

6.0 SAMPLE PROBLEMS

Two example problems are used to demonstrate coupled hydrologic transport and geochemical reactions. Problem No. 1 involves a simple system of calcite precipitation along a one-dimensional transport path. Problem No. 2 deals with an experimental system of EDTA adsorption onto ferrous hydroxide along a one-dimensional space. Each problem includes three cases for reactive transport to demonstrate the ability of the coupled model to deal with both immobile and mobile kinetic species.

The following sections for each example includes a description of the problem, chemical/minerals considered, and thermodynamic data used. The input data for each example is presented in tabular form. The output for each example is contained in the attached floppy disks to allow readers to compare their output from HYDROGEOCHEM to these examples.

For numerical computation, the region of interest for both problems is discretized with 2 square elements of size 0.025 x 0.025 with 6 nodes. A simulation of five time steps with step size of 0.05 is made for all cases. The velocity is 0.0125. The longitudinal dispersivity is assumed to be 0.003. The reaction types for these simulations cases are summarized in Table 6.1.

Table 6.1. Reaction Types for 2 Example Problems Each With 3 Cases
(K_x = kinetically controlled complexed species, K_y = kinetically controlled adsorbed species, K_p = kinetically controlled precipitated species)

Problem	Cases	Reaction Types	Velocity
No. 1	1A	$K_x = 0, K_p = 0$	0.0125
	1B	$K_x = 0, K_p = 1$	
	1C	$K_x = 1, K_p = 1$	
No. 2	2A	$K_x = 0, K_y = 0$	0.0125
	2B	$K_x = 0, K_y = 4$	
	2C	$K_x = 2, K_y = 4$	

6.1 Problem No. 1: A Simple System of Calcite Precipitation

This problem deals with a simple system of calcite precipitation involving three components; calcium, carbonate, and hydrogen. The geochemical problem is defined by three components, six complexed species, and two potentially precipitated species. Thus, a total of 11 species are included: Ca^{2+} , CO_3^{2-} , H^+ , OH^- , $\text{CaCO}_3(\text{aq})$, CaHCO_3^+ , $\text{Ca}(\text{OH})_2$, H_2CO_3 , H_2CO_3^* , HCO_3^- , H_2CO_3 , $\text{Ca}(\text{OH})_2(\text{solid})$, $\text{CaCO}_3(\text{solid})$. Table 6.2 lists the geochemical data.

Three cases are included. Case 1A considers the simplest problem of equilibrium species only. Case 1B deals with the relatively easy problem of including only immobile kinetic species, in which the precipitated species, $\text{CaCO}_3(\text{s})$, will now be forming due to a kinetic reaction, with

logarithm of forward and backward rate constants of 3.30 and -5.00 (Table 6.2) respectively. Case 1C handles the more difficult problem of including both mobile and immobile kinetic species, in which the complexed species, HCO_3^- , will now also be forming due to a kinetic reaction, with logarithm of forward and backward rate constants of 5.0 and -5.2 (Table 6.2) respectively.

Table 6.2. Geochemical Data for Problem No 1.

Species	Ca^{2+}	CO_3^{2-}	H^+	Log(K)	Log (K^b)	Log(K^f)
Ca^{2+}	1	0	0	0.00	-----	-----
O_3^{2-}	0	1	0	0.00	-----	-----
H^+	0	0	1	0.00	-----	-----
OH^-	0	0	-1	-14.00	-----	-----
CaCO_3 (aq)	1	1	0	3.00	-----	-----
CaHCO_3^+	1	1	1	11.60	-----	-----
CaOH^+	1	0	-1	-12.20	-----	-----
HCO_3^-	0	1	1	10.20	-5.2	5.0
H_2CO_3	0	1	2	16.50	-----	-----
$\text{Ca}(\text{OH})_2(\text{s})$	1	0	-2	-21.90	-----	-----
CaCO_3 (s)	1	1	0	8.30	-5.0	3.3

The initial total analytical concentrations of calcium, carbonate, and excessive hydronium are 0.001, 0.001, and 0. M, respectively. The total analytical concentrations of calcium, carbonate, and excessive hydronium at the incoming boundary are also held at 0.001, 0.001, and 0.0 M, respectively. For Case 1B, the initial concentration of the kinetic species calcite is 8.642×10^{-5} M. For Case 1C, the initial concentrations of the kinetic species $\text{CaCO}_3(\text{s})$ and HCO_3^- are 8.642×10^{-5} and 8.404×10^{-6} M, respectively. The concentration of the mobile kinetic species HCO_3^- on the incoming boundary is held at 8.404×10^{-6} .

The input data sets are prepared according to Appendix A and are given in Tables 6.3, 6.4 and 6.5.

Table 6.3. Input Data Set for Problem Number 1, Case A.

```

1 TEST OF HGC2-0: Ca, CO3, and H: Kx=0, ky=0, kz=0, kp=0
0 0 0 0 5
C ***** DATA SET 2: BASIC INTEGER PARAMTERS
6 2 1 0 5 1 4 -1 1 0 1 0 10 1 50 0 0 0 1 12
C ***** DATA SET 3: BASIC REAL PARAMETERS
0.05 0.0D0 1.0 101 1.0D0 1.0D0 1.0D0 1.0D00 1.0D-5 1.0D0 0.0d0 0
C ***** DATA SET 4: PRINT AND AUXILIARY STORGE CONTROL
44444
00000
1.0D38
C ***** DATA SET 5: CHEMICAL OUTPUT AND CHEMICAL PORPerty TYPE INDICATOR
2
1 5 NODEP
C ***** DATA SET 6: MATERIAL PROPERTIES
3.0D-3 0.0D0 0.0D0 1.0D0 AL AT AM RHOB
C ***** DATA SET 7: NODE COORDINATES
1 2 2 0.0 0.0 0.0
2 2 2 0.025D0 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF X-COORD
1 2 2 0.0D0 0.025D0 0.0D0
2 2 2 0.0D0 0.025D0 0.0
0 0 0 0.0D0 0.0D0 0.0D0 END OF Z-COORD
C ***** DATA SET 8: ELEMENT CONNECTIVITY
1 1 2 4 3 1 1 2 IE
C ***** DATA SET 10: CHEMICAL COMPONENT INFORMATION
3 0 0 0 0 0 noha nohs nokx noky nokz nokp
Calcium
1 1
Cabanate
2 1
Hydrogen
3 1
C ***** DATA SET 11: INITIAL CONDITIONS
1 5 1 1.00d-3 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C. Calcium
1 5 1 1.00d-3 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C. Cabonate
1 5 1 0.0d00 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C. HYDROGEN
C ***** DATA SET 12: CONTROL INTEGERS FOR TRANSIENT SOURCE/SINK AND B.C.
0 0 0 0 0 0 2 1 2 2 1 1 2
C ***** DATA SET 14: VARIABLE BOUNDARY CONDITIONS
0.0D0 0.00D00 1.0D38 0.00D00
1 0 0 1 0
0 0 0 0 0 END OF B.C. Calcium
0.0D0 0.000D00 1.0D38 0.000D00
1 0 0 1 0
0 0 0 0 0 END OF B.C. Carbonate
0.0D0 0.0D0 1.0D38 0.0D0
1 0 0 1 0
0 0 0 0 0 END OF B.C. Hydrogen
1 1 1 5 1
0 0 0 0 0 END NPVB
1 0 2 1 2 0 0 0 0
0 0 0 0 0 END OF ISV
C ***** DATA SET 15: DIRICHLET BOUNDARY CONDITIONS
0.0D0 1.0d-3 1.0D38 1.0d-3
1 1 1 1 0
0 0 0 0 0 END OF B.C. Calcium
0.0D0 1.0d-3 1.0D38 1.0d-3

```

```

1 1 1 1 0
0 0 0 0 0
0.0D0 0.0d00 1.0D38 0.0d00
1 1 1 1 0
0 0 0 0 0
1 1 1 1 1
0 0 0 0 0
C ***** DATA SET 16: HYDROLOGICAL VARIABLES
1 5 1 0.0 0.0125 0.0 0.0
0 0 0 0.0 0.0 0.0 0.0
1 1 1 1.0D0 0.0 0.0
0 0 0 0.0 0.0 0.0
C ***** DATA SET 17: NUMBER OF COMPONENTS AND PRODUCT SPECIES
3 0 6 0 0 2 50 50 1.0 1.0D-6 2.0d0 NONA NONS NOMX NOMY NOMZ NOMP
C ***** DATA SET 18: H+, E-, IONIC STRENGTH correction INFORMATION
0.0 2 3 0 SICOR ICOR LNH LNE
c ***** DATA SET 19: temperature, pressure and expected pe and pH
298.0 1.0
-20.0 20.0 0.0 20.0 PEMN PEMX PHMN PHMX
c ***** DATA SET 22: Basic real and integer parameters
1.0 1.0d-6 500 50 2.0d0 1.0d38 omegac epsc niterc npcyl cnstrx cnstry
c ***** DATA SET 23: Component name and component species types
Calcium
1
Cabonate
1
Hydrogen
1
C ***** DATA SET 24: COMPONENT SPECIES AND THEIR ION-EXCHANGE INDEX
FRE Ca++
0 2 0 iscn VJ IONEX
FREE CO32--
0 -2 0 iscn VJ IONEX
FREE H+
0 1 0 iscn VJ IONEX
C ***** DATA SET 25: COMPLEXED SPECIES AND THEIR ION-EXCHANGE INDEX
OH-
0 -14.00 0.0 -14.00 0 0 0 -1 0 0 0 -1
CACO3
0 3.00 0.0 3.00 0 1 1 0 0 1 1 0
CAHCO3+
0 11.60 0.0 11.60 0 1 1 1 0 1 1 1
CAOH+
0 -12.20 0.0 -12.20 0 1 0 -1 0 1 0 -1
HCO3-
0 10.20 0.0 10.20 0 0 1 1 0 0 1 1
H2CO3
0 16.50 0.0 16.50 0 0 1 2 0 0 1 2
C ***** DATA SET 27: PRECIPITATED SPECIES
CA(OH)2
0 -21.90 0.0 -21.90 0 1 0 -2 1 0 -2
CACO3
0 8.30 -5.0 3.30 0 1 1 0 1 1 0
C ***** DATA SET 28: mixed kinetic reaction data
0

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END OF JOB

Table 6.4. Input Data Set for Problem Number 1, Case B.

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2 TEST OF HGC2-0: Ca, CO3, and H: Kx=0, ky=0, kz=0, kp=1
0 0 0 0 5
C ***** DATA SET 2: BASIC INTEGER PARAMTERS
6 2 1 0 5 1 4 -1 1 0 1 0 10 1 50 0 0 0 1 12
C ***** DATA SET 3: BASIC REAL PARAMETERS
0.05 0.0D0 1.0 101 1.0D0 1.0D0 1.0D0 1.0D00 1.0D-5 1.0D0 0.0d0 0
C ***** DATA SET 4: PRINT AND AUXILIARY STORGE CONTROL
444444444444 4 4 4 4 4 4
0 0 0
1.0D38
C ***** DATA SET 5: CHEMICAL OUTPUT AND CHEMICAL PORPerty TYPE INDICATOR
2
1 5 NODEP
C ***** DATA SET 6: MATERIAL PROPERTIES
3.0D-3 0.0D0 0.0D0 1.0D0 AL AT AM RHOB
C ***** DATA SET 7: NODE COORDINATES
1 2 2 0.0 0.0 0.0
2 2 2 0.025D0 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF X-COORD
1 2 2 0.0D0 0.025D0 0.0D0
2 2 2 0.0D0 0.025D0 0.0
0 0 0 0.0D0 0.0D0 0.0D0 END OF Z-COORD
C ***** DATA SET 8: ELEMENT CONNECTIVITY
1 1 2 4 3 1 1 2 IE
C ***** DATA SET 10: CHEMICAL COMPONENT INFORMATION
3 0 0 0 0 1 noha nohs nokx noky nokz nokp
Calcium
1 1
Cabonate
2 1
Hydrogen
3 1
C ***** DATA SET 11: INITIAL CONDITIONS
1 5 1 1.00d-3 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C. Calcium
1 5 1 1.00d-3 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C. Cabonate
1 5 1 0.0d00 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C. HYDROGEN
1 5 1 8.642d-5 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C.kinetic CaCO3
C ***** DATA SET 12: CONTROL INTEGERS FOR TRANSIENT SOURCE/SINK AND B.C.
0 0 0 0 0 0 2 1 2 2 1 1 2
C ***** DATA SET 14: VARIABLE BOUNDARY CONDITIONS
0.0D0 0.00D00 1.0D38 0.00D00
1 0 0 1 0
0 0 0 0 0 END OF B.C. Calcium
0.0D0 0.000D00 1.0D38 0.000D00
1 0 0 1 0
0 0 0 0 0 END OF B.C. Carbonate
0.0D0 0.0D0 1.0D38 0.0D0
1 0 0 1 0
0 0 0 0 0 END OF B.C. Hydrogen
1 1 1 5 1
0 0 0 0 0 END NPVB
1 0 2 1 2 0 0 0 0
0 0 0 0 0 0 0 0 0 END OF ISV
C ***** DATA SET 15: DIRICHLET BOUNDARY CONDITIONS
0.0D0 1.0d-3 1.0D38 1.0d-3
1 1 1 1 0

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0 0 0 0 0 END OF B.C. Calcium
0.0D0 1.0d-3 1.0D38 1.0d-3
1 1 1 1 0
0 0 0 0 0 END OF B.C. Cabonate
0.0D0 0.0d00 1.0D38 0.0d00
1 1 1 1 0
0 0 0 0 0 END OF B.C. Hydrogen
1 1 1 1 1
0 0 0 0 0 END OF NPDB
C ***** DATA SET 16: HYDROLOGICAL VARIABLES
1 5 1 0.0 0.0125 0.0 0.0
0 0 0 0.0 0.0 0.0 0.0 END OF VELOCITY
1 1 1 1.0D0 0.0 0.0
0 0 0 0.0 0.0 0.0 END OF TH
C ***** DATA SET 17: NUMBER OF COMPONENTS AND PRODUCT SPECIES
3 0 6 0 0 2 50 50 1.0 1.0D-6 2.0d0 NONA NONS NOMX NOMY NOMZ NOMP
C ***** DATA SET 18: H+, E-, IONIC STRENGTH correction INFORMATION
0.0 2 3 0 SICOR ICOR LNH LNE
C ***** DATA SET 19: temperature, pressure and expected pe and pH
298.0 1.0
-20.0 20.0 0.0 20.0 PEMN PEMX PHMN PHMX
C ***** DATA SET 22: Basic real and integer parameters
1.0 1.0d-6 500 50 1.0d38 1.0d38 omegac epsc niterc npcyl cnstrx cnstry
C ***** DATA SET 23: Component name and component species types
Calcium
1
Cabonate
1
Hydrogen
1
C ***** DATA SET 24: COMPONENT SPECIES AND THEIR ION-EXCHANGE INDEX
FRE Ca++
0 2 0 iscn VJ IONEX
FREE CO32--
0 -2 0 iscn VJ IONEX
FREE H+
0 1 0 iscn VJ IONEX
C ***** DATA SET 25: COMPLEXED SPECIES AND THEIR ION-EXCHANGE INDEX
OH-
0 -14.00 0.0 -14.00 0 0 0 -1 0 0 0 -1
CACO3
0 3.00 0.0 3.00 0 1 1 0 0 1 1 0
CAHCO3+
0 11.60 0.0 11.60 0 1 1 1 0 1 1 1
CAOH+
0 -12.20 0.0 -12.20 0 1 0 -1 0 1 0 -1
HCO3-
0 10.20 0.0 10.20 0 0 1 1 0 0 1 1
H2CO3
0 16.50 0.0 16.50 0 0 1 2 0 0 1 2
C ***** DATA SET 27: PRECIPITATED SPECIES
CA(OH)2
0 -21.90 0.0 -21.90 0 1 0 -2 1 0 -2
CACO3
0 8.30 -5.0 3.30 2 1 1 0 1 1 0
C ***** DATA SET 28: kinetic reaction data
1
2 1 1 -5.0 3.30
1 1 1
1 2 11

