Table 6.8 Input Data Sets for Problem 6, Case A, buffered pH

```
   1  BENCHMARK PROBLEM - CASE A - BUFFERED PH (IOPTRS=1)
 1 0 0 0 1
C ******* DATA SET 2: BASIC INTEGER PARAMTERS
 202 100 1 0 750   1 4 -1 1 0   0 0 40 1 50   0 1 0 1 11   2 1 1
C ******* DATA SET 3: BASIC REAL PARAMETERS
 0.1 0.0D0 0.1 75 0.0D0   1.0D0 1.0D0 1.0D00 1.0D-6 1.0D0
C ******* DATA SET 4: PRINT AND AUXILIARY STORGE CONTROL
40000000000000000000000000000000000000000000000000000000000000000000000000000000
40000000000000000000000000000000000000000000000000000000000000000000000000000000
40000000000000000000000000000000000000000000000000000000000000000000000000000000
40000000000000000000000000000000000000000000000000000000000000000000000000000000
40000000000000000000000000000000000000000000000000000000000000000000000000000000
40000000000000000000000000000000000000000000000000000000000000000000000000000000
40000000000000000000000000000000000000000000000000000000000000000000000000000000
40000000000000000000000000000000000000000000000000000000000000000000000000000000
40000000000000000000000000000000000000000000000000000000000000000000000000000000
4000000000000000000000000000004
10000000001000000000100000000010000000001000000000100000000010000000001000000000
10000000001000000000100000000010000000001000000000100000000010000000001000000000
10000000001000000000100000000010000000001000000000100000000010000000001000000000
10000000001000000000100000000010000000001000000000100000000010000000001000000000
10000000001000000000100000000010000000001000000000100000000010000000001000000000
10000000001000000000100000000010000000001000000000100000000010000000001000000000
10000000001000000000100000000010000000001000000000100000000010000000001000000000
10000000001000000000100000000010000000001000000000100000000010000000001000000000
10000000001000000000100000000010000000001000000000100000000010000000001000000000
1000000000100000000010000000001
1.0D38
C ******* DATA SET 5: CHEMICAL OUTPUT AND CHEMICAL PORPERTY TYPE INDICATOR
 2
 1  201 NODEP

C ******* DATA SET 6: MATERIAL PROPERTIES
 0.5D-0 0.0D0 0.0D0 1.5D0 AL AT AM RHOB
C ******* DATA SET 7: NODE COORDINATES
    1   100    2      0.0D0   1.0D0  0.0
    2   100    2      0.0D0   1.0D0  0.0D0
    0    0     0      0.0     0.0    0.0           END OF X-COORD
    1   100    2      0.0D0   0.0D0  0.0D0
    2   100    2      1.0D0   0.0D0  0.0
    0    0     0      0.0D0   0.0D0  0.0D0         END OF Z-COORD
C ******* DATA SET 8: ELEMENT CONNECTIVITY
    1    1    3    4    2    1    1   100          IE
C ******* DATA SET 10: CHEMICAL COMPONENT INFORMATION
 7 0 0 2 0 0 0 1   NOhA NOhS NOKX KY KZ KP mb ma
    H+
  1   1
 H2CO3*
  2   1
 NH4+
  3   1
 O2
  4   1
```

