxation,
   1 = exact relaxation,
   1 ~ 2 = over-relaxation.

2. NPCYL = number of cycles allowed for iterating precipitation-dissolution. (Set NPCYL = 1 if precipitation-dissolution is not in the simulation).

3. NITERC = number of iterations allowed.

4. EPSC = error tolerance for iteration.

5. CNSTRNX = a factor for the constraint on complexed species concentration. No complexed species concentration would yield a total component concentration greater than CNSTRNX times of the input total component concentration.

6. CNSTRNY = a factor for the constraint on adsorbed species concentration. No adsorbed species concentration would yield a total component concentration greater than CNSTRNY times of the input total component concentration.

7. IPIV = option for pivoting for solution of the Newton-Raphson matrix equations.
   1 = full pivoting.
   2 = partial pivoting.

DATA SET 23: NAMES AND TYPES OF CHEMICAL COMPONENT SPECIES

For each component, two lines are needed.

Line 1 - FORMAT(A20,*)

1. CNAM(J,2) = Component name of the J-th component.

Line 2 - free format.

1. INDTC(J,2) = Type of the J-th component species,
   1 = mobile aqueous species, e.g, Ca^{2+},
   2 = immobile adsorbent species, e.g., SOH
   3 = fictitious species, e.g., sigmao or sigmab
   4 = mobile adsorbent species, e.g. colloid component species

2. IFCS = Indicator for free component species:
   0 = free component species subject to transport.
   1 = free component species not subject to transport.

DATA SET 24: COMPONENT SPECIES AND THEIR ION-EXCHANGED SPECIES

For each component species, either two lines or (2 + 3*IONEX) lines are needed, depending on whether the species participates in ion-exchange reactions. If the species does not participate in ion-exchange reaction, two lines are needed for the species. If the species is involved in IONEX sites of ion-exchanged reaction, (2+3*IONEX) lines are needed for the species.

Data for the NONA aqueous components should be listed first, then for the NONS adsorbent components. (NONA and NONS are specified in Data Set 17). All information relating to one component species is input (either 2 or (2+3*IONEX) lines), then the information for the next component species. Components should be described in the same order used in Data Set 23.

Line 1: FORMAT(A20)

1. SPECN(I) = Name of the I-th component species.

Line 2: Free format. This line contains three variables:

1. ISCN(I) = Indicator of the I-th species concentration:
   0 = Species concentration or activity will be computed.
   3 = Species concentration or activity is fixed.

2. VJ(I) = Charge of the I-the component species.

3. IONEX = Integer indicating the number of ion exchange sites to which this component species participates:
0 = This component species does not participate in any ion exchange reaction.
IONEX = This component species participates in IONEX ion exchange reactions.

The following sub-data set is needed for a component specie only if IONEX is not equal to zero. When IONEX is not equal to 0, this subdata set is repeated IONEX times. For each of the IONEX ion exchange sites on which this component specie is involved in ion-exchange reactions, the following three lines are needed.

For k = 1, IONEX

Line 3 - This line contains the following variable

1. J = This species participates in the J-th ion exchange site's reaction.

Line 4 - FORMAT(A20):

1. SPECN(II) = Name of the II-th ion-exchanged species resulted from the I-th component species involving in the J-th ion exchange site reaction.
NOTE: II is internally arranged according to the order of ion exchange site.

Line 5 - Free Format. This line contains the following variables

1. ISCN(II) = Indicator of the II-th ion-exchanged species concentration:
0 = species concentration is be computed,
3 = species concentration is fixed.

2. AXYZP(IPD,1) = Stoichiometric coefficient of the first component in the II-th ion exchange species for use in mass action, where IPD=II-NON.

3. AXYZP(I,2) = Stoichiometric coefficient of the second component in the II-th ion exchange species for use in mass action, where IPD=II-NON.

4. AXYZP(I,3) = Stoichiometric coefficient of the third component in the II-th ion exchange species for use in mass action, where IPD=II-NON.