```

END OF JOB

Table 6.5. Input Data Set for Problem Number 1, Case C.

```

3 TEST OF HGC2-0: Ca, CO3, H: kx=1, ky=0, kz=0, kp=1
1 0 0 0 5
C ***** DATA SET 2: BASIC INTEGER PARAMTERS
6 2 1 0 5 1 4 -1 1 0 1 0 10 1 50 0 0 0 1 12
C ***** DATA SET 3: BASIC REAL PARAMETERS
0.05 0.0D0 1.0 101 1.0D0 1.0D0 1.0D0 1.0D00 1.0D-6 1.0D0 0.0d0 0
C ***** DATA SET 4: PRINT AND AUXILIARY STORGE CONTROL
444444444444 4 4 4 4 4
0000000000000000000000000000000000
1.0D38
C ***** DATA SET 5: CHEMICAL OUTPUT AND CHEMICAL PORPerty TYPE INDICATOR
2
1 5 NODEP
C ***** DATA SET 6: MATERIAL PROPERTIES
3.0D-3 0.0D0 0.0D0 1.0D0 AL AT AM RHOB
C ***** DATA SET 7: NODE COORDINATES
1 2 2 0.0 0.0 0.0
2 2 2 0.025D0 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF X-COORD
1 2 2 0.0D0 0.025D0 0.0D0
2 2 2 0.0D0 0.025D0 0.0
0 0 0 0.0D0 0.0D0 0.0D0 END OF Z-COORD
C ***** DATA SET 8: ELEMENT CONNECTIVITY
1 1 2 4 3 1 1 2 IE
C ***** DATA SET 10: CHEMICAL COMPONENT INFORMATION
3 0 1 0 0 1 noha nohs nokx noky nokz nokp
Calcium
1 1
Cabanate
2 1
Hydrogen
3 1
C ***** DATA SET 11: INITIAL CONDITIONS
1 5 1 1.00d-3 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C. Calcium
1 5 1 1.00d-3 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C. Cabonate
1 5 1 0.0d00 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C. HYDROGEN
1 5 1 .8404d-5 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. hco3
1 5 1 8.642d-5 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C.kinetic CaCO3
C ***** DATA SET 12: CONTROL INTEGERS FOR TRANSIENT SOURCE/SINK AND B.C.
0 0 0 0 0 0 2 1 2 2 1 1 2
C ***** DATA SET 14: VARIABLE BOUNDARY CONDITIONS
0.0D0 0.00D00 1.0D38 0.00D00
1 0 0 1 0
0 0 0 0 0 END OF B.C. Calcium
0.0D0 0.000D00 1.0D38 0.000D00
1 0 0 1 0
0 0 0 0 0 END OF B.C. Carbonate
0.0D0 0.0D0 1.0D38 0.0D0
1 0 0 1 0
0 0 0 0 0 END OF B.C. Hydrogen
0.0 .8404d-5 1.0d38 .8404d-5
1 0 0 1 0
0 0 0 0 0 end of b.c. hco3
1 1 1 5 1
0 0 0 0 0 END NPVB
1 0 2 1 2 0 0 0 0

```

```

0 0 0 0 0 0 0 0 0 0 END OF ISV
C ***** DATA SET 15: DIRICHLET BOUNDARY CONDITIONS
0.0D0 1.0d-3 1.0D38 1.0d-3
1 1 1 1 0
0 0 0 0 0 END OF B.C. Calcium
0.0D0 1.0d-3 1.0D38 1.0d-3
1 1 1 1 0
0 0 0 0 0 END OF B.C. Cabonate
0.0D0 0.0d00 1.0D38 0.0d00
1 1 1 1 0
0 0 0 0 0 END OF B.C. Hydrogen
0.0d0 .8404d-5 1.0d38 .8404d-5
1 1 1 1 0
0 0 0 0 0 end of b.c. hco3
1 1 1 1 1
0 0 0 0 0 END OF NPDB
C ***** DATA SET 16: HYDROLOGICAL VARIABLES
1 5 1 0.0 0.0125 0.0 0.0
0 0 0 0.0 0.0 0.0 0.0 END OF VELOCITY
1 1 1 1.0D0 0.0 0.0
0 0 0 0.0 0.0 0.0 END OF TH
C ***** DATA SET 17: NUMBER OF COMPONENTS AND PRODUCT SPECIES
3 0 6 0 0 2 50 50 1.0 1.0D-6 2.0d0 NONA NONS NOMX NOMY NOMZ NOMP
C ***** DATA SET 18: H+, E-, IONIC STRENGTH correction INFORMATION
0.0 2 3 0 SICOR ICOR LNH LNE
c ***** DATA SET 19: temperature, pressure and expected pe and pH
298.0 1.0
-20.0 20.0 0.0 20.0 PEMN PEMX PHMN PHMX
c ***** DATA SET 22: Basic real and integer parameters
1.0 1.0d-6 500 50 2.0d0 1.0d38 omegac epsc niterc npcyl cnstrx cnstry
c ***** DATA SET 23: Component name and component species types
Calcium
1
Cabonate
1
Hydrogen
1
C ***** DATA SET 24: COMPONENT SPECIES AND THEIR ION-EXCHANGE INDEX
FRE Ca++
0 2 0 iscn VJ IONEX
FREE CO32--
0 -2 0 iscn VJ IONEX
FREE H+
0 1 0 iscn VJ IONEX
C ***** DATA SET 25: COMPLEXED SPECIES AND THEIR ION-EXCHANGE INDEX
OH-
0 -14.00 0.0 -14.00 0 0 0 -1 0 0 0 -1
CACO3
0 3.00 0.0 3.00 0 1 1 0 0 1 1 0
CAHCO3+
0 11.60 0.0 11.60 0 1 1 1 0 1 1 1
CAOH+
0 -12.20 0.0 -12.20 0 1 0 -1 0 1 0 -1
HCO3-
0 10.20 -5.2 5.0 2 0 1 1 0 0 1 1
H2CO3
0 16.50 0.0 16.50 0 0 1 2 0 0 1 2
C ***** DATA SET 27: PRECIPITATED SPECIES
CA(OH)2
0 -21.90 0.0 -21.90 0 1 0 -2 1 0 -2
CACO3
0 8.30 -5.0 3.30 2 1 1 0 1 1 0

```

C ***** DATA SET 28: MIXED KINETIC REACTIONS

```
2
2 1 0 -5.2 5.0
1 1 1
2 3 8
2 1 1 -5.0 3.30
1 1 1
1 2 11
```

END OF JOB

6.2 Problem No. 2: An Experimental System of EDTA Adsorption onto Ferrous Hydroxide

To test a more complicated experimental system, data for this example came from laboratory experiments on a system containing six chemical components; calcium, cobalt, hydrogen, EDTA, chlorate, and solid ferric oxide (Szescody, et al., 1994). The ferric component species acts as an adsorption site. In addition to these six free species, six significant complexed species and seven surface or adsorbed species are included for simulation. Thus a total of 19 species are involved. Table 6.6 lists the geochemical data for this problem.

Three cases are included in this problem. For Case 2A, all 13 product species will be considered equilibrium controlled reactions. For Case 2B, all species remain the same as for Case 2A, however the formation of 4 of 7 adsorbed species is now allowed to be a kinetic process. These four kinetic adsorbed species are: $\text{FeOH}_2\text{-FeEDTA}$, $\text{FeOH}_2\text{-CoEDTA}$, FeO-Co , and $\text{FeOH}_2\text{-H}_2\text{EDTA}$. The forward and backward rate constants for these four species are given in Table 6.6. Case 2C involves the same product species as in Cases 2A and 2B, but the complexed species CoEDTA^{2-} , will also be forming due to a kinetic reaction, with logarithm of forward and backward rate constants given in Table 6.6.

The initial total analytical concentrations of calcium, cobalt, EDTA, chlorate, and solid ferric oxide are 2×10^{-3} , 8.51×10^{-6} , 8.51×10^{-6} , 1×10^{-3} , and 1.12×10^{-7} M, respectively, and the activity of hydrogen is fixed at $\text{pH} = 4.5$. When the species CoEDTA^{2-} , $\text{FeOH}_2\text{-FeEDTA}$, $\text{FeOH}_2\text{-CoEDTA}$, FeO-Co^+ , and $\text{FeOH}_2\text{-H}_2\text{EDTA}$ are kinetic species, their initial concentrations are specified as 8.3398×10^{-6} , 1.0×10^{-19} , 1.0×10^{-19} , 1.0×10^{-19} , and 1.0×10^{-19} , respectively. To specify the boundary conditions, the total concentrations of calcium, cobalt, EDTA, and chlorate are assumed to have the same values as their initial concentrations, i.e., 2×10^{-3} , 8.51×10^{-6} , 8.51×10^{-6} , and 1.0×10^{-3} M, respectively. The concentrations of the mobile kinetic species CoEDTA^{2-} in the incoming fluid is also assumed to have same value as its initial conditions of 8.3398×10^{-6} .

The input data sets are prepared according to Appendix A and are given in Tables 6.7, 6.8 and 6.9.