Table 6.8 Input Data Sets for Problem 6, Case A, (continued)

```
 NTA3-
  5   1
 Co 2+
  6   1
 Buffer
  7   1
C ******* DATA SET 11:  INITIAL CONDITIONS (MASS/MEDIA VOLUME)
    1   201   1    2.0034d-4 0.0D0     0.0D0

    0    0    0    0.0        0.0        0.0          END OF I.C. H+ - variable PH
    1   201   1    1.96d-7   0.0D0     0.0D0

    0    0    0    0.0        0.0        0.0          END OF I.C. H2CO3(g)
    1   201   1    0.00d-14  0.0D0     0.0D0

    0    0    0    0.0        0.0        0.0          END OF I.C. NH4+
    1   201   1    1.25d-5   0.0D0     0.0D0

    0    0    0    0.0        0.0        0.0          END OF I.C. O2
    1   201   1    0.00d-14  0.0D0     0.0D0

    0    0    0    0.0        0.0        0.0          END OF I.C. NTA3-
    1   201   1    0.00d-14  0.0D0     0.0D0

    0    0    0    0.0        0.0        0.0          END OF I.C. Co2+
    1   201   1    4.00d-4   0.0D0     0.0D0

    0    0    0    0.0        0.0        0.0          END OF I.C. Buffer
    1   201   1    0.00d-20  0.0D0     0.0D0

    0    0    0    0.0        0.0        0.0          END OF I.C. CoNTA(ads) = Ky1
    1   201   1    0.00d-20  0.0D0     0.0D0

    0    0    0    0.0        0.0        0.0          END OF I.C. Co(ads) = Ky2
    1   201   1    5.44d-5   0.0D0     0.0D0

    0    0    0    0.0        0.0        0.0          END OF I.C. Cells
C ******* DATA SET 12: CONTROL INTEGERS FOR TRANSIENT SOURCE/SINK AND B.C.
    0  0  0    0  0  0    0  0  0    4    2    2    4
C ******* DATA SET 14: VARIABLE BOUNDARY CONDITIONS (MASS/LIQUID VOLUME)
  0.0D0   5.01275D-4  20.0D0   5.01275D-4  20.01D0  5.0085D-4  75.0D0  5.0085D-4
  0.0D0   0.00D0      20.0D0   0.00D0      20.01D0  0.00D0     75.0D0  0.00D0
    1    1    1    1    1
    0    0    0    0    0                          END OF B.C. H+
  0.0D0   4.90D-7  20.0D0   4.90D-7  20.01D0  4.90D-7  75.0D0  4.90D-7
  0.0D0   0.00D0   20.0D0   0.00D0   20.01D0  0.00D0   75.0D0  0.00D0
    1    1    1    1    1
    0    0    0    0    0                          END OF B.C. H2CO3(g)
  0.0D0   0.00D0    20.0D0   0.00D0    20.01D0  0.00D0    75.0D0  0.00D0
  0.0D0   0.00D0    20.0D0   0.00D0    20.01D0  0.00D0    75.0D0  0.00D0
    1    1    1    1    1
    0    0    0    0    0                          END OF B.C. NH4+
```

Table 6.8 Input Data Sets for Problem 6, Case A, (continued)

```
  0.0D0   3.125D-5  20.0D0  3.125D-5  20.01D0  3.125D-5 75.0D0  3.125D-5
  0.0D0   0.00D0    20.0D0   0.00D0   20.01D0  0.00D0   75.0D0  0.00D0
    1    1    1    1    1
    0    0    0    0    0                          END OF B.C. O2
  0.0D0   5.23D-6  20.0D0   5.23D-6  20.01D0  0.00D0   75.0D0  0.00D0
  0.0D0   0.00D0   20.0D0   0.00D0   20.01D0  0.00D0   75.0D0  0.00D0
    1    1    1    1    1
    0    0    0    0    0                          END OF B.C. NTA3-
  0.0D0   5.23D-6  20.0D0   5.23D-6  20.01D0  0.00D0   75.0D0  0.00D0
  0.0D0   0.00D0   20.0D0   0.00D0   20.01D0  0.00D0   75.0D0  0.00D0
    1    1    1    1    1
    0    0    0    0    0                          END OF B.C. Co2+
  0.0D0   1.00D-3  20.0D0   1.00D-3  20.01D0  1.00D-3  75.0D0  1.00D-3
  0.0D0   0.00D0   20.0D0   0.00D0   20.01D0  0.00D0   75.0D0  0.00D0
    1    1    1    1    1
    0    0    0    0    0                          END OF B.C. Buffer
    1    1    1    1    1
    3    1    1    201  1
    0    0    0    0    0                          END NPVB
    1    1    1    1    2    1    99   2    2
    0    0    0    0    0    0    0    0    0       END OF ISV
C ******* DATA SET 16: HYDROLOGICAL VARIABLES
    1   201   1     4.0    0.0    0.0    0.0
    0    0    0     0.0    0.0    0.0    0.0       END OF VELOCITY
    1   99    1     0.4    0.0
    0    0    0     0.0    0.0    0.0              END OF TH
    1   201   1     1.0    0.0    0.0
    0    0    0     0.0    0.0    0.0              END OF RHOL
C ******* DATA SET 17: NUMBER OF COMPONENTS AND PRODUCT SPECIES
7 0 14 2 0 0                        NONA NONS NOMX NOMY NOMZ NOMP
C ******* DATA SET 18: H+, E-, IONIC STRENGTH correction INFORMATION
 0.0 0 1 0 0   SICOR ICOR LNH LNG LNE

c ******* DATA SET 19:  temperature, pressure and expected pe and pH
 298.3 1.0   TEMP PRESSU
 -20.0 20.0 -20.0 20.0   PEMN PEMX PHMN PHMX

c ******* DATA SET 22: Basic real and integer parameters
  1.0 1 1000 1.0d-6 1.0d00 1.0d00 omegac npcyl niterc epsc cnstrx cnstry

c ******* DATA SET 23: Component name and component species types
 H+
  1 0
 H2CO3*
  1 0
 NH4+
  1 0
 O2
  1 0
 NTA-
  1 0
 Co 2+
  1 0
 Buffer
  1 0
```

