6.0 SAMPLE PROBLEMS

Sample problems are presented in this section to demonstrate the application of HYDROBIOGEOCHEM to a variety of problems. Each example includes a description of the physical and biogeochemical aspects of the problem. The input data sets for each example are presented in tabular form in the text. Comments follow some data lines where format allows, and are not required. The input and output data files for each problem can be obtained on floppy disk by contacting the authors as noted in Appendix B.

Examples 1 through 4 were originally presented in the User's Manual for the model LEHGC, Version 1.1 (Yeh et al., 1995); their problem descriptions are taken directly from that document. Examples 1 and 2 are tests of advection and diffusion, respectively. Example 3 is a test of fracture flow with matrix diffusion. Example 4 tests hydrologic transport coupled with simple adsorption. The input data files are modified to meet the new data requirements for HYDROBIOGEOCHEM. The results of these examples as computed by HYDROBIOGEOCHEM are in agreement with those of LEHGC, and with the analytical solution (for Example 1 and 4), other numerical solution (for Example 2), and experimental data (for Example 2 and 3) presented originally in the LEHGC manual (Yeh et al., 1995).

Examples 5 through 8 are new problems which involve reactive contaminant transport. Example 5 couples biodegradation with 1D transport, and examines the impact of differing conditions for biomass mobility on the level of degradation attained. Example 6 is a benchmark reactive transport problem developed by Valocchi and Tebes (1997). It couples biodegradation, adsorption/desorption, and aqueous speciation reactions with 1D transport. The impact of buffered versus variable pH and of kinetic versus fast adsorption/desorption conditions on transport and transformation are examined. Example 7 is a benchmark reactive transport problem developed by Lichtner (1997) simulating mining of a copper ore using an acidic injection solution to leach the ore from the deposit. This problem involves 2D transport under variable pH and redox conditions and with moving, kinetic precipitation/dissolution fronts. Example 8 involves the injection of a microorganism into a contaminated region of an aquifer to achieve remediation of the area. This problem involves biodegradation by both adsorbed and aqueous microorganisms, equilibrium and kinetic geochemistry including pH dependent adsorption and desorption, coupled with 2D transport.

6.1 Problem 1: Test Problem for Advection

An analytical solution described by Martinez and Bixler (1983) was used to benchmark the use of HYDROBIOGEOCHEM in problems involving advection. The solution to the problem defined by

$$\frac{\partial C}{\partial t} + v\frac{\partial C}{\partial z} = D\frac{\partial^2 C}{\partial z^2} \qquad (6.1.1)$$

subject to the boundary and initial conditions

$$\begin{aligned} C(z,0) &= 0 \\ C(0,t) &= 1, \quad t > 0 \\ C(l,t) &= 0, \quad l \Rightarrow \infty \end{aligned} \qquad (6.1.2)$$

is given as

$$C(z,t) = 0.5 * \left[\operatorname{erfc}\left(\frac{z-vt}{2\sqrt{Dt}} \right) + \exp\left(\frac{vz}{D} \right) \operatorname{erfc}\left(\frac{z+vt}{2\sqrt{Dt}} \right) \right] \qquad (6.1.3)$$

In the application presented here, $v = V/\theta$ and $D = [a_L V]/\theta$, where V is the Darcy velocity, θ the moisture content, and a_L the longitudinal dispersivity.

In this example, a steady flow field is established by applying a constant flux, V, of 1.0 cm/dy to the top of a one-dimensional column 100 cm in depth. The moisture content, θ, is 0.18; a dispersivity, a_L, of 5 cm is assumed. At time t = 0, a conservative tracer (Nickel) at a concentration of 1×10^{-7} gm/ml is introduced into the flux applied at the top boundary. The problem was run with a Dirichlet boundary condition (i.e., the top boundary nodes are fixed at a concentration of 1×10^{-7} gm/ml), as defined by the analytical solution. The bottom boundary is defined as variable, and because the flow is directed out of the bottom boundary, the concentration at the bottom nodes will be computed as part of the solution. Note that this representation at a finite boundary is not the same as the infinite boundary suggested by the analytical solution. The computational grid is composed of 58 equally spaced elements, except for the bottom element which is 0.24 cm larger. The vertical axis is the z-axis; in this coordinate system, flow from top to bottom has a negative velocity (V = -1.0 cm/day in Data Set 16). The simulation time was carried out to 30 days (121 time steps of 0.25 days).

The input data sets are prepared according to Appendix A and are given in Table 6.1. The LEHGC code simulates total concentrations in units of M/L^3 of liquid (eg. mol/liter). In HYDROBIOGEOCHEM, however, total concentrations have units of M/L^3 total media (i.e. are different from those of LEHGC by a factor of θ, the volumetric moisture content). Moisture

content in this problem has a constant and uniform value of 0.18. Accounting for this factor of θ, the results computed by HYDROBIOGEOCHEM are in agreement with those of LEHGC, and with the analytical solution.

Table 6.1 Input Data Sets for Problem 1

```
    1 Advection Benchmark: (Units in cm-gm-day)
 0 0 0 10 1
C ******* DATA SET 2: BASIC INTEGER PARAMETERS
 118 58 1  0 121   1 4 -1 1 0   1 0 10 1 150   0 1 0 1 22   1 0 1
C ******* DATA SET 3: BASIC REAL PARAMETERS
 0.25D0 0.0D0 0.25D0 30.0D0 1.0D0   1.0D0 1.0D0 1.0D00 1.0D-5 1.0D0
C ******* DATA SET 4: PRINTER OUTPUT, DISK STORAGE CONTROL AND TIME STEP RESET
4400000000000000000040000000000000000004000000000000000000000000000000000000
4000000000000000000400000000000000004
1100000000000000000010000000000000000001000000000000000000000000000000000000
1000000000000000000100000000000000001
1.0D6
C ******* DATA SET 5: CHEMICAL PRINTOUT
 7
 1 19 39 59 79 99 117
C ******* DATA SET 6: MATERIAL PROPERTIES
 5.0D0  0.0D0 0.0D0 1.5D0
C ******* DATA SET 7: NODAL POINT COORDINATES
    1   58    2      0.0D0   0.0D0     0.0D0           DEFINE X FOR ODD NODES
    2   58    2      1.0D0   0.0D0     0.0D0           DEFINE X FOR EVEN NODES
    0    0    0      0.0       0.0     0.0             END OF X-COORD
    1    1    2      0.0D0   1.96D0    0.0D0           DEFINE Z FOR ALL NODES
    2    1    2      0.0D0   1.96D0    0.0D0           OF VARYING ELEMENT SIZES
    5   56    2      3.68D0  1.72D0    0.0D0
    6   56    2      3.68D0  1.72D0    0.0D0
    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  58
C ******* DATA SET 10: TRANSPORT COMPONENT INFORMATION
 1  0 0 0 0 0 0 0  NOHA HS NOKX KY KZ KP NOMB MA
Nickel
 1 0
C ******* DATA SET 11:  INITIAL CONDITIONS
  1 117 1  1.0D-20 0.0D0 0.0D0            Essentially zero concentration
  0  0 0  0.0     0.0   0.0               END OF I.C. FIRST CHEMICAL
C ******* DATA SET 12: INTEGER PARAMETERS FOR SOURCES AND BOUNDARY CONDITIONS
  0 0 0  0 0 0  2 1 2  2 1 1 2
C ******* DATA SET 14: VARIABLE BOUNDARY CONDITIONS
     0.0D0  0.00D0  1.0D6 0.00D0          BOTTOM BOUNDARY
    1    0    0    1    0
    0    0    0    0    0                END OF B.C. FIRST CHEMICAL
    1    1    1    1    1
    0    0    0    0    0                       END NVNP
    1    0    1    1    2    0    0    0    0
    0    0    0    0    0    0    0    0    0     END OF NVES
C ******* DATA SET 15: DIRICHLET BOUNDARY CONDITIONS
     0.0D0  1.0D-7  1.0D6 1.0D-7          TOP BOUNDARY
    1    1    1    1    0
    0    0    0    0    0                END OF B.C. FIRST CHEMICAL
    1    1    1  117    1
    0    0    0    0    0                       END NDNP
```