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NON+1. AXYZP(I,NON) = Stoichiometric coefficient of the NON-th component in the II-th ion exchange species for use in mass action, where IPD=II-NON.

NON+2. BXYZP(IPD,1) = Stoichiometric coefficient of the first component in the II-th ion exchange species for use in mole balance, where IPD=II-NON.

NON+3. BXYZP(I,2) = Stoichiometric coefficient of the second component in the II-th ion exchange species for use in mole balance, where IPD=II-NON.

NON+4. BXYZP(I,3) = Stoichiometric coefficient of the third component in the II-th ion exchange species for use in mole balance, where IPD=II-NON.

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2*NON+1. BXYZP(I,NON) = Stoichiometric coefficient of the NON-th component in the II-th ion exchange species for use in mole balance, where IPD=II-NON.

DATA SET 25: COMPLEXED SPECIES AND THEIR ION-EXCHANGED SPECIES

This data set is needed only if NOMX .GT. 0. If needed, it is read in similar to DATA SET 24. (NOMX, the number of aqueous complexed species, is specified in Data Set 17).

Line 1: FORMAT(A20)

1. SPECN(II) = Name of the II-th species or the I-th complexed species.

Line 2: Free format contains the following variables:

1. ISCN(II) = Indicator of the II-th species concentration:
   0 = Species concentrtion will be computed.
   3 = Species concentration is fixed.

2. AXYZP(I,1) = Stoichiometric coefficient of the first component in the I-th complexed species, for use in mass action equation.

3. AXYZP(I,2) = Stoichiometric coefficient of the second component in the I-th complexed species, for use in mass action equation.

4. AXYZP(I,3) = Stoichiometric coefficient of the third component in the I-th complexed species, for use in mass action equation.

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NON+1. AXYZP(I,NON) = Stoichiometric coefficient of the NON-th component in the I-th complexed species, for use in mass action equation.

NON+2. IONEX = Integer indicating the number of ion exchange sites on which this complexed species participates in ion-exchange reactions:
0 = This complexed species does not participate in any ion exchange reaction.
IONEX = This complexed species participates in IONEX ion exchange reactions.

NON+3. BXYZP(I,1) = Stoichiometric coefficient of the first component in the I-th complexed species, for use in mole balance equation.

NON+4. BXYZP(I,2) = Stoichiometric coefficient of the second component in the I-th complexed species, for use in mole balance equation.

NON+5. BXYZP(I,3) = Stoichiometric coefficient of the third component in the I-th complexed species, for use in mole balance equation.
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2*NON+1. BXYZP(I,NON) = Stoichiometric coefficient of the NON-th component in the I-th complexed species, for use in mole balance equation.

The following sub-data set is needed for this aqueous complexed species only if IONEX is not equal to zero. When IONEX is not equal to 0, this sub-data set is repeated IONEX times. For each of the IONEX ion exchange sites on which this aqueous complexed specie is involved in ion-exchange reactions, the following three lines are needed to read ion exchanged species information.

For k = 1, IONEX

Line 3 - This line contains the following variable

1. J = This complexed species participates in the J-th ion exchange site's reaction.

Line 4 - FORMAT(A20):

1. SPECN(II) = Name of the II-th ion-exchanged species resulted from the I-th complexed species involving in the J-th ion exchange site reaction.
NOTE: II is internally arranged according to the order of ion exchange site.

Line 5 - Free Format. This line contains the following variables

1. ISCN(II) = Indicator of the II-th ion-exchanged species concentration:
0 = species concentration is be computed,
3 = species concentration is fixed.

2. AXYZP(IPD,1) = Stoichiometric coefficient of the first component in the II-th ion exchange

species for use in mass action, where IPD=II-NON.

3. AXYZP(I,2) = Stoichiometric coefficient of the second component in the II-th ion exchange species for use in mass action, where IPD=II-NON.

4. AXYZP(I,3) = Stoichiometric coefficient of the third component in the II-th ion exchange species for use in mass action, where IPD=II-NON.

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NON+1. AXYZP(I,NON) = Stoichiometric coefficient of the NON-th component in the II-th ion exchange species for use in mass action, where IPD=II-NON.