Table 6.6. List of Geochemical Data for Problem No. 2

Species	Ca ²⁺	Co ²⁺	H ⁺	EDTA ⁴⁻	ClO ₄ ⁻	FeOH	log K ^e	log K ^b	log K ^f
Ca ²⁺	1	0	0	0	0	0	0.00	-----	-----
Co ²⁺	0	1	0	0	0	0	0.00	-----	-----
H ⁺	0	0	1	0	0	0	0.00	-----	-----
EDTA ⁴⁻	0	0	0	1	0	0	0.00	-----	-----
ClO ₄ ⁻	0	0	0	0	1	0	0.00	-----	-----
FeOH	0	0	0	0	0	1	0.00	-----	-----
CaEDTA ²⁻	1	0	0	1	0	0	12.32	-----	-----
CaHEDTA ⁻	1	0	1	1	0	0	15.93	-----	-----
CoEDTA ²⁻	0	1	0	1	0	0	17.97	2.03	20.0
CoHEDTA ⁻	0	1	1	1	0	0	21.40	-----	-----
H ₂ EDTA	0	0	2	1	0	0	17.78	-----	-----
OH ⁻	0	0	-1	0	0	0	-14.0	-----	-----
FeO ⁻	0	0	-1	0	0	1	-11.6	-----	-----
FeOH ₂ ⁺	0	0	1	0	0	1	5.60	-----	-----
FeO-Co ⁺	0	1	-1	0	0	1	-2.69	1.70	-0.99
FeOH ₂ -FeEDTA	0	0	4	1	0	2	36.60	-38.00	-1.40
FeOH ₂ -CoEDTA ⁻	0	1	1	1	0	1	28.49	1.51	30.0
FeOH ₂ -H ₂ EDTA ⁻	0	0	3	1	0	1	30.48	1.52	32.0
FeOH ₂ -CaEDTA ⁻	1	0	1	1	0	1	23.81	-----	-----

Table 6.7. Input Data Set for Problem Number 2, Case A.

```

4 SIMULATION OF CoEDTA-Fe(OH)3 REACTION KINETICS: kx=0,ky=0, kz=0, kp=0
0 0 0 0 5
C ***** DATA SET 2: BASIC INTEGER PARAMTERS
6 2 1 0 5 1 4 -1 1 0 1 0 10 1 50 0 0 0 1 12
C ***** DATA SET 3: BASIC REAL PARAMETERS
0.05 0.0D0 1.0 101 1.0D0 1.0D0 1.0D0 1.0D00 1.0D-6 1.0D0 0.0d0 0
C ***** DATA SET 4: PRINT AND AUXILIARY STORGE CONTROL
444444
000000
1.0D38
C ***** DATA SET 5: CHEMICAL OUTPUT AND CHEMICAL PORPerty TYPE INDICATOR
2
1 5 NODEP
C ***** DATA SET 6: MATERIAL PROPERTIES
3.0D-3 0.0D0 0.0D0 1.0D0 AL AT AM RHOB
C ***** DATA SET 7: NODE COORDINATES
1 2 2 0.0 0.0 0.0
2 2 2 0.025D0 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF X-COORD
1 2 2 0.0D0 0.025D0 0.0D0
2 2 2 0.0D0 0.025D0 0.0
0 0 0 0.0D0 0.0D0 0.0D0 END OF Z-COORD
C ***** DATA SET 8: ELEMENT CONNECTIVITY
1 1 2 4 3 1 1 2 IE
C ***** DATA SET 10: CHEMICAL COMPONENT INFORMATION
5 1 0 0 0 0 NOhA NOhS NOKX NOKY NOKZ NOKP
Calcium
1 1
Cobolt
2 1
Hydrogen
3 3
EDTA
4 1
Chlorate
5 1
FeOH
6 2
C ***** DATA SET 11: INITIAL CONDITIONS
1 5 1 2.00d-3 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C. Calcium
1 5 1 8.51d-6 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C. Cobalt
1 5 1 -4.5 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C. HYDROGEN
1 5 1 8.51d-6 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. EDTA
1 5 1 1.00d-3 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. Chlorate
1 5 1 1.12d-7 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. FeOH
C ***** DATA SET 12: CONTROL INTEGERS FOR TRANSIENT SOURCE/SINK AND B.C.
0 0 0 0 0 0 2 1 2 2 1 1 2
C ***** DATA SET 14: VARIABLE BOUNDARY CONDITIONS
0.0D0 2.00D-3 1.0D38 2.00D-3
1 0 1 1 0
0 0 0 0 0 END OF B.C. Calcium
0.0D0 8.51D-6 1.0D38 8.51D-6
1 0 1 1 0
0 0 0 0 0 END OF B.C. Colbat

```

```

0.0D0 8.51D-6 1.0D38 8.51D-6
1 0 1 1 0
0 0 0 0 0 END OF B.C. EDTA
0.0D0 1.00D-3 1.0D38 1.00D-3
1 0 1 1 0
0 0 0 0 0 END OF B.C. Chlorate
1 1 1 5 1
0 0 0 0 0 END NPVB
1 0 2 1 2 0 0 0 0
0 0 0 0 0 0 0 0 0 END OF ISV
C ***** DATA SET 15: Dirichlet Boundary Condition
0.0D0 2.00D-3 1.0D38 2.00D-3
1 1 1 1 0
0 0 0 0 0 END OF B.C. Calcium
0.0D0 8.51D-6 1.0D38 8.51D-6
1 1 1 1 0
0 0 0 0 0 END OF B.C. Cobalt
0.0D0 8.51D-6 1.0D38 8.51D-6
1 1 1 1 0
0 0 0 0 0 END OF B.C. EDTA
0.0D0 1.00D-3 1.0D38 1.00D-3
1 1 1 1 0
0 0 0 0 0 END OF B.C. Chlorate
1 1 1 1 1
0 0 0 0 0 END NPDB
C ***** DATA SET 16: HYDROLOGICAL VARIABLES
1 5 1 0.0 0.0125 0.0 0.0
0 0 0 0.0 0.0 0.0 0.0 END OF VELOCITY
1 1 1 1.0D0 0.0 0.0
0 0 0 0.0 0.0 0.0 END OF TH
C ***** DATA SET 17: NUMBER OF COMPONENTS AND PRODUCT SPECIES
5 1 6 7 0 0 NONA NONS NOMX NOMY NOMZ NOMP
C ***** DATA SET 18: H+, E-, IONIC STRENGTH correction INFORMATION
0.0 0 3 0 SICOR ICOR LNH LNE
c ***** DATA SET 19: temperature, pressure and expected pe and pH
298.3 1.0 TEMP PRESSU
-20.0 20.0 0.0 20.0 PEMN PEMX PHMN PHMX
C ***** DATA SET 20: ADSORPTION INFORMATION
1 0 nsorb iads
0 0 lona(i), lonb(i) i=1,nsorb lines
0.0 0.0 0.0 cap1m(j,i),cap2m(j,i),sream(j,i), j=1,nsorb, i=1,nmat
c ***** DATA SET 22: Basic real and integer parameters
1.0 1.0d-6 250 1 2.0d0 1.0d38 omegac epsc niterc npcyl cnstrx cnstry
c ***** DATA SET 23: Component name and component species types
Calcium
1 mobile aqueous species
Cobolt
1 mobile aqueous species
Hydrogen
1 mobile aqueous species
EDTA
1 mobile aqueous species
Chlorate
1 mobile aqueous species
FeOH
2 immobile adsobent species
C ***** DATA SET 24: COMPONENT SPECIES AND THEIR ION-EXCHANGE INDEX
Free Calcium
0 2 0 iscn VJ IONEX
Free Cobolt
0 2 0
Free Hydrogen
3 1 0

```

```

Free EDTA
  0 -4 0
Free ClO4-
  0 -1 0
Free FeOH
  0 0 0
C ***** DATA SET 25: COMPLEXED SPECIES AND THEIR ION-EXCHANGE INDEX
CaEDTA
  0 12.32 0.0 12.32 0 1 0 0 1 0 0 0 1 0 0 1 0 0
CaHEDTA
  0 15.93 0.0 15.93 0 1 0 1 1 0 0 0 1 0 1 1 0 0
CoEDTA2-
  0 17.97 2.03 20.00 0 0 1 0 1 0 0 0 0 1 0 1 0 0
CoHEDTA
  0 21.40 0.0 21.40 0 0 1 1 1 0 0 0 0 1 1 1 0 0
H2EDTA
  0 17.78 0.0 17.78 0 0 0 2 1 0 0 0 0 0 2 1 0 0
OH
  0 -14.00 0.0 -14.00 0 0 0 -1 0 0 0 0 0 0 -1 0 0 0
C ***** DATA SET 21: ABSORBED SPECIES
FeO-
  0 -11.60 0.0 -11.60 0 0 0 -1 0 0 1 0 0 -1 0 0 1
FeOH2+
  0 5.60 0.0 5.60 0 0 0 1 0 0 1 0 0 1 0 0 1
FeOH2-FeEDTA
  0 36.60 -38.0 -1.40 0 0 0 4 1 0 2 0 0 4 1 0 2
FeOH2-CoEDTA
  0 28.49 1.51 30.00 0 0 1 1 1 0 1 0 1 1 1 0 1
FeO-Co
  0 -2.69 1.70 -0.99 0 0 1 -1 0 0 1 0 1 -1 0 0 1
FeOH2-CaEDTA
  0 23.81 0.0 23.81 0 1 0 1 1 0 1 1 0 1 1 0 1
FeOH2-H2EDTA
  0 30.48 1.52 32.00 0 0 0 3 1 0 1 0 0 3 1 0 1
C ***** DATA SET 28: kinetic reaction data
0
                                END OF JOB

```

Table 6.8. Input Data Set for Problem Number 2, Case B.

```

5 SIMULATION OF CoEDTA-Fe(OH)3 REACTION KINETICS: kx=4,ky=0, kz=0, kp=0
0 0 0 0 5
C ***** DATA SET 2: BASIC INTEGER PARAMTERS
6 2 1 0 5 1 4 -1 1 0 1 0 10 1 50 0 0 0 1 12
C ***** DATA SET 3: BASIC REAL PARAMETERS
0.05 0.0D0 1.0 101 1.0D0 1.0D0 1.0D0 1.0D00 1.0D-6 1.0D0 0.0d0 0
C ***** DATA SET 4: PRINT AND AUXILIARY STORGE CONTROL
444444
000000
1.0D38
C ***** DATA SET 5: CHEMICAL OUTPUT AND CHEMICAL PROPERTY TYPE INDICATOR
2
1 5 NODEP
C ***** DATA SET 6: MATERIAL PROPERTIES
3.0D-3 0.0D0 0.0D0 1.0D0 AL AT AM RHOB
C ***** DATA SET 7: NODE COORDINATES
1 2 2 0.0 0.0 0.0
2 2 2 0.025D0 0.0D0 0.0D0

```

```

0 0 0 0.0 0.0 0.0 END OF X-COORD
1 2 2 0.0D0 0.025D0 0.0D0
2 2 2 0.0D0 0.025D0 0.0
0 0 0 0.0D0 0.0D0 0.0D0 END OF Z-COORD
C ***** DATA SET 8: ELEMENT CONNECTIVITY
1 1 2 4 3 1 1 2 IE
C ***** DATA SET 10: CHEMICAL COMPONENT INFORMATION
5 1 0 4 0 0 NOhA NOhS NOKX NOKY NOKZ NOKP
Calcium
1 1
Cobolt
2 1
Hydrogen
3 3
EDTA
4 1
Chlorate
5 1
FeOH
6 2
C ***** DATA SET 11: INITIAL CONDITIONS
1 5 1 2.00d-3 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C. Calcium
1 5 1 8.51d-6 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C. Cobalt
1 5 1 -4.5 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C. HYDROGEN
1 5 1 8.51d-6 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. EDTA
1 5 1 1.00d-3 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. Chlorate
1 5 1 1.12d-7 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. FeOH
1 5 1 1.00d-19 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. Fe(OH)2-FeEDTA
1 5 1 1.00d-19 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. Fe(OH)3-CoEDTA
1 5 1 1.00d-19 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. Fe-Co
1 5 1 1.00d-19 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. Fe(OH)3-H2EDTA
C ***** DATA SET 12: CONTROL INTEGERS FOR TRANSIENT SOURCE/SINK AND B.C.
0 0 0 0 0 0 2 1 2 2 1 1 2
C ***** DATA SET 14: VARIABLE BOUNDARY CONDITIONS
0.0D0 2.00D-3 1.0D38 2.00D-3
1 0 1 1 0
0 0 0 0 0 END OF B.C. Calcium
0.0D0 8.51D-6 1.0D38 8.51D-6
1 0 1 1 0
0 0 0 0 0 END OF B.C. Colbat
0.0D0 8.51D-6 1.0D38 8.51D-6
1 0 1 1 0
0 0 0 0 0 END OF B.C. EDTA
0.0D0 1.00D-3 1.0D38 1.00D-3
1 0 1 1 0
0 0 0 0 0 END OF B.C. Chlorate
1 1 1 5 1
0 0 0 0 0 END NPVB
1 0 2 1 2 0 0 0 0
0 0 0 0 0 0 0 0 0 END OF ISV
C ***** DATA SET 15: DIRICHLET BOUNDARY CONDITIONS
0.0D0 2.00D-3 1.0D38 2.00D-3
1 1 1 1 0