Table 6.1 Input Data Sets for Problem 1 (continued)

```
C ******* DATA SET 16: VELOCITY AND MOISTURE CONTENT
   1 117 1  0.0D0  -1.0D0  0.0D0 0.0D0
   0   0 0  0.0     0.0    0.0   0.0        END OF VELOCITY
   1  57 1  0.18D0  0.0D0
   0  0  0  0.0     0.0                     END OF THETA
   1 117 1  1.0D0   0.0D0 0.0D0
   0  0  0  0.0     0.0   0.0               END OF RHOL
C ******* DATA SET 17: NUMBER OF COMPONENTS AND PRODUCT SPECIES
 1 0 0 0 0 0
C ******* DATA SET 18: H+, e-, IONIC STRENGTH CORRECTION INFORMATION
 0.0 0 0 0 0
C ******* DATA SET 19: TEMPERATURE, PRESSURE, AND EXPECTED pe AND pH
 298.0 1.0
 -20.0 20.0 0.0 20.0
C ******* DATA SET 22: BASIC REAL AND INTEGER PARAMETERS
 1.0  50 50 1.0D-6  2.0  1.0D38
C ******* DATA SET 23: NAME OF CHEMICAL COMPONENTS AND TYPES OF COMPONENT SPECIES
Nickel
 1 0
C ******* DATA SET 24: COMPONENT SPECIES AND THEIR ION-EXCHANGE SPECIES
Nickel
0 0 0
C ******* DATA SET 28: REACTIONS
0
                    End of Job
```

6.2 Problem 2: Test Problem for Diffusion

To validate transport by diffusion, HYDROBIOGEOCHEM was benchmarked against LEHGC Version 1.1 and against a well-established finite element code for nonlinear heat conduction, COYOTE (Gartling, 1982). The problem solved is based on an experiment involving the diffusion of a conservative tracer (tritium) through a 1.43 cm wafer of dolomite (Dyhuizen and Casey, 1989). The wafer was placed between two reservoirs, or cells, each with a volume of 381.1 cm^3. The cell, wafer and background solution were allowed to approach chemical and thermal equilibrium before adding the tritium tracer to the bottom cell. The cells were periodically rotated so that a nearly uniform solution concentration was produced in the cells. Tritium activity in the top cell was then measured as a function of time.

The experiment was modeled as a one-dimensional column. The material properties used were those inferred by the analysis of the experimental results of Dykhuizen and Casey. The thickness and diameter of the wafer were 1.43 and 6.1 cm, respectively. Given the cell volume and wafer diameter, a corresponding cell height was computed (13.1 cm) for each cell. Although the model geometry does not correspond exactly to the experimental design, the wafer surface area in contact with the solution (which is mixed), and the ratio of volumes (wafer to cell) are maintained. The computational mesh is made up of 54 elements (110 nodes) with the largest vertical spacing of 1.0 cm in the cell regions away from the wafer, decreasing to 0.0715 cm adjacent to and within the wafer. The wafer perimeter is impermeable.

Concentrations were normalized to the initial concentration in the bottom cell (C_0). In the original LEHGC problem formulation, the initial normalized concentration (C/C_0) in the bottom cell was 1.0 and in the wafer and top cell, 1.0×10^{-11}(essentially zero). The simulation was run allowing the bottom-cell concentration to vary as time progresses and the tracer source is depleted. The cell mixing (by rotation in the experiment) was simulated by assigning a very large diffusion coefficient in the cells. The top and bottom boundaries are defined as variable boundaries which, with no flow in or out of the boundaries, indicates that the concentration at these nodes is to be determined as part of the solution procedure. The wafer moisture content and effective diffusion coefficient are 0.045 and 6.89×10^{-7} cm^2/s, respectively.

The LEHGC code requires initial conditions have units of M/L^3 of liquid (i.e. mol/liter). In HYDROBIOGEOCHEM, however, initial conditions must have units of M/L^3 total media. Thus the initial conditions specified in the LEHGC problem formulation have to be adjusted by the volumetric moisture content, θ, to produce consistent results in HYDROBIOGEOCHEM. For the nodes within the bottom cell, the moisture content, θ, equals 1, and the LEHGC concentration is 1.0, so the initial condition for HYDROBIOGEOCHEM is also 1.0. For the cells in the interior of the wafer, the moisture content equals 0.045 and the LEHGC concentration is 1.0×10^{-11}, so the initial condition for HYDROBIOGEOCHEM is 0.045×10^{-11}. The nodes at the transitions between reservoirs and the wafer have a moisture content in the element on the reservoir side of the node 1.0 and a moisture content in the element on the wafer side of the node of 0.045. The elements adjacent to and within the wafer all have a uniform size. Thus, the moisture content used to compute the initial condition for these transition nodes is (1.0 + 0.045)/2 or 0.5225. The initial concentrations at these nodes are 0.5225×10^{-11}. Finally, for the top cell, the moisture content equals 1, the LEHGC concentration is 1.0×10^{-11}, so the corresponding HYDROBIOGEOCHEM initial condition is also 1.0×10^{-11}.

The simulation was carried out to 1200 hours (100 time steps of 4.32×10^4 sec each). The input data sets are prepared according to Appendix A and are given in Table 6.2. Note that the units in this problem are consistently cm-gm-sec. The results computed by HYDROBIOGEOCHEM are in agreement with those of LEHGC, and with those of COYOTE, as presented in the LEHGC Version 1.1 User Manual.

Table 6.2 Input Data Sets for Problem 2

```
    2 Caseys Diffusion Experiment: (Units in cm-gm-sec) **T=ORIG*THETA***
 1 0 0 10 0
C ******* DATA SET 2: BASIC INTEGER PARAMTERS
 110 54 2 20 100   1 4 -1 1 0   1 0 10 1 150   0 1 0 1 22   1 0 1
C ******* DATA SET 3: BASIC REAL PARAMETERS
 4.32D4 0.0D0 4.32D4 4.32D6 1.0D0   1.0D0 1.0D0 1.0D00 1.0D-5 1.0D0
C ******* DATA SET 4: PRINTER OUTPUT, DISK STORAGE CONTROL AND TIME STEP RESET
440000000400000000040000000004000000000400000000040000000004000000000400000000004
00000000040000000004
101000100100100010010010001001001000100100100010010010001001001000100100100010001001
00100010010010001001
1.0D38
C ******* DATA SET 5: CHEMICAL PRINTOUT
 7
 1 25 35 55 75 85 109
C ******* DATA SET 6: MATERIAL PROPERTIES
 0.0D0  0.0D0 3.00D-3 1.0D0
 0.0D0  0.0D0 6.89D-7 2.7D0
C ******* DATA SET 7: NODAL POINT COORDINATES
    1   54    2      0.0D0   0.0D0     0.0D0           DEFINE X FOR ODD NODES
    2   54    2      6.1D0   0.0D0     0.0D0           DEFINE X FOR EVEN NODES
    0    0    0      0.0       0.0       0.0           END OF X-COORD
    1   12    2      0.0D0   1.0D0     0.0D0           DEFINE Z FOR ALL NODES
    2   12    2      0.0D0   1.0D0     0.0D0           OF VARYING ELEMENT SIZES
   27    1    2     12.5D0   0.3D0     0.0D0
   28    1    2     12.5D0   0.3D0     0.0D0
   31   24    2     12.957D0 0.0715D0  0.0D0
   32   24    2     12.957D0 0.0715D0  0.0D0
   81    1    2     14.83D0  0.3D0     0.0D0
   82    1    2     14.83D0  0.3D0     0.0D0
   85   12    2     15.63D0  1.0D0     0.0D0
   86   12    2     15.63D0  1.0D0     0.0D0
    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   54               IE
C ******* DATA SET 9: MATERIAL TYPE CORRECTION
   18 19  1   2  0   MAKE WAFER MATERIAL TYPE 2
    0  0  0   0  0   END OF MATERIAL CORRECTION
C ******* DATA SET 10: TRANSPORT COMPONENT INFORMATION
 1 0 0 0 0 0 0 0
Tritium
 1    0
C ******* DATA SET 11:  INITIAL CONDITIONS
  1 33 1  1.0D0       0.0D0 0.0D0            Bottom cell
 35  1 1  0.5225D-11  0.0D0 0.0D0            Transition nodes: Bottom cell/Wafer
 37 37 1  0.045D-11   0.0D0 0.0D0            Wafer
 75  1 1  0.5225D-11  0.0D0 0.0D0            Transition nodes: Wafer/Top cell
 77 33 1  1.0D-11     0.0D0 0.0D0            Top cell
  0  0 0  0.0         0.0   0.0              END OF I.C. FIRST CHEMICAL
```