Table 6.8 Input Data Sets for Problem 6, Case A, (continued)

```
C ******* DATA SET 24: COMPONENT SPECIES AND THEIR ION-EXCHANGE INDEX
H+
  0  1 0  iscn VJ IONEX
H2CO3*
  0  0 0  iscn VJ IONEX
NH4+
  0  1 0  iscn VJ IONEX
O2
  0  0 0  iscn VJ IONEX
NTA3-
  0 -3 0  iscn VJ IONEX
Co2+
  0  2 0  iscn VJ IONEX
Buffer
  0 -1 0  iscn VJ IONEX
C ******** DATA SET 25:  COMPLEXED SPECIES
H3NTA
0    3  0  0  0  1  0  0   0   3  0  0  0  1  0  0
H2NTA-
0    2  0  0  0  1  0  0   0   2  0  0  0  1  0  0
HNTA2-
0    1  0  0  0  1  0  0   0   1  0  0  0  1  0  0
CoNTA-
0    0  0  0  0  1  1  0   0   0  0  0  0  1  1  0
CoNTA2 4-
0    0  0  0  0  2  1  0   0   0  0  0  0  2  1  0
CoOHNTA 2-
0   -1  0  0  0  1  1  0   0  -1  0  0  0  1  1  0
CoOH+
0   -1  0  0  0  0  1  0   0  -1  0  0  0  0  1  0
Co(OH)2
0   -2  0  0  0  0  1  0   0  -2  0  0  0  0  1  0
Co(OH)3-
0   -3  0  0  0  0  1  0   0  -3  0  0  0  0  1  0
HCO3-
0   -1  1  0  0  0  0  0   0  -1  1  0  0  0  0  0
CO3 2-
0   -2  1  0  0  0  0  0   0  -2  1  0  0  0  0  0
NH3
0   -1  0  1  0  0  0  0   0  -1  0  1  0  0  0  0
OH-
0   -1  0  0  0  0  0  0   0  -1  0  0  0  0  0  0
HBuffer
0    1  0  0  0  0  0  1   0   1  0  0  0  0  0  1
C ******** DATA SET 26:  ADSORBED SPECIES
CoNTA(ads)
0    0  0  0  0  1  1  0       0  0  0  0  1  1  0
Co(ads)
0    0  0  0  0  0  1  0       0  0  0  0  0  1  0
C ******** DATA SET 28:  MICROBIAL SPECIES
C5H7O2N(cells)
  0  -2.681936665037 0
```