```

```

0 0 0 0 0 END OF B.C. Calcium
0.0D0 8.51D-6 1.0D38 8.51D-6
1 1 1 1 0
0 0 0 0 0 END OF B.C. Colbat
0.0D0 8.51D-6 1.0D38 8.51D-6
1 1 1 1 0
0 0 0 0 0 END OF B.C. EDTA
0.0D0 1.00D-3 1.0D38 1.00D-3
1 1 1 1 0
0 0 0 0 0 END OF B.C. Chlorate
1 1 1 1 1
0 0 0 0 0 END NPDB
C ***** DATA SET 16: HYDROLOGICAL VARIABLES
1 5 1 0.0 0.0125 0.0 0.0
0 0 0 0.0 0.0 0.0 0.0 END OF VELOCITY
1 1 1 1.0D0 0.0 0.0
0 0 0 0.0 0.0 0.0 END OF TH
C ***** DATA SET 17: NUMBER OF COMPONENTS AND PRODUCT SPECIES
5 1 6 7 0 0 50 50 1.0 1.0d-6 2.0d0 NONA NONS NOMX NOMY NOMZ NOMP
C ***** DATA SET 18: H+, E-, IONIC STRENGTH correction INFORMATION
0.0 0 3 0 SICOR ICOR LNH LNE
c ***** DATA SET 19: temperature, pressure and expected pe and pH
298.3 1.0 TEMP PRESSU
-20.0 20.0 0.0 20.0 PEMN PEMX PHMN PHMX
C ***** DATA SET 20: ADSORPTION INFORMATION
1 0 nsorb iads
0 0 lona(i), lonb(i) i=1,nsorb lines
0.0 0.0 0.0 cap1m(j,i),cap2m(j,i),sream(j,i), j=1,nsorb, i=1,nmat
c ***** DATA SET 22: Basic real and integer parameters
1.0 1.0d-6 250 1 2.0d0 1.0d38 omegac epsc niterc npcyl cnstrx cnstry
c ***** DATA SET 23: Component name and component species types
Calcium
1 mobile aqueous species
Cobolt
1 mobile aqueous species
Hydrogen
1 mobile aqueous species
EDTA
1 mobile aqueous species
Chlorate
1 mobile aqueous species
FeOH
2 immobile adsorbent species
C ***** DATA SET 24: COMPONENT SPECIES AND THEIR ION-EXCHANGE INDEX
Free Calcium
0 2 0 iscn VJ IONEX
Free Cobolt
0 2 0
Free Hydrogen
3 1 0
Free EDTA
0 -4 0
Free ClO4-
0 -1 0
Free FeOH
0 0 0
C ***** DATA SET 25: COMPLEXED SPECIES AND THEIR ION-EXCHANGE INDEX
CaEDTA
0 12.32 0.0 12.32 0 1 0 0 1 0 0 0 1 0 0 1 0 0
CaHEDTA
0 15.93 0.0 15.93 0 1 0 1 1 0 0 0 1 0 1 1 0 0
CoEDTA2-
0 17.97 2.03 20.00 0 0 1 0 1 0 0 0 0 1 0 1 0 0

```

```

CoHEDTA
 0 21.40 0.0 21.40 0 0 1 1 1 0 0 0 0 1 1 1 0 0
H2EDTA
 0 17.78 0.0 17.78 0 0 0 2 1 0 0 0 0 0 2 1 0 0
OH
 0 -14.00 0.0 -14.00 0 0 0 -1 0 0 0 0 0 0 -1 0 0 0
C ***** DATA SET 21: ABSORBED SPECIES
FeO-
 0 -11.60 0.0 -11.60 0 0 0 -1 0 0 1 0 0 -1 0 0 1
FeOH2+
 0 5.60 0.0 5.60 0 0 0 1 0 0 1 0 0 1 0 0 1
FeOH2-FeEDTA
 0 36.60 -38.00 -1.40 2 0 0 4 1 0 2 0 0 4 1 0 2
FeOH2-CoEDTA
 0 28.49 1.51 30.00 2 0 1 1 1 0 1 0 1 1 1 0 1
FeO-Co
 0 -2.69 1.70 -0.99 2 0 1 -1 0 0 1 0 1 -1 0 0 1
FeOH2-CaEDTA
 0 23.81 0.0 23.81 0 1 0 1 1 0 1 1 0 1 1 0 1
FeOH2-H2EDTA
 0 30.48 1.52 32.00 2 0 0 3 1 0 1 0 0 3 1 0 1
C ***** DATA SET 28: kinetic reaction data
4
3 1 0 -38.0 -1.40
4 1 2 1
3 4 6 15
4 1 0 1.51 30.00
1 1 1 1 1
2 3 4 6 16
3 1 0 1.70 -0.99
1 -1 1 1
2 3 6 17
3 1 0 1.52 32.00
3 1 1 1
3 4 6 19

```

END OF JOB

Table 6.9. Input Data Set for Problem Number 2, Case C.

```

6 SIMULATION OF CoEDTA-Fe(OH)3 REACTION KINETICS: kx=1,ky=4, kz=0, kp=0
1 0 0 0 5
C ***** DATA SET 2: BASIC INTEGER PARAMTERS
6 2 1 0 5 1 4 -1 1 0 1 0 20 1 50 0 0 0 1 12
C ***** DATA SET 3: BASIC REAL PARAMETERS
0.05 0.0D0 1.0 101 1.0D0 1.0D0 1.0D0 1.0D00 1.0D-6 1.0D0 1.0d0 1
C ***** DATA SET 4: PRINT AND AUXILIARY STORGE CONTROL
444444
000000
1.0D38
C ***** DATA SET 5: CHEMICAL OUTPUT AND CHEMICAL PORPERTY TYPE INDICATOR
2
1 5 NODEP
C ***** DATA SET 6: MATERIAL PROPERTIES
3.0D-3 0.0D0 0.0D0 1.0D0 AL AT AM RHOB
C ***** DATA SET 7: NODE COORDINATES
1 2 2 0.0 0.0 0.0
2 2 2 0.025D0 0.0D0 0.0D0

```

```

0 0 0 0.0 0.0 0.0 END OF X-COORD
1 2 2 0.0D0 0.025D0 0.0D0
2 2 2 0.0D0 0.025D0 0.0
0 0 0 0.0D0 0.0D0 0.0D0 END OF Z-COORD
C ***** DATA SET 8: ELEMENT CONNECTIVITY
1 1 2 4 3 1 1 2 IE
C ***** DATA SET 10: CHEMICAL COMPONENT INFORMATION
5 1 1 4 0 0 NOhA NOhS NOKX NOKY NOKZ NOKP
Calcium
1 1
Cobolt
2 1
Hydrogen
3 3
EDTA
4 1
Chlorate
5 1
FeOH
6 2
C ***** DATA SET 11: INITIAL CONDITIONS
1 5 1 2.00d-3 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C. Calcium
1 5 1 8.51d-6 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C. Cobalt
1 5 1 -4.5 0.0D0 0.0D0
0 0 0 0.0 0.0 0.0 END OF I.C. HYDROGEN
1 5 1 8.51d-6 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. EDTA
1 5 1 1.00d-3 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. Chlorate
1 5 1 1.12d-7 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. FeOH
1 5 1 8.3398d-6 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. CoEDTA
1 5 1 1.00d-19 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. Fe(OH)2-FeEDTA
1 5 1 1.00d-19 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. Fe(OH)3-CoEDTA
1 5 1 1.00d-19 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. Fe-Co
1 5 1 1.00d-19 0.0 0.0
0 0 0 0.0 0.0 0.0 end of i.c. Fe(OH)3-H2EDTA
C ***** DATA SET 12: CONTROL INTEGERS FOR TRANSIENT SOURCE/SINK AND B.C.
0 0 0 0 0 0 2 1 2 2 1 1 2
C ***** DATA SET 14: VARIABLE BOUNDARY CONDITIONS
0.0D0 2.00D-3 1.0D38 2.00D-3
1 0 1 1 0
0 0 0 0 0 END OF B.C. Calcium
0.0D0 8.51D-6 1.0D38 8.51D-6
1 0 1 1 0
0 0 0 0 0 END OF B.C. Colbat
0.0D0 8.51D-6 1.0D38 8.51D-6
1 0 1 1 0
0 0 0 0 0 END OF B.C. EDTA
0.0D0 1.00D-3 1.0D38 1.00D-3
1 0 1 1 0
0 0 0 0 0 END OF B.C. Chlorate
0.0D0 8.3398d-6 1.0D38 8.3398d-7
1 0 1 1 0
0 0 0 0 0 END OF B.C. CoEDTA
1 1 1 5 1
0 0 0 0 0 END NPVB

```

```

1 0 2 1 2 0 0 0 0
0 0 0 0 0 0 0 0 0 END OF ISV
C ***** DATA SET 15: DIRICHLET BOUNDARY CONDITIONS
0.0D0 2.00D-3 1.0D38 2.00D-3
1 1 1 1 0
0 0 0 0 0 END OF B.C. Calcium
0.0D0 8.51D-6 1.0D38 8.51D-6
1 1 1 1 0
0 0 0 0 0 END OF B.C. Colbat
0.0D0 8.51D-6 1.0D38 8.51D-6
1 1 1 1 0
0 0 0 0 0 END OF B.C. EDTA
0.0D0 1.00D-3 1.0D38 1.00D-3
1 1 1 1 0
0 0 0 0 0 END OF B.C. Chlorate
0.0D0 8.3398d-6 1.0D38 8.3398d-7
1 1 1 1 0
0 0 0 0 0 END OF B.C. CoEDTA
1 1 1 1 1
0 0 0 0 0 END NPDB
C ***** DATA SET 16: HYDROLOGICAL VARIABLES
1 5 1 0.0 0.0125 0.0 0.0
0 0 0 0.0 0.0 0.0 0.0 END OF VELOCITY
1 1 1 1.0D0 0.0 0.0
0 0 0 0.0 0.0 0.0 END OF TH
C ***** DATA SET 17: NUMBER OF COMPONENTS AND PRODUCT SPECIES
5 1 6 7 0 0 50 50 1.0 1.0d-6 2.0d0 NONA NONS NOMX NOMY NOMZ NOMP
C ***** DATA SET 18: H+, E-, IONIC STRENGTH correction INFORMATION
0.0 0 3 0 SICOR ICOR LNH LNE
c ***** DATA SET 19: temperature, pressure and expected pe and pH
298.3 1.0 TEMP PRESSU
-20.0 20.0 0.0 20.0 PEMN PEMX PHMN PHMX
C ***** DATA SET 20: ADSORPTION INFORMATION
1 0 nsorb iads
0 0 lona(i), lonb(i) i=1,nsorb lines
0.0 0.0 0.0 cap1m(j,i),cap2m(j,i),sream(j,i), j=1,nsorb,i=1,nmat
c ***** DATA SET 22: Basic real and integer parameters
1.0 1.0d-6 700 1 2.0 2.0 omegac epsc niterc npcyl cnstrx cnstry
c ***** DATA SET 23: Component name and component species types
Calcium
1 mobile aqueous species
Cobolt
1 mobile aqueous species
Hydrogen
1 mobile aqueous species
EDTA
1 mobile aqueous species
Chlorate
1 mobile aqueous species
FeOH
2 immobile adsobent species
C ***** DATA SET 24: COMPONENT SPECIES AND THEIR ION-EXCHANGE INDEX
Free Calcium
0 2 0 iscn VJ IONEX
Free Cobolt
0 2 0
Free Hydrogen
3 1 0
Free EDTA
0 -4 0
Free ClO4-
0 -1 0
Free FeOH

```

```

0 0 0
C ***** DATA SET 25: COMPLEXED SPECIES AND THEIR ION-EXCHANGE INDEX
CaEDTA
0 12.32 0.0 12.32 0 1 0 0 1 0 0 0 1 0 0 1 0 0
CaHEDTA
0 15.93 0.0 15.93 0 1 0 1 1 0 0 0 1 0 1 1 0 0
CoEDTA2-
0 17.97 2.03 20.00 2 0 1 0 1 0 0 0 0 1 0 1 0 0
CoHEDTA
0 21.40 0.0 21.40 0 0 1 1 1 0 0 0 0 1 1 1 0 0
H2EDTA
0 17.78 0.0 17.78 0 0 0 2 1 0 0 0 0 0 2 1 0 0
OH
0 -14.00 0.0 -14.00 0 0 0 -1 0 0 0 0 0 0 -1 0 0 0
C ***** DATA SET 21: ABSORBED SPECIES
FeO-
0 -11.60 0.0 -11.60 0 0 0 -1 0 0 1 0 0 -1 0 0 1
FeOH2+
0 5.60 0.0 5.60 0 0 0 1 0 0 1 0 0 1 0 0 1
FeOH2-FeEDTA
0 36.60 -38.00 -1.40 2 0 0 4 1 0 2 0 0 4 1 0 2
FeOH2-CoEDTA
0 28.49 1.51 30.00 2 0 1 1 1 0 1 0 1 1 1 0 1
FeO-Co
0 -2.69 1.70 -0.99 2 0 1 -1 0 0 1 0 1 -1 0 0 1
FeOH2-CaEDTA
0 23.81 0.0 23.81 0 1 0 1 1 0 1 1 0 1 1 0 1
FeOH2-H2EDTA
0 30.48 1.52 32.00 2 0 0 3 1 0 1 0 0 3 1 0 1
***** DATA SET 28: kinetic reaction data
5
2 1 0 2.03 20.00
1 1 1
2 4 9
3 1 0 -38.0 -1.40
4 1 2 1
3 4 6 15
4 1 0 1.51 30.00
1 1 1 1 1
2 3 4 6 16
3 1 0 1.70 -0.99
1 -1 1 1
2 3 6 17
3 1 0 1.52 32.00
3 1 1 1
3 4 6 19

```

END OF JOB

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APPENDIX A

Data Input Guide for HYDROGEOCHEM

Data Input Guide for HYDROGEOCHEM

In this version, the unit of length should be decimeter (dm) and the unit of mass for any chemical species should be mole. The density of water and solid should be expressed in kg/dm³ (liter). The ion-exchange capacity is in equivalents/M of solid. The corresponding concentration unit of all species (aqueous, sorbed, and precipitated species) is mole/liter of fluid (Molar); the corresponding unit for the sorption distribution coefficient is dm³/kg (= ml/g). Any units of time may be used as long as the same unit is used throughout the input file.