Table 6.2 Input Data Sets for Problem 2 (continued)

```
C ******* DATA SET 12: INTEGER PARAMETERS FOR SOURCES AND BOUNDARY CONDITIONS
  0 0 0  0 0 0  0 0 0  4 2 2 2
C ******* DATA SET 14: VARIABLE BOUNDARY CONDITIONS
     0.0D0   0.00D00    1.0D38   0.00D00
     0.0D0   0.00D00    1.0D38   0.00D00
    1    1    1    1    1
    0    0    0    0    0                 END OF B.C. FIRST CHEMICAL
    1    1    1    1    1
    3    1    1  109    1
    0    0    0    0    0                          END NVNP
    1    1    1    1    2    1   53    2    2
    0    0    0    0    0    0    0    0    0     END OF NVES
C ******* DATA SET 16: VELOCITY AND MOISTURE CONTENT
   1 109 1  0.0   0.0  0.0  0.0
   0  0  0  0.0   0.0  0.0  0.0         END OF VELOCITY
   1 16  1  1.0   0.0  0.0
  18 19  1  0.045 0.0  0.0
  38 16  1  1.0   0.0  0.0
   0  0  0  0.0   0.0  0.0             END OF TH
   1 109 1  1.0   0.0  0.0  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
 1 0 0 0 0 0 0
C ******* DATA SET 18: H+, e-, IONIC STRENGTH CORRECTION INFORMATION
 0.0 0 0 0 0
C ******* DATA SET 19: TEMPERATURE, PRESSURE, AND EXPECTED pe AND pH
 298.0 1.0
 -20.0 20.0 0.0 20.0
C ******* DATA SET 22: BASIC REAL AND INTEGER PARAMETERS
 1.0 50 50 1.0D-6 2.0  1.0D38
C ******* DATA SET 23: NAME OF CHEMICAL COMPONENTS AND TYPES OF COMPONENT SPECIES
Tritium
 1 0
C ******* DATA SET 24: COMPONENT SPECIES AND THEIR ION-EXCHANGE SPECIES
Tritium                  0
  0 0 0
C ******* DATA SET 28: REACTIONS
0
                         END OF JOB
```

6.3 Problem 3: Test Problem for Fracture Flow and Matrix Diffusion

This problem simulates the effect of matrix diffusion on solute transport through fractured media and is based on a model tested by Grisak and Pickens (1980). The model was based on a longitudinal cross-section of a 0.76 meter high column with a 120 μm wide fracture in the center, running the length of the column. Due to symmetry, one-half of the cross-section can be used; the resulting domain is 7.6 dm high by 0.325 dm wide with a 6 x 10^{-4} dm wide fracture on the left hand side. The fracture is simulated by assigning specific elements to the fracture. The fracture elements are then assigned a moisture content, θ, of 1.0 and a bulk density, ρ_b, of 1.0 x 10^{-20} kg/dm^3 (to avoid a "divide-by-zero" error if a bulk density of zero is used). The matrix elements have a moisture content and bulk density of 0.35 and 1.7 kg/dm^3, respectively. The diffusion coefficient D, is 3.6 x 10^{-4} dm^2/hr in the fracture cells and 3.6 x 10^{-5} dm^2/hr in the matrix cells. Longitudinal dispersivity, a_L, for all elements is set to 7.6 dm while lateral dispersivity, a_T, is set to 0.0 dm for all elements.

The grid is made up of 21 rows by 17 columns of rectangular elements, with the three left-hand columns of elements representing the fracture and the remaining elements representing the matrix. The fracture element widths (x-direction) are 1.2 x 10^{-4} dm in the first column and 2.4 x 10^{-4} dm in the second and third columns. The matrix element widths gradually increased from being equal to the fracture element width, 2.4 x 10^{-4} dm, at the fracture side to 0.1 dm at the opposite side. The heights (z-direction) of rows of elements gradually increase from 6 x 10^{-4} dm to 0.2 dm, from the top to the bottom.

The upper boundary of the model has a constant concentration, Dirichlet boundary. The specified concentration along this boundary in the original LEHGC problem formulation was 1.0 mol/liter. For HYDROBIOGEOCHEM, this is adjusted by volumetric moisture content, θ, for units of mol/dm^3 of total media. In the fracture θ = 1.0, in the matrix θ = 0.35, and at the fracture/matrix interface nodes θ = 0.675, since the elements to either side of this interface have equal size and therefore equal contribution to moisture content at these nodes. The specified initial and boundary concentrations along the upper boundary are therefore 1.0, 0.675, and 0.35 mol/dm^3 media for the fracture nodes, interface node, and matrix nodes, respectively.

The other three boundaries are treated as Cauchy boundaries with zero total flux. In the LEHGC problem formulation, this was implemented using the variable boundary condition with a zero total flux specified for the inflow condition. In HYDROBIOGEOCHEM, this boundary specification introduced a problem in the simulation. Diffusion creates a very small component of velocity from outside of the left edge of the domain (i.e. the centerline of the fracture), giving an incoming concentration of 0.0 rather than 1.0 from points on this edge of the domain. This is not consistent with the physical system being simulated. The HYDROBIOGEOCHEM input is revised to simply leave these three boundaries as unspecified, creating the Cauchy condition with zero total flux.

Vertical velocity values at each node in the fracture are calculated assuming a parabolic velocity profile and an average fracture velocity of -0.313 dm/hr (downward). This results in velocities

of
-0.469 dm/hr, -0.45 dm/hr and -0.3 dm/hr in the first, second and third columns respectively. Since the fourth column of nodes represents the boundary between the matrix and fracture, these nodes have velocities equal to those in the matrix. The vertical Darcy velocity in the matrix is derived by first solving equation (6.3.1), which describes fracture flow velocity, to obtain the hydraulic gradient.

$$V_f = \frac{\rho\ g\ (2b)^2\ \frac{dh}{dx}}{12\ \mu} \qquad \textbf{(6.3.1)}$$

where: dh/dx is the hydraulic gradient (L/L), ρ is density of the fluid (M/L^3), g is gravitational acceleration (L/T^2), 2b is the width of the fracture (L), μ is dynamic viscosity of the fluid (M/LT), and V_f is the average velocity of the fluid in the fracture (L/T).

Equation (6.3.2) is then used to solve for the vertical Darcy velocity in the matrix using the calculated value for the hydraulic gradient.

$$V_m = -K\ \frac{dh}{dx} \qquad \textbf{(6.3.2)}$$

where: K is the hydraulic conductivity (L/T), and V_m is the Darcy velocity of the fluid in the matrix (L/T). The value of the hydraulic conductivity, 2.16×10^{-6} dm/hr (6×10^{-9} cm/s), is obtained from Grisak et al. (1980) whose column study was the basis for Grisak and Pickens' model.

A time step of 0.24 hours was used; a total of six days (144 hours) are simulated using 600 time steps. The input data sets are prepared according to Appendix A and are given in Table 6.3. The results computed by HYDROBIOGEOCHEM are in agreement with those of LEHGC, and with those of Grisak and Pickens, as presented in the LEHGC Version 1.1 User Manual.