NON+2. BXYZP(IPD,1) = Stoichiometric coefficient of the first component in the II-th ion exchange species for use in mole balance, where IPD=II-NON.

NON+3. BXYZP(I,2) = Stoichiometric coefficient of the second component in the II-th ion exchange species for use in mole balance, where IPD=II-NON.

NON+4. BXYZP(I,3) = Stoichiometric coefficient of the third component in the II-th ion exchange species for use in mole balance, where IPD=II-NON.

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2*NON+1. BXYZP(I,NON) = Stoichiometric coefficient of the NON-th component in the II-th ion exchange species for use in mole balance, where IPD=II-NON.

DATA SET 26: ADSORBED SPECIES

This data set is needed only if NOMY .GT. 0. Two lines per adsorbed species are needed. (NOMY, the number of adsorbed species, is specified in Data Set 17).

Line 1 - FORMAT(A20)

1. SPECN(II) = Name of the II-th species or the I-th adsorbed species.

Line 2 - Unformatted input containing the following variables

1. ISCN(II) = Indicator of the II-th species concentration:
   0 = species concentration is to be computed,
   3 = species concentration is fixed.

2. AXYZP(II,1) = Stoichiometric coefficient of the first component in the II-th product species or in the I-th adsorbed species, for use in mass action equation.

3. AXYZP(II,2) = Stoichiometric coefficient of the second component in the II-th product species or in the I-th adsorbed species, for use in mass action equation.

4. AXYZP(II,3) = Stoichiometric coefficient of the third component in the II-th product species or in the I-th adsorbed species, for use in mass action equation.

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NON+1. AXYZP(II,NON) = Stoichiometric coefficient of the NON-th component in the II-th product species or in the I-th adsorbed species, for use in mass action equation.

NON+2. BXYZP(II,1) = Stoichiometric coefficient of the first component in the II-th product species or in the I-th adsorbed species, for use in mole balance equation.

NON+3. BXYZP(II,2) = Stoichiometric coefficient of the second component in the II-th product species or in the I-th adsorbed species, for use in mole balance equation.

NON+4. BXYZP(II,3) = Stoichiometric coefficient of the third component in the II-th product species or in the I-th adsorbed species, for use in mole balance equation.

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2*NON+1. BXYZP(II,NON) = Stoichiometric coefficient of the NON-th component in the II-th product species or in the I-th adsorbed species, for use in mole balance equation.

DATA SET 27: PRECIPITATED/DISSOLVED SPECIES

This data set is needed only if NOMP .GT. 0. Two lines per precipitated species are needed. (NOMP, the number of precipitated species, is specified in Data Set 17).

Line 1 - FORMAT(A20)

1. SPECN(II) = Name of the II-th product species or the I-th precipipated/dissolved species.

Line 2 - Unformatted input containing the following variables

1. ISCN(II) = Indicator of the II-th species concentration:
0 = species concentration is to be computed,
3 = species concentration is fixed.

2. PKIPD = Log10 of the equilibrium formation constant for the I-th precipitated species.

3. AXYZP(II,1) = Stoichiometric coefficient of the first component in the II-th product species or in the I-th precipitated/dissolved species, for use in mass action equation.

4. AXYZP(II,2) = Stoichiometric coefficient of the second component in the II-th product species or in the I-th precipitated/dissolved species, for use in mass action equation.

5. AXYZP(II,3) = Stoichiometric coefficient of the third component in the II-th product species or in the I-th precipitated/dissolved species, for use in mass action equation.

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NON+2. AXYZP(II,NON) = Stoichiometric coefficient of the NON-th component in the II-th product species or in the I-th precipitated/dissolved species, for use in mass action equation.

NON+3. BXYZP(II,1) = Stoichiometric coefficient of the first component in the II-th product species or in the I-th precipitated/dissolved species, for use in mole balance equation.

NON+4. BXYZP(II,2) = Stoichiometric coefficient of the second component in the II-th product species or in the I-th precipitated/dissolved species, for use in mole balance equation.