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

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 chemical equilibrium computation to be printed:
1 = yes.
0 = no.
4. NHGCI = Integer indicating if chemical information is to be printed:
0 = no.
> 0 = print every NHGC 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-field format input contains 19 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 is wanted.
7. NMPPM = Number of material properties per material: must be 8 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 indicator:
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 = Is the pointwise iteration method to be used to solve the matrix equations:
0 = No.
1 = Yes.
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.

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

I1 = Largest integer not exceeding $\text{Log}(\text{DELMAX}/\text{DEL T})/\text{LOG}(1 + \text{CHNG})$.

I2 = Largest integer not exceeding $(\text{RTIME}-\text{DEL T}*((1 + \text{CHNG})^{**}(I1 + 1)-1)/\text{CHNG})/\text{DELMAX}$.

RTIME = Real simulation time.

DELMAX, DEL T, and CHNG are defined in Data Set 3.

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.
11. APC = Indicator for solution technique for kinetically controlled complexed species when IALT = 1 is chosen.
0 = use the operator splitting method,
1 = use the predictor-corrector method.
12. IALT = Indicator for solution technique for kinetically controlled complexed species:
0 = use direct iteration method. This option can be selected only when all kinetic reactions are "basic" kinetic reactions.
1 = use either the operator splitting or the predictor-corrector method, as specified by APC.

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)

```
-----
KPRO  KPR(1) KPR(2) -----KPR(NTI)
-----
1      2      3                               80
```

KPRO = Printer control for steady-state and initial conditions:
 0 = Print nothing.
 1 = Print FLOW, FRATE, and TFLOW.
 2 = Print above (1) plus concentration.
 3 = Print above (2) plus material flux.
 4 = Print above (3) plus detailed chemical equilibrium information.

KPR(I) = Printer control for the I-th time step, the same allowable values as for KPRO.

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

```
-----
KDSK0 KDSK(1) KDSK(2) --- KDSK(I) --- KDSK(NTI)
-----
1      2      3                               80
```

KDSK0 = Auxiliary storage control for steady-state and initial conditions:
 0 = No storage.
 1 = Store on Logical Unit 12.

KDSK(I) = Auxiliary storage control for the I-th time-step, the same allowable values as for KDSK0.

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

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: CHEMICAL PRINTOUT AND CHEMICAL PROPERTY 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 where detailed chemical 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 $1 \leq I \leq \text{NCPRT}$ 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. NODEP(NP) is an indicator to print detailed chemical information for the NP-th node. 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 described below are not needed if Logical Unit 11 is used as input (i.e., $KVI > 0$).

DATA SET 7: NODAL POINT COORDINATES

Typically, a total of $2 \times NNP$ lines are required: NNP lines for the x-coordinate and NNP lines for the z-coordinate. 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 $XAD \cdot (1 + XRD)$, the second increment is $XAD \cdot (1 + XRD)^2$, the third increment is $XAD \cdot (1 + XRD)^3$, and so on.

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

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

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 facility.

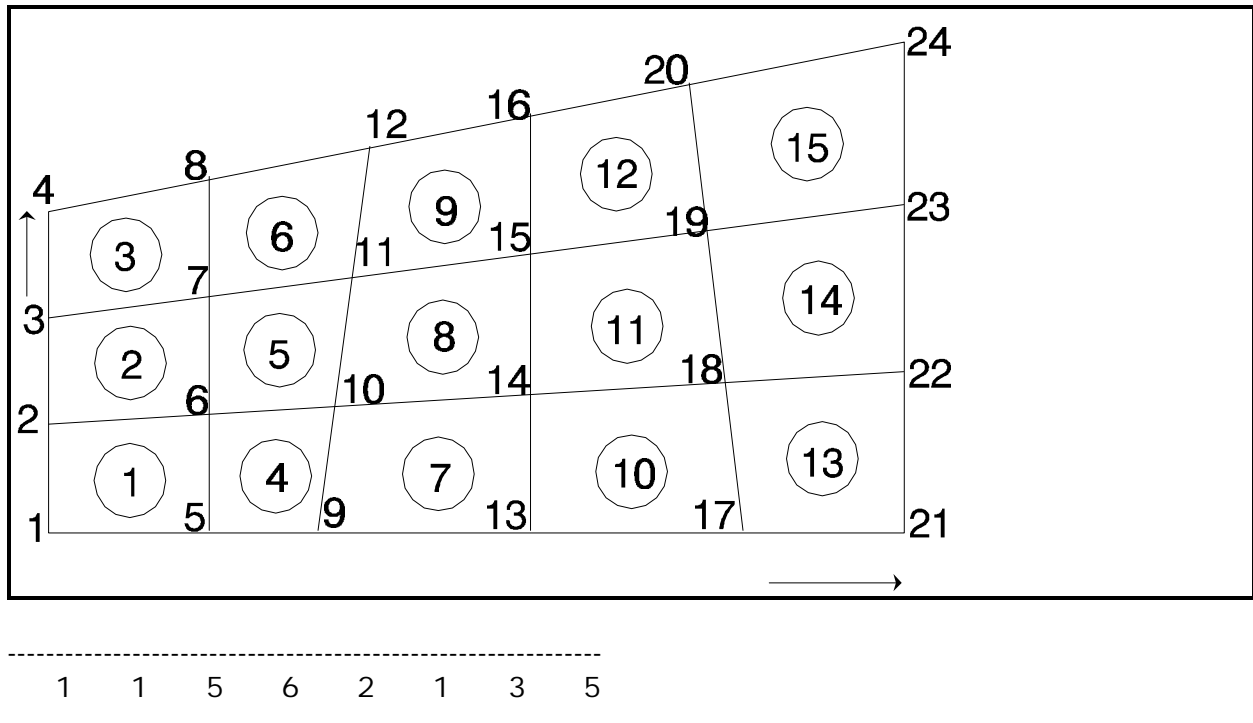


Fig. A.1

DATA SET 9: MATERIAL TYPE CORRECTION

This data set is required only if $NCM > 0$. Normally NCM lines are required. However, if the elements to be corrected 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 six integers.

1. NOHA = Number of mobile components
2. NOHS = Number of immobile components
3. NOKX = Number of kinetic complexed species
4. NOKY = Number of kinetic adsorbed species
5. NOKZ = Number of kinetic ion-exchanged species
6. NOKP = Number of kinetic precipitated 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. 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 and for the NOKX + NOKY + NOKZ + NOKP kinetic product species. (NOHA, NOHS, NOKX, NOKY, NOKZ, NOKP 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/liter).
5. RAD = Increment of initial or pre-initial total concentration for each of the NSEQ nodes (moles/liter).
6. RRD = Percent increase of the increment over its preceding increment (decimal fraction):
0 = All increments, XAD's, are the same.
> 0 = The first increment is $XAD \cdot (1 + XRD)$, the second increment is $XAD \cdot (1 + XRD)^2$, the third increment is $XAD \cdot (1 + XRD)^3$, 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 chemical component or species.

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.

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 $KSTR > \text{zero}$, 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 $NSTR = 0$.

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 $KSS > 0$, 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 ≥ 1 if $NDNP \geq 1$).
9. NDDP = Number of data points in each of the NDPR profiles (should be ≥ 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

(1) Element Source/Sink: Subdata sets (a) through (c) are needed if and only if $NSEL > 0$. When $NSEL > 0$, subdata sets (b) and (c) should be repeated ($NOHA + NOHS + 1 + NOKX$) times. ($NOHA$, $NOHS$ and $NOKX$ are specified in Data Set 10).

(a) 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.

(b) 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 $K = 1, NOH + 1 + NOKX$ (where $NOH = NOHA + NOHS$)

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:
 Value is concentration (moles/liter) if $K \leq NOH$,
 Value is flow rate of water (L^{**3}/T) if $K = (NOH + 1)$, and
 Value is concentration (moles/liter) if $(NOH + 1) < K \leq NOKX$.

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:
 Value is concentration (moles/liter) if $K \leq NOH$,
 Value is flow rate of water (L^{**3}/T) if $K = (NOH + 1)$, and
 Value is concentration (moles/liter) if $(NOH + 1) < K \leq NOKX$.

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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::
 Value is concentration (moles/liter) if $K \leq NOH$,
 Value is flow rate of water (L^{**3}/T) if $K = (NOH + 1)$, and
 Value is concentration (moles/liter) if $(NOH + 1) < K \leq NOKX$.

(c) 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.

(2) Point source/sink: Subdata sets (a) through (c) are needed if and only if $NWNP > 0$. When $NWNP > 0$, subdata sets (b) and (c) should be repeated for $(NOH + 1 + NOKX)$ times.

(a) 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.

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

For $K = 1, NOH + 1 + NOKX$ (where $NOH = NOHA + NOHS$)

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::
 Value is concentration (moles/liter) if $K \leq NOH$,
 Value is flow rate of water (L^{**3}/T) if $K = (NOH + 1)$, and
 Value is concentration (moles/liter) if $(NOH + 1) < K \leq NOKX$.

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:
 Value is concentration (moles/liter) if $K \leq NOH$,

Value is flow rate of water (L^3/T) if $K = (NOH + 1)$, and
Value is concentration (moles/liter) if $(NOH + 1) < K \leq NOKX$.

.

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::

Value is concentration (moles/liter) if $K \leq NOH$,

Value is flow rate of water (L^3/T) if $K = (NOH + 1)$, and

Value is concentration (moles/liter) if $(NOH + 1) < K \leq NOKX$.

- (c) 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) and for all kinetic aqueous complexed product species. ($INDTC$ 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 $NOH + NOKX$ times, once for each of the NOH chemical components and $NOKX$ kinetic complexed 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 ≤ 1).

(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) and for all kinetic aqueous complexed product species. ($INDTC$ is specified in Data Set 10).

Subdata sets (a) and (b) should be repeated $NOH + NOKX$ times, once for each of the NOH components and $NOKX$ kinetic complexed 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 ≤ 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/liter).
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/liter).
- ⋮
- 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/liter).

- (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 integers:

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 AND MOISTURE CONTENT

If KVI > 0, this data set is not needed because these will be read via Logical Unit 11.

- (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 is used to signal 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 node 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.

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 4 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. 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. This set reads information of NSORB adsorbing sites.

Record 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

Record 2 to Record NSORB + 1.

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

1. LNOA(I) = Location of the $\exp(-e*\psi_{io}/kt)$ 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 $\exp(-e*\psi_{ib}/kt)$ 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 mass),
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 mass),
.
.
.
- 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 mass),
.
.
.
- 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,
- 3NSORB. SREAM(NSORBI) = Surface area of the NSORB-th adsorbing site in material I, (L**2/M of solid mass).

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 solids) for the first site in material I.
2. CECM(2,I) = Ion-exchange capacity (equivalents per unit mass of solids) for the second site in material I.
- .
- J. CECM(J,I) = Ion-exchange capacity (equivalents per unit mass of solids) for the J-th site in material I,
- .
- NSITE. CECM(NSITE,I) = Ion-exchange capacity (equivalents per unit mass of solids) 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. EPSC = error tolerance for iteration.
3. NITERC = number of iterations allowed.
4. NPCYL = number of cycles allowed for iterating precipitation-dissolution. (Set NPCYL = 1 if precipitation-dissolution is not in the simulation).
5. CNSTRNX = a factor for the constraint on complexed species concentration. No complexed species concentration would yield a total component concentration greater than CNSTRN 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 CNSTRN times of the input total component concentration.