Table 6.3 Input Data Sets for Problem 3

```
 3   FRACTURE FLOW & MATRIX DIFFUSION: (Units in dm-kg-hr) *** removed var bc
0  0  0 0  1
C ******* DATA SET 2: BASIC INTEGER PARAMETERS
 396 357 2 63 600   1 4 -1 1 0   1 0 30 1 150   0 1 0 1 22  1 0 1
C ******* DATA SET 3: BASIC REAL PARAMETERS
2.4D-1  0.0D00  2.4D-1  1.0D03  1.0   1.0  1.0  1.0  1.0D-5  1.0D0
C ******* DATA SET 4: PRINTER OUTPUT, DISK STORAGE CONTROL AND TIME STEP RESET
20000000000000000000000000000000000000000000000000200000000000000000000000000000
00000000000000000000200000000000000000000000000000000000000000000000002000000000
00000000000000000000000000000000000000002000000000000000000000000000000000000000
00000000002000000000000000000000000000000000000000000000000020000000000000000000
00000000000000000000000000000020000000000000000000000000000000000000000000000000
20000000000000000000000000000000000000000000000000200000000000000000000000000000
00000000000000000000200000000000000000000000000000000000000000000000002000000000
00000000000000000000000000000000000000002
10000100001000010000100001000010000100001000010000100001000010000100001000010000
10000100001000010000100001000010000100001000010000100001000010000100001000010000
10000100001000010000100001000010000100001000010000100001000010000100001000010000
10000100001000010000100001000010000100001000010000100001000010000100001000010000
10000100001000010000100001000010000100001000010000100001000010000100001000010000
10000100001000010000100001000010000100001000010000100001000010000100001000010000
10000100001000010000100001000010000100001000010000100001000010000100001000010000
10000100001000010000100001000010000100001
1.0D38
C ******* DATA SET 5: CHEMICAL OUTPUT
 4
 23  44  131  141
C ******* DATA SET 6: MATERIAL PROPERTIES
 7.6D00  0.0D00  3.6D-5  1.7D00    Matrix
 7.6D00  0.0D00  3.6D-4  1.0D-20   Fracture
C ******* DATA SET 7: NODAL POINT COORDINATES
   1   21    1    0.0        0.0     0.0
  23   21    1    1.2D-4     0.0     0.0
  45   21    1    3.6D-4     0.0     0.0
  67   21    1    6.0D-4     0.0     0.0
  89   21    1    8.4D-4     0.0     0.0
 111   21    1    1.2D-3     0.0     0.0
 133   21    1    1.8D-3     0.0     0.0
 155   21    1    3.0D-3     0.0     0.0
 177   21    1    5.0D-3     0.0     0.0
 199   21    1    1.0D-2     0.0     0.0
 221   21    1    1.8D-2     0.0     0.0
 243   21    1    3.0D-2     0.0     0.0
 265   21    1    4.5D-2     0.0     0.0
 287   21    1    6.5D-2     0.0     0.0
 309   21    1    1.0D-1     0.0     0.0
 331   21    1    1.5D-1     0.0     0.0
 353   21    1    2.25D-1    0.0     0.0
 375   21    1    3.25D-1    0.0     0.0
   0    0    0    0.0        0.0     0.0   END OF X-COORD
   1   17   22    0          0.0     0.0
   2   17   22    0.8        0.0     0.0
```

Table 6.3 Input Data Sets for Problem 3 (continued)

```
   3   17   22    1.6       0.0    0.0
   4   17   22    2.4       0.0    0.0
   5   17   22    3.2       0.0    0.0
   6   17   22    4         0.0    0.0
   7   17   22    4.8       0.0    0.0
   8   17   22    5.5       0.0    0.0
   9   17   22    6.1       0.0    0.0
  10   17   22    6.6       0.0    0.0
  11   17   22    7         0.0    0.0
  12   17   22    7.3       0.0    0.0
  13   17   22    7.45      0.0    0.0
  14   17   22    7.523     0.0    0.0
  15   17   22    7.5616    0.0    0.0
  16   17   22    7.5808    0.0    0.0
  17   17   22    7.5904    0.0    0.0
  18   17   22    7.5952    0.0    0.0
  19   17   22    7.5976    0.0    0.0
  20   17   22    7.5988    0.0    0.0
  21   17   22    7.5994    0.0    0.0
  22   17   22    7.6       0.0    0.0
   0    0    0    0.0       0.0    0.0    END OF Z-COORD
C ******* DATA SET 8: ELEMENT CONNECTIVITY
    1    1   23   24    2    1   21   17
C ******* DATA SET 9: MATERIAL TYPE CORRECTION
   1  62  1  2  0
   0   0  0  0  0
C ******* DATA SET 10: TRANSPORT COMPONENT INFORMATION
 1   0  0 0 0 0  0 0
  TRACER
  1    0
C ******* DATA SET 11: INITIAL CONDITIONS
    1   20    1    1.0D-20   0.0D0   0.0D0   Fracture centerline (left boundary)
   22    2   22    1.0D00    0.0D0   0.0D0   Nodes along top of fracture
   88    0    0    0.675D0   0.0D0   0.0D0   Node at top of interface fract/matr
  110   13   22    0.35D00   0.0D0   0.0D0   Nodes along top of matrix
   23   20    1    1.0D-20   0.0D0   0.0D0   Nodes in fracture
   45   20    1    1.0D-20   0.0D0   0.0D0
   67   20    1    0.675D-20 0.0D0   0.0D0   Nodes along interface
   89   20    1    0.35D-20  0.0D0   0.0D0   Nodes in matrix
  111   20    1    0.35D-20  0.0D0   0.0D0
  133   20    1    0.35D-20  0.0D0   0.0D0
  155   20    1    0.35D-20  0.0D0   0.0D0
  177   20    1    0.35D-20  0.0D0   0.0D0
  199   20    1    0.35D-20  0.0D0   0.0D0
  221   20    1    0.35D-20  0.0D0   0.0D0
  243   20    1    0.35D-20  0.0D0   0.0D0
  265   20    1    0.35D-20  0.0D0   0.0D0
  287   20    1    0.35D-20  0.0D0   0.0D0
  309   20    1    0.35D-20  0.0D0   0.0D0
  331   20    1    0.35D-20  0.0D0   0.0D0
  353   20    1    0.35D-20  0.0D0   0.0D0
  375   20    1    0.35D-20  0.0D0   0.0D0
    0    0    0    0.0D00    0.0D0   0.0D0
```

Table 6.3 Input Data Sets for Problem 3 (concluded)

```
C ******* DATA SET 12: INTEGER PARAMETERS FOR SOURCES AND BOUNDARY CONDITIONS
  0  0  0    0  0  0   18 3  2      0  0  1   2
C ******* DATA SET 15: DIRICHLET BOUNDARY CONDITIONS
  0.0D0  1.0D0    1.0D38  1.0D0    BC for top of fracture
  0.0D0  0.675D0  1.0D38  0.675D0  BC for top of fracture/matrix interface
```

```
  0.0D0  0.35D0   1.0D38  0.35D0   BC for top of matrix
    1    2    1    1    0          DIR nodes along top of fracture
    4    0    0    2    0          DIR nodes at top of fracture/matrix interface
    5   13    1    3    0          DIR nodes along top of matrix
    0    0    0    0    0                      END OF B.C. SOLUTE
    1   17    1   22   22
    0    0    0    0    0                      END OF NDNP
C ******* DATA SET 16: VELOCITY AND MOISTURE CONTENT
    1   21    1    0.0  -0.469      0.0  0.0
   23   21    1    0.0  -0.450      0.0  0.0
   45   21    1    0.0  -0.300      0.0  0.0
   67  329    1    0.0   0.0D00     0.0  0.0
    0    0    0    0.0   0.0        0.0  0.0     END OF VELOCITY
    1   62    1    1.0   0.0
   64  293    1    0.35  0.0
    0    0    0    0.0   0.0                    END OF TH
    1  395    1    1.0   0.0  0.0  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
  1  0       0  0  0  0
C ******* DATA SET 18: H+, e-, IONIC STRENGTH CORRECTION INFORMATION
    0.0   0    0  0  0
C ******* DATA SET 19: TEMPERATURE, PRESSURE, AND EXPECTED pe AND pH
  298.0   1.0
  -20.0  20.0  0.0  20.0
C ******* DATA SET 22: BASIC REAL AND INTEGER PARAMETERS
  1  1 50 1.0d-6  2.0D0  1.0D38
C ******* DATA SET 23: NAME OF CHEMICAL COMPONENTS AND TYPES OF COMPONENT SPECIES
  TRACER
  1  0
C ******* DATA SET 24: COMPONENT SPECIES AND THEIR ION-EXCHANGE SPECIES
  FREE TRACER
    0    0.0    0
C ******* DATA SET 28: REACTIONS
0
          END OF JOB
```

6.4 Problem 4: Test Hydrologic Transport and Simple Adsorption

This problem involves transport in a 1 dm long, one-dimensional column. The flow velocity is -1.0×10^{-2} dm/hr (flow is from top to bottom). The effective porosity is 0.3, the bulk density is 1.2 kg/dm^3, and the dispersivity is 2×10^{-3} dm. The transport involves four chemical components. The initial condition is a total analytical concentration of 10^{-4} M, or 0.3×10^{-4} mol/dm^3 media, for all four chemical components. The boundary conditions are as follows: at the top of the column (z = 1.0 dm), the total analytical concentrations are 10^{-3} M, or 0.3×10^{-3} mol/dm^3 media; at z = 0.0 dm, variable boundary conditions with zero concentration gradients specified for all four components.