NON+5. BXYZP(II,3) = Stoichiometric coefficient of the third component in the II-th product species or in the I-th precipitated/dissolved species, for use in mole balance equation.

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2*NON+2. BXYZP(II,NON) = Stoichiometric coefficient of the NON-th component in the II-th product species or in the I-th precipitated/dissolved species, for use in mole balance equation.

DATA SET 14: MICROBIAL SPECIES

This data set is needed only if NOMB or NOMA .GT. 0. For each species, two lines are needed. The NOMB aqueous microbial species should be listed first, then the NOMA adsorbed microbial components. (NOMB and NOMA are specified in Data Set 10).

Line 1 - FORMAT(A20, I5)

1. SPECN(II) = Name of the II-th species

Line 2 - (FREE FORMAT) contains the following variables

1. ISCN(II) = Indicator of the II-th species concentration
   0 = species concentration is to be computed.
   3 = species concentration is fixed.

2. PKD = Log10 of the death/decay constant of the I-th microbial species.

3. NER = Number of chemical species affected by endogenous respiration of this microbial species.

The following lines are needed only if NER .GT. 0. Two lines are needed for each of the NER species affected by endogenous respiration.

Line 3 - (FREE FORMAT) contains the following variable

1. IGER(II,J) = global species number of the J-th chemical species affected by endogenous respiration of the II-th microbial species.

Line 4 - (FREE FORMAT) contains the following variables

1. ERAIJ = stoichiometric coefficient for use of the J-th chemical species due to maintenance/decay processes of this microbial species.

2. ERKIJ = half saturation constant for the J-th chemical species in the maintenance/decay processes of this microbial species.

DATA SET 29: REACTION DATA

NOTE: Equilibrium chemical reactions involving aqueous complexation, adsorption or precipitation may involve as many reactants as necessary but must be written as the formation of only one equilibrium product species. Each equilibrium product species may participate in only one equilibrium reaction.

Ion exchange reactions, whether equilibrium or kinetic, must have one aqueous species and one ion exchanged species both as reactants and as products. The reactant ion exchanged species must be the reference ion exchange species for the site involved, i.e.:
Aqueous Species + Reference IE Species $\leftrightarrow$ New Aqueous Species + New IE Species

All other kinetic chemical reactions may involve any species as reactants or products.

Microbiological reactions may involve any chemical species as reactants and products. One reactant may be identified as the substrate, one as the electron acceptor, one as the nutrient, and one as the inhibitor for use in the Monod kinetic expressions.

One line is needed specifying the number of mixed kinetic reactions in the simulation.

Line 1 - (FREE FORMAT) contains the following variable:

1. NRXN = The number of kinetic reactions in this simulation

The following subset is needed only if NRXN is greater than zero. For each of the NRXN kinetic reactions four lines are needed.

Line 1 - (FREE FORMAT) contains the following variables:

1. NRTS = The number of reactant species participating in this kinetic reaction.

2. NPDS = The number of product species participating in this kinetic reaction.

3. KRTYP(I) = Kinetic reaction type of the I-th reaction.
   - 0 = Equilibrium reaction.
   - 1 = Kinetic chemical reaction.
   - 2 = Monod kinetic microbial reaction.
   - 3 = Microbial phase transfer reaction.

Line 2 - (FREE FORMAT) contains the following variables:

If KRTYP(I) = 0,
1. PEQK = Log10 of the equilibrium constant for this reaction.

If KRTYP(I) = 1 or 3,

1. PBK = Log10 of the backward rate constant for this kinetic reaction.
2. PFK = Log10 of the forward rate constant for this kinetic reaction.

If KRTYP(I) = 2,

1. GRMAXK = maximum specific growth rate of the i-th reaction, μ_{max}, (1/T).

2. HSCS = half saturation constant for the substrate in the i-th reaction, K_S, , mass/mass of phase (M/M). (If the substrate availability is not to be incorporated in the Monod kinetic expressions for this reaction, set = 0).