DATA SET 23: NAME OF CHEMICAL COMPONENTS AND TYPES OF 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 1 - free format.

2. 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

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

For each component species, either two lines or $(2 + 3 \cdot \text{IONEX})$ lines are needed, depending on whether the species participates in an ion-exchange reaction. 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, $(2 + 3 \cdot \text{IONEX})$ 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 specie is input (either 2 or $(2 + 3 \cdot \text{IONEX})$ lines), then the information for the next component specie. 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.
1 = Not implemented in this version.
2 = Not implemented in this version.
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 to be computed,
3 = species concentration is fixed.

2. PKIPD = Log10 of the selectivity of the II-th ion-exchanged species resulted from the I-th component species involving in the J -th ion exchange site reaction.

3. PBIPD = Log10 of the backward rate constant of the II-th ion-exchanged species resulted from the I-th component species involving in the ISITE-th ion-exchange site reaction.

4. PFIPD = Log10 of the forward rate constant of the II-th ion-exchanged species resulted from the I-th component species involving in the ISITE-th ion-exchange site reaction.

5. KI(IPD) = Kinetic indicator of the ion-exchanged species resulted from the I-th component species,
0 = equilibrium reaction
1 = kinetic reaction

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

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

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

$NON + 5$. $AXYZP(I, NON)$ = Stoichiometric coefficient of the NON -th component in the II-th ion exchange species for use in mass action, where $IPD = II - NON$.

$NON + 6$. $BXYZP(IPD,1)$ = Stoichiometric coefficient of the first component in the II-th ion exchange species for use in mole balance, where $IPD = II - NON$.

NON + 7. 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 + 8. 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 + 5. 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 concentration will be computed.

1 = Not implemented in this version.

2 = Not implemented in this version.

3 = Species concentration is fixed.

2. PKIPD = Log10 of the equilibrium constant of the I-th complexed species.

3. PBIPD = Log10 of the backward rate constant of the I-th complexed species in its elementary kinetic reaction

4. PFIPD = Log10 of the forward rate constant of the I-th complexed species in its elementary kinetic reaction

5. KI = Kinetic indicator of the I-th complexed species
0 = participates in an equilibrium reaction only
1 = participates in an elementary kinetic reaction
2 = participates in mixed kinetic reaction(s)

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

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

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

NON+ 6. 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+ 7. BXYZP(I,1) = Stoichiometric coefficient of the first component in the I-th complexed species, for use in mole balance equation.

NON+ 8. BXYZP(I,2) = Stoichiometric coefficient of the second component in the I-th complexed species, for use in mole balance equation.

NON+ 9. BXYZP(I,3) = Stoichiometric coefficient of the third component in the I-th complexed species, for use in mole balance equation.

2*NON+ 6. 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 species 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 to be computed,
3 = species concentration is fixed.

2. PKIPD = Log10 of the selectivity of the II-th ion-exchanged species resulted from the I-th complexed species involving in the J-th ion exchange site reaction.

3. PBIPD = Log10 of the backward rate constant of the II-th ion-exchanged species resulted from the I-th complexed species involving in the ISITE-th ion-exchange site reaction.

4. PFIPD = Log10 of the forward rate constant of the II-th ion-exchanged species resulted from the I-th complexed species involving in the ISITE-th ion-exchange site reaction.

5. KI(IPD) = Kinetic indicator of the ion exchanged species resulted from the I-th complexed species,
 0 = equilibrium reaction
 1 = kinetic reaction
6. 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.
7. 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.
8. 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+ 5. 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+ 6. 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+ 7. 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+ 8. 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+ 5. 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. PKIPD = Log10 of the equilibrium constant of the I-th adsorbed species.
3. PBIPD = Log10 of the backward rate constant of the I-th adsorbed species in its elementary kinetic reaction

4. PFIPD = Log10 of the forward rate constant of the I-th adsorbed species in its elementary kinetic reaction
5. KI(I)= Kinetic indicator of the I-th adsorbed species
 0 = participates in an equilibrium reaction only
 1 = participates in an elementary kinetic reaction
 2 = participates in mixed kinetic reaction(s)
6. XYZP(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.
7. XYZP(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.
8. XYZP(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+ 5. XYZP(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+ 6. 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+ 7. 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+ 8. 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+ 5. 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 $NOMP > 0$. 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 precipitated/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 constant of the I-th precipitated/dissolved species.
3. PBIPD = Log10 of the backward rate constant of the I-th precipitated species in its elementary kinetic reaction
4. PFIPD = Log10 of the forward rate constant of the I-th precipitated species in its elementary kinetic reaction
5. KI(I) = Kinetic indicator of the I-th precipitated species
0 = participates in an equilibrium reaction only
1 = participates in an elementary kinetic reaction
2 = participates in mixed kinetic reaction(s)
6. 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.
7. 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.
8. 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 + 5. 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 + 6. 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+ 7. 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+ 8. 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+ 5. 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 28: MIXED KINETIC REACTION DATA

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 three 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 = Kinetic reaction with no precipitate
1 = Kinetic reaction involving precipitation-dissolution

4. PBK = Log10 of the backward rate constant for this kinetic reaction.

5. PFK = Log10 of the forward rate constant for this kinetic reaction.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

	<u>Global Species Number:</u>
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)

Within the NONA, NONS, NOMX, NOMY and NOMP 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.

APPENDIX B

List of Symbols Used in Report

List of Symbols Used in Report

A = area of a triangular element, (L^2); or constant in Debye-Huckel equation.

A_1, A_2, A_3 = area of a triangular element, (L^2).

A_i, B_i = activity of the i -th aqueous species denoting either A_i or B_i ,
(dimensionless).

A_j, B_j = activity of the j -th ion-exchanged species denoting either exchanged A_j or B_j , (dimensionless).

A_i^x = activity of the i -th complexed species, (dimensionless).

a_j, z_j = molar concentration of the j -th ion exchanged species.

a_L = longitudinal diffusivity, (L),

a_m = molecular diffusion coefficient, (L^2/T),

a_T = transverse diffusivity, (L),

a_i = molar concentration of the i -th aqueous species denoting either c_j or x_i , (M/L^3).

\hat{a}_i, \hat{z}_i = chemical formula for the i -th aqueous species, (dimensionless).

\hat{a}_j, \hat{z}_j = chemical formula for the j -th ion-exchanged species,
(dimensionless).

a_{je}^a = stoichiometric coefficient of the electron in the j -th aqueous component species, (dimensionless).

a_{ie}^x = stoichiometric coefficient of the electron in the i -th complexed species, (dimensionless).

a_{je}^s = stoichiometric coefficient of the electron in the j -th adsorbent component species, (dimensionless).

a_{ie}^y = stoichiometric coefficient of the electron in the i-th adsorbed species, (dimensionless).

a_{ie}^z = stoichiometric coefficient of the electron in the i-th ion-exchanged species, (dimensionless).

a_{ie}^p = stoichiometric coefficient of the electron in the i-th precipitated species, (dimensionless).

a_{ij}^p, a_{ik}^p = stoichiometric coefficient of the j-th or k-th aqueous component in the i-th precipitated species, (dimensionless).

a_{ij}^x, a_{ik}^x = stoichiometric coefficient of the j-th or k-th aqueous component in the i-th complexed species, (dimensionless).

a_{ij}^y, a_{ik}^y = stoichiometric coefficient of the j-th or k-th aqueous component in the i-th adsorbed species, (dimensionless).

a_{ik}^z, a_{ik}^z = stoichiometric coefficient of the j-th or k-th aqueous component in the i-th ion-exchanged species, (dimensionless).

a_{ib}^y = stoichiometric coefficient of c_b in the i-th adsorbed species.

a_{io}^y = stoichiometric coefficient of c_o in the i-th adsorbed species.

B = a conversion factor from charge per unit area to moles per unit volume; or a constant in the Debye-Huckel equation.

B' = a constant in the Debye-Huckel equation.

B_i^y = activity of the i-th adsorbed species of surface complexation (dimensionless).

B_D, B_N, B_C, B_V = boundary segments for Dirichlet, Neumann, Cauchy, and Variable boundaries respectively.

B_e = the length of boundary segment e, (L).

$\{B\}$ = load vector from the boundary source.

$\{B_D^e\}, \{B_N^e\}, \{B_C^e\}, \{B_V^e\}$ = boundary element column vectors for Dirichlet, Neumann, Cauchy, and Variable boundaries respectively.

b_{ij}^y, b_{ik}^y = stoichiometric coefficient of the j-th or k-th adsorbent component in the i-th adsorbed species of surface complexation, (dimensionless).

C = the capacitance term in constant capacitance model.

C_e = concentration of operational electrons in the aqueous phase, (M/L³).

C_j^* = input concentration of the j-th aqueous component if Q is a source (injection), (M/L³); = C_j if Q is a sink (withdrawal), (M/L³).

C_j = total dissolved concentration of the j-th aqueous component, (M/L³).

C_i = the value of C at node i, (M/L³).

C_{in} = total dissolved concentration of incoming fluid through variable boundaries, (M/L³).

C_1 = capacitance of the region between the "o" plane and "b" plane, (Farady/L²).

C_2 = capacitance of the region between "b" plane and "d" plane, (Farady/L²).

C_{ci}^* = Lagrangian concentration at the i-th Cauchy boundary node, (M/L³).

C_{vi}^* = Lagrangian concentration at the i-th variable-boundary node, (M/L³).

$\{C^*\}$ = column vector representing the Lagrangian concentration at all nodes, (M/L³).

$C_j(t)$ = the value of concentration C_j at time t, (M/L³).

c_j, c_k = concentration of j-th or k-th aqueous component species, (M/L³).

\hat{c}_j = chemical formula for the j-th aqueous component species,
(dimensionless).

c_b, c_o = capacitance terms in electrostatic models (equations 3.3.33 -
3.3.53).

\mathbf{D} = dispersion coefficient tensor, (L^2/T).

$[D^e]$ = dispersion matrix.

$\left\{ \frac{DC}{DT} \right\}$ = column vector containing the value of $\left\{ \frac{DC}{DT} \right\}$ at all nodes.

$\left\{ \frac{d(S+P)}{dt} \right\}$ = column vector containing the value of $\frac{d(S+P)}{dt}$ at all nodes.

$\frac{d\theta}{dh}$ = specific water capacity, ($1/L$).

$[E]$ = growth matrix representing the effect of the rate of change of
moisture content.

e = electronic charge, ($1.6021892 \times 10^{-19}$ Coulomb/Electron).

$[F^e]$ = fluid source matrix.

$[G], [H]$ = matrices used in FDM approximation of time derivative (equations
3.2.23, 3.2.24, 3.2.42).

H = total head, (L).

h = pressure head, (L).

h_{jk}^a = stoichiometric coefficient of the k-th chemical element in the j-th
aqueous component species, (dimensionless).

h_{ik}^x = stoichiometric coefficient of the k-th chemical element in the i-th
complexed component species, (dimensionless).

h_{jk}^s = stoichiometric coefficient of the k-th chemical element in the j-th
adsorbent component species, (dimensionless).

h_{ik}^y = stoichiometric coefficient of the k-th chemical element in the i-th adsorbed species.

h_{ik}^z = stoichiometric coefficient of the k-th chemical element in the i-th ion-exchanged species, (dimensionless).

h_{ik}^p = stoichiometric coefficient of the k-th chemical element in the i-th precipitated component species, (dimensionless).

I = ionic strength.

J_j = $\theta c_j(\mathbf{V}_j - \mathbf{V}_f)$ is the surface flux of the j-th aqueous component species with respect to fluid velocity \mathbf{V}_f , [(M/T)/L²].

K = hydraulic conductivity tensor, (L/T); or an operator denoting $K(I) = \left(-\nabla \cdot \theta D \cdot \nabla + Q - \frac{\delta \theta}{\delta t} \right) (I)$.

K_{dj} = distribution coefficient of the j-th aqueous component, (L³/M).

K_i^x = equilibrium constant of the i-th complexed species,
(dimensionless).

K_i^y = equilibrium constant of the i-th adsorbed species, (dimensionless).

K_{ij} = selectivity coefficient of the i-th species with respect to the j-th species, or the effective equilibrium constant of i-th ion-exchanged species, (dimensionless).

K_i^p = equilibrium constant of the i-th precipitated species,
(dimensionless).