To mimic the hydrologic transport without interaction among four chemical components, we assume that each chemical component has two species: a free species and an adsorbed species. The ratios of the adsorbed species to the free species are assumed to be 0, 1/9, 1, and 9, respectively, for chemical components 1, 2, 3, and 4 (i.e., 0%, 10%, 50%, and 90% adsorption, respectively). To apply the no-interaction scenario among four components, the adsorbing site is not a constraint for the equilibrium between free species and adsorbed species for each component. In the original LEHGC problem formulation, which treats all concentrations as mol/L, the geochemical equilibrium constants for the formation of the four adsorbed species were 0 (log K = -38), 1/9, 1, and 9, respectively. These reactions are of the form:

$$\mathrm{C} \leftrightarrow \mathrm{S}\ , \qquad \text{with } K = \frac{[\mathrm{S\ mol/L}]}{[\mathrm{C\ mol/L}]} \tag{6.4.1}$$

For HYDROBIOGEOCHEM, all individual species concentrations are in units of mol/mass of phase. The adsorption/desorption reactions are of the form:

$$\mathrm{C} \leftrightarrow \mathrm{S}\ , \qquad \text{with } K' = \frac{[\mathrm{S\ mol/mass\ of\ solid}]}{[\mathrm{C\ mol/mass\ of\ liquid}]}$$

$$\text{where} \quad K' = K * \frac{1}{\rho_b} * \rho_\ell \theta \tag{6.4.2}$$

As noted above, $\theta = 0.3$, $\rho_b = 1.2$ kg/dm^3, and ρ_ℓ is assumed equal to 1.0 kg/dm^3. For the HYDROBIOGEOCHEM input, the equilibrium constants for the formation of the four adsorbed species were therefore 0, 0.027778, 0.25, and 2.25, respectively.

For numerical simulation, the column is discretized into 1 x 40 elements of size 0.025 dm by 0.025 dm, resulting in 82 nodes; the horizontal axis is the z-axis. The simulation is conducted for three time steps only because the purpose of this simulation is to verify the hydrologic module against LEHGC. The time-step size is 0.5 hr. The input data sets are prepared according to Appendix A and are given in Table 6.4. With the adjustments noted above, the results computed by HYDROBIOGEOCHEM are in agreement with those of LEHGC.

Table 6.4 Input Data Sets for Problem 4

```
    1 TEST OF LEHGC: TRANSPORT MODULE - FOUR COMPONENTS units in (dm-kg-hr) **logK's
  0 0 0 1 0
C ******* DATA SET 2: BASIC INTEGER PARAMTERS
 82 40 1 0 3   1 4 -1 1 0   1 0 30 1 150   0 1 0 1 12   1 0 1
C ******* DATA SET 3: BASIC REAL PARAMETERS
 0.50D0 0.0D0 0.50D00 15.0D0 1.0D0   1.0D0 1.0D0 1.0D00 1.0D-5 1.0D0
C ******* DATA SET 4: PRINT AND AUXILIARY STORGE CONTROL
4444
0001
1.0D38
C ******* DATA SET 5: CHEMICAL PRINTOUT AND CHEMICAL PROPERTY TYPE INDICATOR
 3
 1 41 82       NODEP
C ******* DATA SET 6: MATERIAL PROPERTIES
 2.0D-3 0.0D0 0.0D0 1.2D0 AL AT AM RHOB
C ******* DATA SET 7: NODE COORDINATES
    1   40    2      0.0          0.0     0.0
    2   40    2      0.025D0   0.0D0     0.0D0
    0    0    0      0.0          0.0     0.0             END OF X-COORD
    1   40    2      0.0D0    0.025D0     0.0D0
    2   40    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   40                IE
C ******* DATA SET 10: CHEMICAL COMPONENT INFORMATION
 4 0  0 0 0 0  0 0
  CHEM 1
  1    0
  CHEM 2
  2    1
  CHEM 3
  3    1
  CHEM 4
  4    1
C ******* DATA SET 11:  INITIAL CONDITIONS
  1 81 1  0.3D-4  0.0D0 0.0D0
  0  0 0  0.0     0.0   0.0               END OF I.C. FIRST CHEMICAL
  1 81 1  0.3D-4  0.0D0 0.0D0
  0  0 0  0.0     0.0   0.0               END OF I.C. SECOND CHEMICAL
  1 81 1  0.3D-4  0.0D0 0.0D0
  0  0 0  0.0     0.0   0.0               END OF I.C. THIRD CHEMICAL
  1 81 1  0.3D-4  0.0D0 0.0D0
  0  0 0  0.0     0.0   0.0               END OF I.C. FOURTH CHEMICAL
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  NSEL NSPR NSDP  NWNP NWPR NWDP  NDNP NDPR NDDP
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. FIRST CHEMICAL
     0.0D0  0.000D00    1.0D38   0.00D00
    1    0    0    1    0
    0    0    0    0    0                 END OF B.C. SECOND CHEMICAL
```

Table 6.4 Input Data Sets for Problem 4 (continued)

```
     0.0D0     0.0D00     1.0D38    0.00D00
    1     0     0     1     0
    0     0     0     0     0                   END OF B.C. THIRD CHEMICAL
     0.0D0      0.0D0     1.0D38    0.00D00
    1     0     0     1     0
    0     0     0     0     0                   END OF B.C.  FOURTH CHEMICAL
    1     1     1     1     1
    0     0     0     0     0                           END NPVB
    1     0     1     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 0.3D-3  1.0D38 0.3D-3
    1     1     1     1     0
    0     0     0     0     0                   END OF B.C.  FIRST CHEMICAL
   0.0D0 0.3D-3  1.0D38 0.3D-3
    1     1     1     1     0
    0     0     0     0     0                   END OF B. C. SECOND CHEMICAL
   0.0D0 0.3D-3  1.0D38 0.3D-3
    1     1     1     1     0
    0     0     0     0     0                   END OF B.C. THIRD CHEMICAL
   0.0D0 0.3D-3  1.0D38 0.3D-3
    1     1     1     1     0
    0     0     0     0     0                   END OF B.C.  FOURTH CHEMICAL
   1 1 1  81 1
   0 0 0 0 0                                    END OF NPDB
C ******* DATA SET 16: HYDROLOGICAL VARIABLES
   1 81 1  0.0  -1.000D-2  0.0    0.0
   0  0 0  0.0   0.0       0.0    0.0   END OF VELOCITY
   1 39 1  0.3   0.0
   0  0 0  0.0   0.0                   END OF TH
   1 81 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
 4 0 0 4 0 0
C ******* DATA SET 18: H+, E-, IONIC STRENGTH correction INFORMATION
 0.0 0 0 0 0
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 information
 1.0  1  50  1.0d-6  2.0d0  1.0d38
c ******* Date Set 23:  Name of chemical components and type of component species
  CHEM 1
  1  0
  CHEM 2
  1  0
  CHEM 3
  1  0
  CHEM 4
  1  0
```