3. HSCA = half saturation constant for the electron acceptor in the i-th reaction, K_A, , mass/mass of phase (M/M). (If electron acceptor availability is not to be incorporated in the Monod kinetic expressions for this reaction, set = 0).

4. HSCN = half saturation constant for the nutrient in the i-th reaction, K_N, , mass/mass of phase (M/M). (If nutrient availability is not to be incorporated in the Monod kinetic expressions for this reaction, set = 0).

5. LOCS = reactant which is the substrate in the i-th reaction. (Set = 0 if not used).

6. LOCA = reactant which is the electron acceptor in the i-th reaction. (Set = 0 if not used).

7. LOCN = reactant which is the nutrient in the i-th reaction. (Set = 0 if not used).

8. TAUL = lag time for the i-th reaction.

9. TAUE = time to reach exponential growth for the i-th reaction.

Line 3 - (FREE FORMAT) contains the following variables:

1. CXYZP(I,1) = stoichiometric coefficient of the 1st reactant species in the I-th reaction.

2. CXYZP(I,2) = stoichiometric coefficient of the 2nd reactant species in the I-th reaction.

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NRTS. CXYZP(I,NRTS) = stoichiometric coefficient of the NRTS-th reactant species in the I-th reaction.

NRTS+1. DXYZP(I,1) = stoichiometric coefficient of the 1-st product species in the I-th reaction.

NRTS+2. DXYZP(I,2) = stoichiometric coefficient of the 2nd product species in the I-th reaction.

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NRTS+NPDS. DXYZP(I,NPDS) = stoichiometric coefficient of the NPDS-th product species in the I-th reaction.

Line 4 - (FREE FORMAT) contains the following variables:

1. IGSNRT(I,1) = global species number of the 1-st reactant species in the I-th reaction.

2. IGSNRT(I,2) = global species number of the 2-nd reactant species in the I-th reaction.

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NRTS. IGSNRT(I,NRTS) = global species number of the NRTS-th reactant species in the I-th reaction.

NRTS+1. IGSNPD(I,1) = global species number of the 1-st product species in the I-th reaction.

NRTS+2. IGSNPD(I,2) = global species number of the 2-nd product species in the I-th reaction.

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NRTS+NPDS. IGSNPD(I,NPDS) = global species number of the NPDS-th product species in the I-th reaction.

NOTE: The total, or global, number of species in the simulation is NONA + NONS + NOMX + NOMY + NOMZ. + NOMP + NOMB + NOMA. (All specified in Data Set 17). These species are stored in the following order:

	Global Species Number:
NONA aqueous component species	1 through NONA
NONS adsorbent component species	(NONA+1) through (NONA+NONS)
NOMX aqueous complexed species	(NONA+NONS+1) through (NONA+NONS+NOMX)
NOMY adsorbed species	(NONA+NONS+NOMX+1) through (NONA+NONS+NOMX+NOMY)

NOMZ ion-exchange species	(NONA+NONS+NOMX+NOMY+1) through (NONA+NONS+NOMX+NOMY+NOMZ)
NOMP precipitated species	(NONA+NONS+NOMX+NOMY+NOMZ+1) through (NONA+NONS+NOMX+NOMY+NOMZ+NOMP)
NOMB aqueous phase microbial species	(NONA+NONS+NOMX+NOMY+NOMZ+NOMP) through (NONA+NONS+NOMX+NOMY+NOMZ +NOMP +NOMB)
NOMA adsorbed phase microbial species	(NONA+NONS+NOMX+NOMY+NOMZ+NOMP +NOMB) through (NONA+NONS+NOMX+NOMY+NOMZ+NOMP +NOMB+NOMA)

Within the NONA, NONS, NOMX, NOMY, NOMP, NOMB, and NOMA groups of species, the species are stored in the same order in which they are input. Within the NOMZ group of species, the ion exchanged species are internally rearranged and are stored in order first by ion exchange site and then by the order of the aqueous species corresponding to the ion exchange species at that site.

DATA SET 29: END-OF-JOB CARD LINE

A blank line must be used to signal the end of the job.