[K] = modified stiff matrix resulting from the action of dispersion, source of water, and the rate of change of moisture content.

k = Boltzman constant, (1.380662 x 10⁻²³ Joule/K); or an indexing variable.

k_i^{bx} = backward rate constant associated with the formation of the i-th

complexed species by its "elementary" kinetic reaction.

k_i^{fx} = forward rate constant associated with the formation of the i-th

complexed species by its "elementary" kinetic reaction.

k_i^{by} = backward rate constant associated with the formation of the i-th

adsorbed species by its "elementary" kinetic reaction.

k_i^{fy} = forward rate constant associated with the formation of the i-th

adsorbed species by its "elementary" kinetic reaction.

K_k^{bz} = backward rate constant associated with the formation of the k-th

ion-exchanged species by its "elementary" kinetic reaction.

K_k^{fz} = forward rate constant associated with the formation of the k-th

ion-exchanged species by its "elementary" kinetic reaction.

k_i^{bp} = backward rate constant associated with the formation of the i-th

precipitated species by its "elementary" kinetic reaction.

k_i^{fp} = forward rate constant associated with the formation of the i-th

precipitated species by its "elementary" kinetic reaction.

k_k^b = backward rate constant for the k-th "mixed" kinetic reaction.

k_k^f = forward rate constant for the k-th "mixed" kinetic reaction.

L_1, L_2, L_3 = three area coordinates of a triangular element, (L).

{L} = the load vector.

M_j^s = total rate of source/sink of the j-th adsorbent component,

(M/L³/T).

M_j^a = total rate of source/sink of the j-th aqueous component, (M/L³/T).

M_{eq} = total rate of source/sink of the ion-exchange site, $(M/L^3/T)$.

M_e^a = external source/sink rate of the free electron species, $[(M/L^3)/T]$.

M_a = the number of aqueous species, equal to the number of aqueous component species plus the number of complexed species.

M_e = the set of elements that have a local side α - β coinciding with the global side i - j , (dimensionless).

M_x = number of complexed species, (dimensionless).

M_y = number of adsorbed species, (dimensionless).

M_p = number of potentially precipitated species, (dimensionless).

M_z = number of ion-exchanged species, (dimensionless).

$[M]$ = mass matrix resulting from the storage term.

m = an indexing variable.

m_j^a = external source/sink rate of the j -th aqueous component species, $[(M/L^3)/T]$.

m_i^x = external source/sink rate of the i -th complexed species, $[(M/L^3)/T]$.

m_j^s = external source/sink rate of the j -th adsorbent component species, $(M/L^3)/T]$.

m_i^y = external source/sink rate of the i -th adsorbed species, $[(M/L^3)/T]$.

m_i^z = external source/sink rate of the i -th ion-exchanged species, $[(M/L^3)/T]$.

m_i^p = external source/sink rate of the i -th precipitated species, $[(M/L^3)/T]$.

NOMZJ(i) = number of ion exchanged species from the first site through the (i-1)th site.

NOMZI(i) = number of ion exchanged species in the i -th site.

N_a = number of aqueous component species, (dimensionless).

N_s = number of adsorbent component species, (dimensionless).

- N_{eq} = number of equivalents of the ion-exchange sites per liter of solution, (M/L³).
- N_{eqj} = value of N_{eq} at node j , (M/L³).
- $(N_{eqj})_t$ = value of N_{eqj} at time t , (M/L³).
- N_e = number of chemical elements considered in the system, (dimensionless).
- N_{eq0} = initial number of equivalents of the ion exchange site, (M/L³).
- N_j = the basis function of the spatial coordinate for the j -th node, (dimensionless).
- $N_j(x_i^*)$ = the interpolation function associated with node j , evaluated at the Lagrangian point x_i^* .
- N_α^e = the α -th local basis function of element e , (dimensionless).
- N_{se} = set of boundary segments having a local node α coinciding with global node i , (dimensionless).
- N_{ce} = number of Cauchy boundary segments, (dimensionless).
- N_{ne} = number of Neumann boundary segments, (dimensionless).
- N_{ve} = number of variable-boundary segments, (dimensionless).
- \mathbf{n} = an outward unit vector normal to the boundary, (L).
- n = number of nodes in the region, (dimensionless); or an indexing variable.
- NSITE = number of ion-exchange sites.
- NSORB = number of adsorbing sites.
- P_j = value of P at node j , (M/L³); or the total precipitated concentration of the j -th aqueous component, (M/L³).
- P_e = concentration of operational electrons in solid phase, (M/L³).
- {P} = column vector containing the value of P at all nodes.
- {P}_t = value of {P} at time t , (M/L³).

- $\{P\}_{t+\Delta t}$ = column vector representing the value of $\{P\}$ at time $(t + \Delta t)$,
(M/L³).
- p_i = concentration of the i -th precipitated species per unit fluid volume
(M/L³).
- \hat{p}_i = chemical formula for the i -th precipitated species, (dimensionless).
- Q = source or sink representing the artificial injection or withdrawal of water, [(L³/L³)/T].
- $\{Q\}$ = load vector from the internal source/sink.
- $\{Q^e\}$ = element column vector.
- q_{jN} = normal Neumann flux, (M/L²/T).
- q_{jC} = normal Cauchy flux, (M/L²/T).
- $\{q_N^e\}, \{q_C^e\}, \{q_V^e\}$ = boundary flux vector for Neumann, Cauchy or Variable boundaries respectively.
- R = universal constant, (8.314 Joule/Mole/K).
- R_e = the region of element e , (L²).
- R_{dj} = retardation factor of the j -th component, (dimensionless).
- r_j^a = production rate of the j -th aqueous component species per unit fluid volume due to all chemical reactions, [(M/L³)/T].
- r_i^x = production rate of i -th complexed species per unit fluid volume due to all chemical reactions, [(M/T)/L³].
- r_j^s = production rate of the j -th adsorbent component species per unit fluid volume due to all sorption reactions, [(M/L³)/T].
- r_i^y = production rate of the i -th adsorbed species per unit fluid volume due to all adsorption reactions, [(M/T)/L³].
- r_i^z = production rate of the i -th ion-exchanged species per unit fluid volume due to all ion-exchange reactions, [(M/T)/L³].
- r_i^p = production rate of the i -th precipitated species per unit fluid volume due to all precipitation reactions, [(M/T)/L³].
- S = total sorbed concentration.

- S_j = the value of S at node j, (M/L³); or the total sorbed concentration of the j-th aqueous component, (M/L³).
- S_e = concentration of operational electrons in sorbent phase, (M/L³).
- {S} = column vector containing the value of S at all nodes, (M/L³).
- {S}_t = value of {S} at time t, (M/L³).
- {S}_{t+Δt} = column vector representing the value of {S} at time (t + Δt), (M/L³).
- s_j = concentration of the j-th adsorbent component species, (M/L³).
- \hat{S}_j = chemical formula for j-th adsorbent component species, (dimensionless).
- s_T = total concentration of all ion-exchanged species, (M/L³).
- T = total analytical concentration of any component, (M/L³); or absolute temperature, (°K).
- T_i = the value of T (total analytical concentration) at node i, (M/L³).
- T_j = total analytical concentration of the j-th aqueous component, (M/L³).
- T_e = total concentration of operational electrons, (M/L³).
- T_{j0} = initial total analytical concentration of j-th aqueous component, (M/L³).
- T_{jD} = prescribed Dirichlet total analytical concentration, (M/L³).
- {T} = column vector containing the value of T (total analytical concentration) at all nodes, (M/L³).
- {T}_{t+Δt} = column vector representing the value of {T} at time (t + Δt), (M/L³).
- {T^{k+1}} = new estimate of {T} during the nonlinear iteration, (M/L³).
- {T^k} = previous estimate of {T} during the nonlinear iteration, (M/L³).

t = time, (T).

\mathbf{V} = Darcy's velocity, (L/T).

$|\mathbf{V}|$ = the magnitude of the Darcy velocity \mathbf{V} , (L/T).

$[V_c^e], [V_v^e]$ = boundary matrix for Cauchy or Variable boundaries respectively.

\mathbf{V}_{fs} = fluid velocity relative to the solid, (1/L).

\mathbf{V}_s = solid velocity, (1/L).

v_{jk}^a = valence of the k-th chemical element in the j-th aqueous component species, (dimensionless).

v_{ik}^x = valence of the k-th chemical element in the i-th complexed species, (dimensionless).

v_{jk}^s = valence of the k-th chemical element in the j-th adsorbent component species, (dimensionless).

v_{ik}^y = valence of the k-th chemical element in the i-th adsorbed species, (dimensionless).

v_{ik}^z = valence of the k-th chemical element in the i-th ion-exchanged species, (dimensionless).

v_{ik}^p = valence of the k-th chemical element in the i-th precipitated species, (dimensionless).

v_{mk} = valence of the k-th chemical element in its maximum oxidation state, except for oxygen in which $v_{ik} = -2$, (dimensionless).

W_j = total analytical concentration of the j-th adsorbent component, (M/L³).

W_{j0} = Initial total analytical concentration of j-th adsorbent component, (M/L³).

w = time weighting factor.

X_k = activity of the k-th aqueous component species, (dimensionless).

- x_i = concentration of the i-th complexed species, (M/L³).
- x_i^* = location of a fictitious particle that would arrive at node i at time (n+ 1), (L), also called the Lagrangian point.
- \hat{x}_i = chemical formula for the i-th complexed species., (dimensionless).
- Y = residues.
- Y_k = activity of the k-th adsorbent component species, (dimensionless).
- y_i = concentration of the i-th adsorbed species, (M/L³).
- \hat{y}_i = chemical formula for i-th adsorbed species i, (dimensionless).
- Z = Jacobian of Y with respect to X.
- z = potential head, (L); or the valence of the ion.
- z_i = molar concentration of the i-th ion-exchanged species, (M/L³); or charge of the i-th aqueous species.
- α_i^p = modified stability constant for the i-th precipitated species.
- α_i^x = modified stability constant for the i-th complexed species.
- α_i^y = modified stability constant for the i-th adsorbed species.
- Γ = surface enclosing the material volume v, (L²).
- γ_i = activity coefficient of the i-th aqueous species denoting either γ_i^a or γ_i^x , (L³/M).
- γ_j = activity coefficient of the J-th ion exchanged species (L³/M).
- γ_i^x = activity coefficient of the i-th complexed species, (L³/M.).
- γ_j^a, γ_k^a = activity coefficient of the j-th or k-th aqueous component species, (L³/M).

- γ_i^y = activity coefficient of the i-th adsorbed species, (L³/M).
- γ_j^s = activity coefficient of the j-th adsorbent component species,
(L³/M).
- γ_i^p = activity coefficient of the i-th precipitated species, (L³/M).
- Δt = time-step size, (T).
- $\Delta \tau$ = time interval.
- $\delta \tau$ = time-step size, along the characteristic line, (T).
- δ = Kronecker delta tensor, (dimensionless).
- ϵ = relative dielectric constant, (= 78.84, dimensionless).
- ϵ_o = permittivity of the free space, (8.85 x 10⁻¹³ Coulomb²/Joule/dm).
- η = local coordinate of a hexahedral element, (dimensionless).
- η_α = coordinate of the corner node of a hexahedral element,
(dimensionless).
- θ = moisture content, (L³/L³).
- I_j^a = rate of decay of the j-th aqueous component species, [(M/L³)/T].
- I_i^x = rate of decay of the i-th complexed species, [(M/L³)/T].
- I_j^s = rate of decay of the j-th adsorbent component species, [(M/L³)/T].
- I_i^y = rate of decay of the i-th adsorbed species, [(M/L³)/T].
- I_i^z = rate of decay of the i-th ion-exchanged species, [(M/L³)/T].
- I_i^p = rate of decay of the i-th precipitated species, [(M/L³)/T].
- I_e^a = rate of decay of the free electron species, [(M/L³)/T].

i_j = modified selectivity coefficient of the i-th ion-exchanged species with respect to the J-th ion-exchanged species.

λ_j^a = total decay rate of the j-th aqueous component, (M/L³/T).

λ_j^s = total decay rate of the j-th adsorbent component, (M/L³/T).

λ_{eq} = total decay rate of the ion-exchange site, (M/L³/T).

Λ_e^a = total rate of decay of the operational electron, [(M/L³)/T].

λ_j^a = rate constant of the j-th aqueous component, (1/T).

λ_j^s = rate constant of the j-th adsorbent component, (1/T).

λ_{eq} = decay rate constant of the ion-exchange site, (1/T).

v = material volume containing constant amount of media, (L³).

v_i = charge of the i-th aqueous species, (dimensionless).

v_j = charge of the J-th ion-exchanged species, (dimensionless).

η = local coordinate of a hexahedral element, (dimensionless).

α = corner node of the local coordinate of a hexahedral element, (dimensionless).

b = bulk density of the medium, (M/L³).

b = charge density in moles per unit volume on the "b" plane, (Coulomb/L²).

d = charge density in moles per unit volume on the diffuse layer, (Coulomb/L²).

o = charge density in moles per unit volume on the "o" plane, (Coulomb/L²).