Table 6.4 Input Data Sets for Problem 4 (concluded)

```
C ******* DATA SET 24: COMPONENT SPECIES AND THEIR ION-EXCHANGE INDEX
FREE CHEMICAL 1
  0 0 0  ISCN VJ IONEX
FREE CHEMICAL 2
  0 0 0  ISCN VJ IONEX
```

```
FREE CHEMICAL 3
  0 0 0  ISCN VJ IONEX
FREE CHEMICAL 4
  0 0 0  ISCN VJ IONEX
C ******** DATA SET 25:  ADSORBED SPECIES
SORBED CHEMICAL 1
 0       1 0 0 0   1 0 0 0
SORBED CHEMICAL 2
 0       0 1 0 0   0 1 0 0
SORBED CHEMICAL 3
 0       0 0 1 0   0 0 1 0
SORBED CHEMICAL 4
 0       0 0 0 1   0 0 0 1
C ******** DATA SET 28:  REACTIONS
4
 1 1  0          NRTS   NPDS   KRTYP  - RXN1
 -38.0           LOGKEQ
 1 1             CXYZP  DXYZP
 1 5             IGSNRT IGSNPD
 1 1  0          NRTS   NPDS   KRTYP - RXN2 (log k for conc in mol/mass phase)
 -1.5563025      LOGKEQ
 1 1             CXYZP  DXYZP
 2 6             IGSNRT IGSNPD
 1 1  0          NRTS   NPDS   KRTYP  - RXN3
 -0.60206        LOGKEQ
 1 1             CXYZP  DXYZP
 3 7             IGSNRT IGSNPD
 1 1  0          NRTS   NPDS   KRTYP  - RXN4
 0.352182518     LOGKEQ
 1 1             CXYZP  DXYZP
 4 8             IGSNRT IGSNPD
                                END OF JOB
```

6.5 Problem 5: Biodegradation Coupled with Transport

This example addresses bioremediation in a hypothetical aquifer system. The physical system is represented using one dimensional transport through a region 100 dm long. Initially, a zone located at 20 dm ≤ x ≤ 30 dm contains a biodegradable substrate and the microorganism capable of doing so. The initial concentration of substrate and biomass are S_0 = 200 mg/L and b_0 = 0.001 U.O.D., respectively. The biodegradation reaction parameters are K_S = 7.5 mg/L, Y_S = 0.130E-3, and μ_{max} = 0.0387 hr^{-1}. The substrate is present in the aqueous phase and its mobility is assumed not to be retarded by interactions with the porous media. The physical parameters selected to describe the system are porosity = 0.2, bulk density = 1.5 kg/dm^3, pore water velocity = 0.1 dm/hr, and longitudinal dispersivity = 0.5 dm. Eighty-one nodes and fifty-two elements (two rows of twenty-six elements) were used to discretize the region of interest. A uniform time step of 0.1 hours is used.

Three cases are considered in which different assumptions are made about the mobility of the biomass. Case A is transport of a non reactive tracer through the media; this represents the migration of the contaminant either when microorganisms are not present or are present but not acclimated to the substrate. Case B reflects the condition that biomass colonies have become established only in the zone in which the substrate is initially present and are adsorbed to the porous media (i.e. the biomass is immobile). Case C is when the biomass is present initially only in the zone in which the substrate is initially present and the biomass exists in the aqueous phase (i.e. the biomass is subject to transport). The input data sets for Case C are given in Table 6.5; the input files for all cases can be obtained on floppy disk.

Figure 6.1 compares the transported substrate concentration when the different assumptions are made about the mobility of the biomass. The progress of a non reactive tracer through the column is shown in Figure 6.1a for comparison. If biomass colonies have become established only in the zone in which the substrate was initially present and are assumed to be adsorbed to the porous media, there is significant reduction in contaminant levels throughout the column due to the degradation which is able to occur within the bioactive zone (Figure 6.1b). If the biomass is assumed to exist in the aqueous phase, additional removal of the pollutant is achieved as biodegradation of the substrate continues to occur as both it and the microorganisms are transported through the entire region of interest (Figure 6.1c). Figure 6.2 contrasts the substrate levels encountered at a location 20 dm down gradient from the initial edge of the plume (x = 50 dm). Over 40% removal is predicted when the biomass is present only in the original zone of contamination, over 90% removal is predicted if the biomass is mobile.

It is interesting to note that Case C is equivalent to the bioremoval of the contaminant that would be achieved in a batch system, regardless of whether the biomass exists in the aqueous or adsorbed phase in such a system (assuming the rate at which the microorganisms can degrade the substrate is the same when the microorganism is associated with either phase). This is equivalent to saying that achieving 90% removal in a batch experiment does not necessarily imply the same percentage of removal at a field site under transport conditions.

Table 6.5 Input Data Sets for Problem 5, Case C

```
    5  N. winogradski on N-NO2 + Transport (Units: m,kg,hr) *** S(aq),B(aq) ***
 1 0 0 10 0
C ******* DATA SET 2: BASIC INTEGER PARAMTERS
 81 52 1 0 8000   1 4 -1 1 0   1 0 30 1 150   0 1 0 1 22   1 0 1
C ******* DATA SET 3: BASIC REAL PARAMETERS
 0.10 0.0D0 0.10 800D0 1.0D0   1.0D0 1.0D0 1.0D00 1.0D-5 1.0D0
C ******* DATA SET 4: PRINTER OUTPUT, DISK STORAGE CONTROL AND TIME STEP RESET
44000000004000000000400000000040000000004000000000400000000040000000004000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000
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Table 6.5 Input Data Sets for Problem 5, Case C (continued)

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Table 6.5 Input Data Sets for Problem 5, Case C (continued)

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Table 6.5 Input Data Sets for Problem 5, Case C (continued)

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10000000001000000000100000000010000000001000000000100000000010000000001000000000
10000000001000000000100000000010000000001000000000100000000010000000001000000000
10000000001000000000100000000010000000001000000000100000000010000000001000000000
10000000001000000000100000000010000000001000000000100000000010000000001000000000
10000000001000000000100000000010000000001000000000100000000010000000001000000000
10000000001000000000100000000010000000001000000000100000000010000000001000000000
10000000001000000000100000000010000000001000000000100000000010000000001000000000
10000000001000000000100000000010000000001000000000100000000010000000001000000000
1
1.0D38
```

Table 6.5 Input Data Sets for Problem 5, Case C (continued)

```
C ******* DATA SET 5: CHEMICAL PRINTOUT
 4
 20  26  32  38
C ******* DATA SET 6: MATERIAL PROPERTIES
 5.0D-3 0.0D0 0.00D0  1.5D0
C ******* DATA SET 7: NODAL POINT COORDINATES
    1    2    1      0.0D0     0.0D0     0.0D0           DEFINE X
    4    2    1      0.5D0     0.0D0     0.0D0           DEFINE X
    7    2    1      1.0D0     0.0D0     0.0D0           DEFINE X
   10    2    1      1.5D0     0.0D0     0.0D0           DEFINE X
   13    2    1      1.75D0    0.0D0     0.0D0           DEFINE X
   16    2    1      1.875D0   0.0D0     0.0D0           DEFINE X
   19    2    1      2.0D0     0.0D0     0.0D0           DEFINE X
   22    2    1      2.25D0    0.0D0     0.0D0           DEFINE X
```

```
   25    2    1      2.5D0     0.0D0     0.0D0          DEFINE X
   28    2    1      2.75D0    0.0D0     0.0D0          DEFINE X
   31    2    1      3.0D0     0.0D0     0.0D0          DEFINE X
   34    2    1      3.125D0   0.0D0     0.0D0          DEFINE X
   37    2    1      3.25D0    0.0D0     0.0D0          DEFINE X
   40   13    3      3.5D0     0.5D0     0.0D0          DEFINE X
   41   13    3      3.5D0     0.5D0     0.0D0          DEFINE X
   42   13    3      3.5D0     0.5D0     0.0D0          DEFINE X
    0    0    0      0.0       0.0       0.0            END OF X-COORD
    1   26    3      0.0D0     0.0D0     0.0D0          DEFINE Z FOR ALL NODES
    2   26    3      0.25D0    0.0D0     0.0D0          DEFINE Z FOR ALL NODES
    3   26    3      0.5D0     0.0D0     0.0D0          DEFINE Z FOR ALL NODES
    0    0    0      0.0D0     0.0D0     0.0D0          END OF Z-COORD
C ******* DATA SET 8: ELEMENT CONNECTIVITY
    1    1    4    5    2    1    2   26              IE
C ******* DATA SET 10: TRANSPORT COMPONENT INFORMATION
 1 0 0 0 0 0 1 0
Na-NO2
 1    0
C ******* DATA SET 11:  INITIAL CONDITIONS
  1   18   1  0.0D0  0.0D0 0.0D0
  19  14   1  40.0D0 0.0D0 0.0D0
  34  46   1  0.0D0  0.0D0 0.0D0
  0   0    0  0.0     0.0   0.0              END OF I.C. SUBSTRATE
  1   18   1  0.0D0  0.0D0 0.0D0
  19  14   1  2.0D-4 0.0D0 0.0D0
  34  46   1  0.0D0  0.0D0 0.0D0
  0   0    0  0.0     0.0   0.0              END OF I.C. MICROBE
C ******* DATA SET 12: INTEGER PARAMETERS FOR SOURCES AND BOUNDARY CONDITIONS
  0 0 0  0 0 0  0 0 0  6 4 1 2
C ******* DATA SET 14: VARIABLE BOUNDARY CONDITIONS
    0.0D0   0.00D00    1.0D38   0.00D00
    1    3    1    1    0
    0    0    0    0    0                  END OF B.C. SUBSTRATE
    0.0D0   0.00D00    1.0D38   0.00D00
    1    3    1    1    0
    0    0    0    0    0                  END OF B.C. MICROBE
    1    2    1    1    1
    4    2    1   79    1
```