Table 6.8 Input Data Sets for Problem 6, Case A, (continued)

```
C ******** DATA SET 29:  reaction data
17

2 1 0    NRTS NPDS KRTYP            REACTION 1 - H3NTA
14.9     LOGKEQ
3  1  1
1  5  8
2 1 0    NRTS NPDS KRTYP            REACTION 2 - H2NTA
13.3     LOGKEQ
2  1  1
1  5  9
2 1 0    NRTS NPDS KRTYP            REACTION 3 - HNTA
10.3     LOGKEQ
1  1  1
1  5  10
2 1 0    NRTS NPDS KRTYP            REACTION 4 - CoNTA
11.7     LOGKEQ
1  1  1
5  6  11
2 1 0    NRTS NPDS KRTYP            REACTION 5 - CoNTA2
14.5     LOGKEQ
2  1  1
5  6  12
3 1 0    NRTS NPDS KRTYP            REACTION 6 - CoOHNTA
0.5     LOGKEQ
-1  1  1  1
1   5  6  13
2 1 0    NRTS NPDS KRTYP            REACTION 7 - CoOH
-9.7     LOGKEQ
 -1  1  1
 1  6  14
2 1 0    NRTS NPDS KRTYP            REACTION 8 - CoOH2
-22.9     LOGKEQ
 -2  1  1
 1  6  15
2 1 0    NRTS NPDS KRTYP            REACTION 9 - CoOH3
-31.5     LOGKEQ
 -3  1  1
 1  6  16
2 1 0    NRTS NPDS KRTYP            REACTION 10 - HCO3
-6.35     LOGKEQ
 -1  1  1
 1  2  17
2 1 0    NRTS NPDS KRTYP            REACTION 11 - CO3
-16.68    LOGKEQ
 -2  1  1
 1  2  18
2 1 0    NRTS NPDS KRTYP            REACTION 12 - NH3
-9.3      LOGKEQ
 -1  1  1
 1  3  19
```

Table 6.8 Input Data Sets for Problem 6, Case A, (concluded)

```
1 1 0    NRTS NPDS KRTYP           REACTION 13 - OH
-14.0      LOGKEQ
 -1  1
 1   20
2 1 0    NRTS NPDS KRTYP           REACTION 14 - HBuffer
6.0      LOGKEQ
 1  1  1
 1  7  21
1 1 1           NRTS NPDS KRTYP    REACTION 15 - CoNTA (ads)
-0.30075847675 -0.574031267728  LOGKB  LOGKF
 1    1
 11   22
1 1 1           NRTS NPDS KRTYP    REACTION 16 - Co(ads)
-1.279039227   -0.574031267728  LOGKB  LOGKF
 1    1
 6   23
3 3 2           NRTS NPDS KRTYP    REACTION 18 - Microbial rxn
0.0916519  7.64D-7 6.25D-6 0.0 1 2 0 0.0 0.0 grmax ks ks kn locs loca locn taul taue
1  1.620  2.424    17.370666  3.120  0.424
10 4      1        24         2      3
0 0 0 0 0             inhib hscinh hscinh p q
                                 END OF JOB
```

6.7 Problem 7: Copper Leaching from a Five-Spot Well Pattern

This application involves the kinetic dissolution and formation of ten mineral species. It simulates the leaching of copper from an ore deposit using an acidic injection solution and is a benchmark reactive transport problem developed by Lichtner (1997). The region of interest is assumed to be homogeneous, having porosity of 5 % and a permeability of 1.5E-13 m^2. One central injection well and four evenly placed extraction wells are screened over 1200 dm and flow is distributed evenly over this depth. The injection and extraction rates are 2.52 L/s. Because of symmetry of the flow field, only one quarter of the entire region is simulated using one quarter of the total injection and extraction rates. This quarter region is 150 dm on each side and is discretized using 30 x 30 uniformly sized elements. An impervious boundary condition is imposed on each side of the region. The simulation is performed in two dimensions using a unit thickness of the 1200 dm depth and a steady state flow field. Figure 6.4 shows the flow field. The injection and extraction wells are at the lower left (x = 0, y = 0) and upper right (x = 150, y = 150) corners of the region, respectively.