τ = tortuosity, (dimensionless).

b = electric potential at the surface "b", (Volt = Joules/Coulomb).

d = electric potential at the surface "d", (Volt = Joules/Coulomb).

ϕ_0 = electric potential at the surface "o", (Volt = Joules/Coulomb).

n = iteration parameter, (dimensionless).

Indices

Subscripts

J - species sorbed by ion exchange.

i - aqueous species.

j, k - used for components in reactions and equilibrium constants.

Superscripts

x - denotes complexed species.

y - denotes adsorbed species.

z - denotes ion exchanged species.

p - denotes precipitated species.

APPENDIX C

List of HYDROGEOCHEM Code Parameters

List of HYDROGEOCHEM Code Parameters

The first column of the following list, alphabetically names each parameter used in the data entry sets. The second column shows where the parameter is specified: the data set number, the group or line number when applicable, and the item number. The third column lists those data sets which will be affected by the parameter in the first column. For example, the entry:

IMID	DS 2, #10	DS 3, #5
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shows that parameter IMID is specified in data set 2, item #10, and that data set 3, item #5 is dependent. The dependency arises because, if IMID is specified as equal to "1", then W, which is specified by data set 3, item #5, should also equal "1".

<u>Parameter</u>	<u>Data set, number</u>	<u>Dependent data sets</u>
APC	DS 3,#11	
APHAG	DS 3, #10	
AXYZP(I,NON)	DS 24, Line 5, #(NON+2)	
"	DS 25, Line 2 &5, #(NON+2)	
AXYZP(II,NON)	DS 26, Line 2, #(NON+2)	
"	DS 27, Line 2, #(NON+2)	
BXYZP(I,NON)	DS 24, Line 5, #(2*NON+2)	
"	DS25, Line 2 &5,	
BXYZP(II,NON)	#(2*NON+2)	
"	DS 26, Line 2, #(NON+3)	
	DS27, Line 2, #(NON+3)	
CAP1M(J,I)		
CAP2M(J,I)	DS 20, Record NSORB+2,	
	#(3J-2)	
	DS 20, Record NSORB+2,	
	#(3J-1)	
CDBF(J,I,K)	DS 15, Group a	
CECM(J,I)	DS 21, Record NSITE+2,#(1- NSITE)	
CHNG	DS 3, #2	DS 2, #5
CNAM(I)	DS 10, Lines 2..I+1, #1	
"	DS 23, #1	
CNSTRNX	DS 22, #5	
CNSTRNY	DS 22, #6	
CVBF(J,I,K)	DS 14, Group a	
CXYZP(I,J)	DS 28, Line 2, #(1-NRTS)	
DELMAX	DS 3, #3	DS 2, #5
DELT	DS 3, #1	DS 2, #5
DXYZP(I,J)	DS 28, Line 2, #(NRTS+1)	
ESPC	DS22, #2	
I1		DS 2, #5
I2		DS 2, #5
IADS	DS 20, Record 1, #2	
IALT	DS 3, #12	

<u>Parameter</u>	<u>Data set, number</u>	<u>Dependent data sets</u>
ICOND	DS 1,Line 2, #3	
ICOR	DS 18, #2	
IDNTC(I,1)	DS 10, Lines 2..I+1, #2	
IE(MI,1)	DS 8, #2	
IE(MI,2)	DS 8, #3	
IE(MI,3)	DS 8, #4	
IE(MI,4)	DS 8, #5	
IE(MI,5)	DS 8, #6	
IGEOM	DS 1, Line 2, #5	
IGSNPD	DS 28, Line 3, #(NRTS+1)	
IGSNRT	DS 28, Line 3, #(1-NRTS)	
IITR	DS 1, Line 2, #1	
ILUMP	DS 2, #9	
IMID	DS 2, #10	DS 3, #5
INDTC(I,1)	DS 10, Lines 2..I+1, #3	DS 11
"	DS 23, #2	
INTER	DS 1, Line2, #2	
IONEX	DS 24, Line 2, #3	DS 24, Lines 3,4, & 5,
"	DS 25, Line 2, #(NON+3)	DS 24, Lines 3,4, & 5
IOPTIM	DS 2, #12	DS3, #10
IPNTS	DS 2, #16	
IQUAD	DS 2, #20	
IS1	DS 14, Group d, #4	
IS1AD	DS 14, Group d, #8	
IS2	DS 14, Group d, #5	
IS2AD	DS 14, Group d, #9	
ISCN(I)	DS 24, Line 1, #2	
ISCN(II)	DS 24, Line 5, #1	
"	DS 25, Lines 2 & 5, #1	
"	DS 26, Line 2, #1	
"	DS 27, Line 2, #1	
IWET	DS 2, #11	
IWRK(N)	DS 5, Line 2, #N	
KDSK0	DS 4	
KDSK(I)	DS 4	
KI	DS 24, Line 5, #5	
"	DS 25, Line 2, #5	
"	DS 25, Line 5, #5	
"	DS 26, Line 2, #5	
"	DS 27, Line 2, #5	
KPRO	DS 4	
KPR(I)	DS 4	
KRTYP	DS 28, Line 2, #3	
KSS	DS 2, #6	DS 11
KSTR	DS 2, #17	DS 11
KVI	DS 2, #8	DS 7
"		DS 8
"		DS 11
"		DS 16

<u>Parameter</u>	<u>Data set, number</u>	<u>Dependent data sets</u>
LES(N)	DS 13, Group 1a, #1..N	
LGRN	DS 2, #19	
LNBA(I)	DS 20, Record 2..NSORB+1, #2	
LNE	DS 18, #4	
LNH	DS 18, #3	
LNI(I)	DS 21, Record 2..NSITE+1, #2	
LNOA(I)	DS 20, Record 2..NSORB+1, #1	
M	DS 14, Group d, #3	
MAD	DS 9, #3	
"	DS 13, Group 1c, #3	
"	DS 14, Group d, #7	
MI	DS 8, #1,	
"	DS 9, #1	
"	DS 13, Group 1c, #1	
"	DS 14 Groups b & d, #1	
MIAD	DS 14, Group b, #3, Group d, #6	
MITYP	DS 9, #4	DS 8
"	DS 13, Group 1c, #4	
"	DS 14, Group b, #4	
MODL	DS 8, #7	
MTYPAD	DS 9, #5	
"	DS 13, Group 1c, #5	
"	DS 14, Group b, #5	
NAD	DS 7, #3	
"	DS 11, #3	
"	DS 15, Group b, #3	
"	DS 16, Groups a & b, #3	
NCM	DS 2, #4	DS 9
NCPRT	DS 5, Line 1, #1	DS 5, Grp 1, Ln 2
NDDP	DS 12, #9	DS 15, Grp a
NDNP	DS 12, #7	DS 15
NDPR	DS 12, #8	DS 15, Grp a
NDTCHG	DS 2, #14	DS 4
NEL	DS 2, #2	DS 8, #7
"		DS 16, Grp b, #2
NHGCI	DS 1, Line 2,#4	
NI	DS 7, #1	
"	DS 11, #1	
"	DS 13, Group 2c, #1	
"	DS 14, Group c #1	
"	DS 15, Groups b & c, #1	
"	DS 16, Groups a & b, #1	
NIAD	DS 13, Group 2c, #3	
"	DS 14, Group c, #3	
"	DS 15, Group c, #3	
NITER	DS 2, #13	

<u>Parameter</u>	<u>Data set, number</u>	<u>Dependent data sets</u>
NITERC	DS 22, #3	
NITYP	DS 13, Group 2c, #4	
"	DS 15, Group b, #4	
NITYPA	DS 13, Group 2c, #5	
NLAY	DS 8, #8	
NLINE		DS 4
NMAT	DS 2, #3	DS 6
NMPPM	DS 2, #7	
NNP	DS 2, #1	DS 5, Grp 2
"		DS 7
"		DS 11
"		DS 15, #4
"		DS 16, Grp a, #2
NODE	DS 14, Group c, #4	
"	DS 15 Group c, #4	
NODEAD	DS 14, Group c, #5	
"	DS 15, Group c, #5	
NODEP(NP)		DS 5
NOHA	DS 10, Line 1, #1	
NOHS	DS 10, Line 1, #2	
NOKX	DS 10, Line 1, #3	
NOKY	DS 10, Line 1, #4	
NOKZ	DS 10, Line 1, #5	
NOKP	DS 10, Line 1, #6	
NOMP	DS 17, #6	
NOMX	DS 17, #3	
NOMY	DS 17, #4	
NOMZ	DS 17, #5	
NOMZI(I)	DS 21, Record 2..NSITE+1, #1	
NONA	DS 17, #1	
NONS	DS 17, #2	
NPCYL	DS 22, #4	
NPDS	DS 28, Line 2, #2	
NPITER	DS 2, #15	
NPROB	DS 1, #1	
NPW(N)	DS 13, Group 2a, #N	
NRTS	DS 28, Line 2, #1	
NRXN	DS 28, Line 1, #1	
NSDP	DS 12, #3	DS 13, Grp 1b
NSEL	DS 12, #1	DS 13, Grps 1a, 1b & 1c

<u>Parameter</u>	<u>Data set, number</u>	<u>Dependent data sets</u>
NSEQ		
"	DS 7, #2	
"	DS 9, #2	
"	DS 11, #2	
"	DS 13, Group 1c, #2	
"	DS 13, Group 2c, #2	
"	DS 14, Groups b, c & d, #2	
"	DS 15, Groups b & c, #2	
"	DS 16, Groups a & b, #2	
NSITE		
NSORB	DS 21, Record 1, #1	
	DS 20, Line 1, #1	
NSPR	DS 12, #2	DS 13, Grp 1b
NSTR	DS 2, #18	DS 11
NTI	DS 2, #5	DS 4
"		DS 11
NTYPAD	DS 15, Group b, #5	
NVDP	DS 12, #13	DS 14, Grp 1a
NVES	DS 12, #11	DS 14, Grp d
NVNP	DS 12, #10	DS 14, Grp c
NVPR	DS 12, #12	DS 14, Grp a
NWDP	DS 12, #6	DS 13, Grp 2b
NWNP	DS 12, #4	DS 13, Grps 2a, 2b & 2c
NWPR	DS 12, #5	DS 13, Grp 2b
OME	DS 3, #7	
OMEGAC	DS 22, #1	
OMI	DS 3, #8	
PBIPD	DS 24, Line 5, #3	
"	DS 25, Line 2, #3	
"	DS 25, Line 5, #3	
"	DS 26, Line 2, #3	
"	DS 27, Line 2, #3	
PBK	DS 28, Line 2, #4	
PEMN	DS 19, Line 2, #1	
PEMX	DS 19, Line 2, #2	
PHMN	DS 19, Line 2, #3	
PHMX	DS 19, Line 2, #4	
PFIPD	DS 24, Line 5, #4	
"	DS 25, Line 2, #4	
"	DS 25, Line 5, #4	
"	DS 26, Line 2, #4	
"	DS 27, Line 2, #4	
PFK	DS 28, Line 2, #5	
PKIPD	DS 24, Line 5, #2	
"	DS 25, Lines 2 & 5, #2	
"	DS 26, Line 2, #2	
"	DS 27, Line 2, #2	
PRESU	DS 19, Line 1, #2	
PROP(N,I)	DS 6, Lines 1..I, #N	

<u>Parameter</u>	<u>Data set, number</u>	<u>Dependent data sets</u>
RAD	DS 11, #5	
RNI	DS 11, #4	
RTIME		DS 2, #5
SICOR	DS 18, #1	
SOSF(J,I,K)	DS 13, Group 1b	
SPECN(I)	DS 24, Line 1, #1	
SPECN(II)	DS 24, Line 4, #1	
"	DS 25, Lines 1 & 4, #1	
"	DS 26, Line 1, #1	
"	DS 27, Line 1, #1	
SREAM(J,I)	DS 20, Record NSORB+2, #3J	
TCDBF(J,I,K)	DS 15, Group a	
TCVBF(J,I,K)	DS 14, Group a	
TDTCH(N)	DS 4, #N	
TEMP	DS 19, Line 1, #1	
THNI	DS 16, Group b, #4	
THNIAD	DS 16, Group b, #5	
TITLE	DS 1, #2	
TMAX	DS 3, #4	
TOLA	DS 3, #9	
TSOSF(J,I,K)	DS 13, Group 1b	
TWSSF(J,I,K)	DS 13, Group 2b	
VJ(I)	DS 24, Line 2, #2	
VXAD	DS 16, Group a, #6	
VXNI	DS 16, Group a, #4	
VZAD	DS 16, Group a, #7	
VZNI	DS 16, Group a, #5	
W	DS 3, #5	
WSSF(J,I,K)	DS 13, Group 2b	
WV	DS 3, #6	
XAD	DS 7, #5	
XNI	DS 7, #4	
XRD	DS 7, #6	