Table 6.5 Input Data Sets for Problem 5, Case C (concluded)

```
    0    0    0    0    0                          END NVNP
    1    1    1    1    2    1    1    1    1
    3    1   51    4    5    1    1    1    1
    0    0    0    0    0    0    0    0    0     END OF NVES
C ******* DATA SET 16: VELOCITY AND MOISTURE CONTENT
   1  80 1  0.002  0.0  0.0  0.0
   0   0 0  0.0    0.0  0.0  0.0         END OF VELOCITY
   1  51 1  0.20   0.0  0.0
   0  0  0  0.0    0.0  0.0              END OF TH
   1  80 1  1.0    0.0  0.0  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
 1 0 0 0 0 0 0
C ******* DATA SET 18: H+, e-, IONIC STRENGTH CORRECTION INFORMATION
 0.0 0    0 0 0
C ******* DATA SET 19: TEMPERATURE, PRESSURE, AND EXPECTED pe AND pH
 310.15 1.0
 -20.0 20.0 0.0 20.0
C ******* DATA SET 22: BASIC REAL AND INTEGER PARAMETERS
```

```
 1.0 1 100 1.0D-6 2.0  2.0
C ******* DATA SET 23: NAME OF CHEMICAL COMPONENTS AND TYPES OF COMPONENT SPECIES
Na-NO2
 1 0
C ******* DATA SET 24: COMPONENT SPECIES AND THEIR ION-EXCHANGE SPECIES
Na-NO2
0 0 0
C ******* DATA SET 28:  Microbial Species
NITROBACTER
0 -38.00 0
C ******* DATA SET 28: REACTIONS
1
1 1 2
0.0387 7.5 0.0 0.0   1 0 0  0 0
1  0.130D-3
1  2
0 0.0 0.0 0.0 0.0
                          END OF JOB
```

Figure 6.2 Concentration profiles versus time at location x = 5 m for example problem 6.5.

6.6 Problem 6: Microbiological and Chemical Reactions Coupled with Transport

This example is a benchmark problem for the simulation of reactive transport developed by Valocchi and Tebes (1997). It includes kinetic adsorption/desorption, equilibrium aqueous complexation and biodegradation as well as advective-dispersive transport. The problem description is directly from the formulation of Valocchi and Tebes, except as noted.

This problem involves one dimensional transport of multiple reacting species through a 100 dm long column over a seventy-five hour period. The physical parameters describing the system are porosity = 0.4, bulk density = 1.5 kg/dm^3, pore water velocity = 10 dm/hr, and longitudinal dispersivity = 0.5 dm. The domain was discretized using 100 elements and 202 nodes and a uniform time step size of 0.10 hours was used for all simulations. Activity corrections were not used.

Aqueous speciation is simulated using fourteen equilibrium chemical reactions (Table 6.6). Two of the aqueous species, Co^{2+} and $CoNTA^-$, may be removed from solution by adsorption to the media in the column. In addition, there is one kinetic biodegradation reaction affecting the chemical distribution within the column. Initially, the column is free from the biodegradation substrate, $HNTA^{2-}$, and the adsorbing species, then for a period of twenty hours a pulse

containing Co^{2+} and NTA^{-} is injected into the column. For the remaining fifty-five hours, the injection fluid has the same chemical composition as the fluid initially present in the column. Table 6.7 summarizes the concentrations initially present in the column and in the injected pulse. Three variations are simulated: (1) the adsorption reactions are kinetic and the pulse and the background solutions are buffered to keep pH =6, (2) the adsorption reactions are kinetic and the pH levels in both the pulse and the background solutions are allowed to vary, and (3) the adsorption reactions are fast, approximating an equilibrium rather than a kinetic process, and the pH levels in both the pulse and the background solutions are allowed to vary.

Table 6.6. Tableau for equilibrium reactions included in example problem 6.6.

	H^+	NTA^{3-}	Co^{2+}	$H_2CO_3^*$	NH_4^+	O_2	Buffer	log K_{eq}
H_3NTA	3	1	0	0	0	0	0	14.9
H_2NTA^-	2	1	0	0	0	0	0	13.3
$HNTA^{2-}$	1	1	0	0	0	0	0	10.3
$CoNTA^-$	0	1	1	0	0	0	0	11.7
$Co(NTA)_2^{4-}$	0	2	1	0	0	0	0	14.5
$CoOHNTA^{2-}$	-1	1	1	0	0	0	0	0.5
$CoOH^+$	-1	0	1	0	0	0	0	-9.7
$Co(OH)_2$	-2	0	1	0	0	0	0	-22.9
$Co(OH)_3^-$	-3	0	1	0	0	0	0	-31.5
HCO_3^-	-1	0	0	1	0	0	0	-6.35
CO_3^{2-}	-2	0	0	1	0	0	0	-16.68
OH^-	-1	0	0	0	0	0	0	-14.0
NH_3	-1	0	0	0	1	0	0	-9.3
HBuffer	1	0	0	0	0	0	1	6.0

Table 6.7. Concentration of component species in the column and in the incoming pulse for example problem 6.6.

Component	Type	Background Concentration	Pulse Concentration
H^+	Aqueous	pH = 6	pH = 6
NTA^{3-}	Aqueous	0.0	5.23E-6 mol/L
Co^{2+}	Aqueous	0.0	5.23E-6 mol/L
$H_2CO_3^*$	Aqueous	4.9E-7 mol/L	4.9E-7 mol/L
NH_4^+	Aqueous	0.0	0.0
O_2	Aqueous	3.125E-5 mol/L	3.125E-5 mol/L
Buffer	Aqueous	1.0E-3 mol/L or 0.0	1.0E-3 mol/L or 0.0
Biomass	Adsorbed	5.44E-5 g/dm^3 media	N/A
$CoNTA_{(ads)}$	Adsorbed	0.0	N/A
$Co_{(ads)}$	Adsorbed	0.0	N/A

Transport of the free cobalt species, Co^{2+}, and $CoNTA^-$ through the column is retarded due to adsorption. The availability of adsorbent sites is considered nonlimiting and the adsorption process is assumed to be kinetic. Valocchi and Tebes use a linear kinetic model to represent the adsorption process; the reactions and reaction rates have been reformulated to express adsorption in terms of forward and backward rate constants for use in HYDROBIOGEOCHEM. The parameters describing adsorption were selected by Valocchi and Tebes to make adsorption a significant kinetic process in the system; they do not necessarily represent realistic adsorption behavior for Co^{2+} or $CoNTA^-$. The two adsorption reactions simulated are:

$$CoNTA^-_{(aq)} \underset{k_{b1}}{\overset{k_{f1}}{\rightleftharpoons}} CoNTA_{(ads)} \qquad (6.6.1)$$

$$Co^{2+}_{(aq)} \underset{k_{b2}}{\overset{k_{f2}}{\rightleftharpoons}} Co_{(ads)} \qquad (6.6.2)$$

where k_{f1} = 0.26667 hr^{-1}, k_{b1} = 0.5003127 hr^{-1}, and k_{f2} = 0.26667 hr^{-1}, k_{b2} = 0.05259697 hr^{-1} for simulations (1) and (2), and where the forward and backward rate constants are all increased by a factor of 10^3 for simulation (3) to approximate adsorption as an equilibrium process.

Biodegradation of $HNTA^-$ removes NTA from the system through the following reaction:

$$HNTA^{2-} + 1.620\ O_2 + 1.272\ H_2O + 2.424\ H^+ \rightarrow 17.3707\ C_5H_7O_2N + 3.120\ H_2CO_3^* + 0.424\ NH_4^+ \qquad (6.6.3)$$

where K_S = 7.64E-7 mol/L, K_O = 6.25E-6 mol/L, μ_{max} = 0.0916519 hr^{-1}, b_0 = 5.44E-5 gram/dm^3 of media, and K_d = 0.00208 hr^{-1}.

The HYDROBIOGEOCHEM results compare well with those supplied by Valocchi and Tebes (Figure 6.3). In Figure 6.3, the solid lines denote the results supplied by Valocchi and Tebes, the symbols denote the HYDROBIOGEOCHEM results. The input data sets for Case A are provided in Table 6.8; the input data files for all three cases can be obtained on floppy disk.

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.

Figure 6.4. Steady State Flow Field

The injection and extraction wells are for the mining of copper from the deposit. The initial mineral composition based on volume is 0.5% chrysocolla, 2.5% goethite, 5% kaolinite, 5% muscovite, and 82% quartz. The copper containing ore is chrysocolla.

Twelve chemical components are included in the simulation: Na^{+}, K^{+}, Ca^{2+}, H^{+}, Cu^{2+}, Al^{3+}, Fe^{2+}, $SiO_{2\,(aq)}$, HCO_3^{-}, SO_4^{2-}, Cl^{-}, and $O_{2\,(aq)}$. In addition to the five primary minerals which exist at the start of the simulation, five secondary minerals may form as the geochemical conditions change within the region. The reactions governing the formation and dissolution of all minerals are simulated as kinetic and are listed below. The rates of these reactions and the molar volumes of these minerals are summarized in Table 6.9.

$$\text{Chrysocolla} + 0.39H^+ \rightleftharpoons -1.61H^+ + Cu^{2+} + SiO_{2(aq)} + 3H_2O \quad (6.7.1)$$

$$\text{Jurbanite} \rightleftharpoons Al^{3+} - H^+ + SO_4^{2-} + 6H_2O \quad (6.7.2)$$

$$\text{Alunite} \rightleftharpoons 3Al^{3+} - 6H^+ + K^+ + 2SO_4^{2-} + 6H_2O \quad (6.7.3)$$

$$\text{Goethite} \rightleftharpoons Fe^{2+} - 2H^+ + 0.25O_2 + 1.5H_2O \quad (6.7.4)$$

$$\text{Gypsum} \rightleftharpoons Ca^{2+} + SO_4^{2-} + 2H_2O \quad (6.7.5)$$

$$\text{Jarosite} \rightleftharpoons K^+ - 3H^+ + 3Fe^{2+} + 2SO_4^{2-} + 0.75O_2 + 4.5H_2O \quad (6.7.6)$$

$$\text{Kaolinite} \rightleftharpoons 2Al^{3+} - 6H^+ + 2SiO_{2(aq)} + 5H_2O \quad (6.7.7)$$

$$\text{Muscovite} \rightleftharpoons 3Al^{3+} + K^+ - 10H^+ + 3SiO_{2(aq)} + 6H_2O \quad (6.7.8)$$

$$\text{Quartz} \rightleftharpoons SiO_{2(aq)} \quad (6.7.9)$$

$$SiO_{2(am)} \rightleftharpoons SiO_{2(aq)} \quad (6.7.10)$$

Table 6.9. Molar Volumes, Initial Conditions and Kinetic Rates for Precipitated Species.

Mineral	Molar Volume (dm^3/mol)	Initial Volume Fraction	Initial Concentration (mol/dm^3)	log k_f (yr^{-1})	log k_b (yr^{-1})
Chyrsocolla	0.07319	0.005	6.83153E-2	0.49881	-3.42919
Jurbanite	0.1260	0.000	0.00000D00	-0.50119	2.72881
Alunite	0.29360	0.000	0.00000D00	-0.50119	-0.15329
Goethite	0.02082	0.025	1.20077E+0	-0.50119	7.45381
Gypsum	0.07469	0.000	0.00000E00	0.49881	4.98081
Jarosite	0.15675	0.000	0.00000E00	-0.50119	34.33881
Kaolinite	0.09952	0.050	5.02412E-1	-2.50119	- 9.31119

Muscovite	0.14071	0.050	3.55341E-1	-2.50119	-16.09119
Quartz	0.022688	0.820	3.61425E+1	-3.50119	0.49781
Amorphous Silica	0.0290	0.000	0.00000E00	-0.50119	2.21281

The fluid composition is simulated using thirty-four soluble product species as well as the twelve aqueous component species. The formation of all aqueous complexed species is assumed to be equilibrium. Table 6.10 lists the reaction tableau for these aqueous species and the equilibrium constants for their formation. Table 6.11 summarizes the total initial concentration of each of the twelve chemical components present in solution in the matrix. The program determines the initial equilibrium aqueous speciation and the activity coefficients for all aqueous species. The pH of the fluid initially in the matrix is 8. The initial conditions in the matrix reflect a partial pressure of $CO_{2(g)}$ and $O_{2(g)}$ of 1E-3 and 0.20 atm, respectively. The density of the initial matrix fluid is 1.0005 kg/dm^3.

Table 6.10. Tableau of Equilibrium Aqueous Reactions for Copper Leaching Application.

	Na^+	K^+	Ca^{2+}	H^+	Cu^{2+}	Al^{3+}	Fe^{2+}	$SiO_{2\,(aq)}$		HCO_3^-		SO_4^{2-}	Cl^-	$O_{2\,(aq)}$
													log K	
OH-	0	0	0	-1	0	0	0	0	0	0	0	0	-13.995	
Fe^{3+}	0	0	0	1	0	0	1	0	0	0	0	0.25	8.490	
$Al(OH)_2^+$	0	0	0	-2	0	1	0	0	0	0	0	0	-10.595	
$Al(OH)_{3\,(aq)}$	0	0	0	-3	0	1	0	0	0	0	0	0	-16.158	
$Al(OH)_4^-$	0	0	0	-4	0	1	0	0	0	0	0	0	-22.883	
$Al(SO4)_2^-$	0	0	0	0	0	1	0	0	0	2	0	0	4.9	
$AlOH^{2+}$	0	0	0	-1	0	1	0	0	0	0	0	0	-4.9571	
$AlSO_4^+$	0	0	0	0	0	1	0	0	0	1	0	0	3.01	
H_2CO3^*	0	0	0	1	0	0	0	0	1	0	0	0	6.3447	
CO_3^{-2}	0	0	0	-1	0	0	0	0	1	0	0	0	-10.329	
$CaCO_{3\,(aq)}$	0	0	1	-1	0	0	0	0	1	0	0	0	-7.0017	
$CaHCO_3^+$	0	0	1	0	0	0	0	0	1	0	0	0	1.0467	
$CaOH^+$	0	0	1	-1	0	0	0	0	0	0	0	0	-12.8500	
$CaSO_{4(aq)}$	0	0	1	0	0	0	0	0	0	1	0	0	2.1111	
$CuOH^+$	0	0	0	-1	1	0	0	0	0	0	0	0	-7.2875	
$CuSO_{4(aq)}$	0	0	0	0	1	0	0	0	0	1	0	0	2.31	
$Fe[II](OH)_{2\,(aq)}$	0	0	0	-2	0	0	1	0	0	0	0	0	-20.6000	
$Fe[III](OH)_2^+$	0	0	0	-1	0	0	1	0	0	0	0	0.25	2.820	
$Fe[III](OH)_{3\,(aq)}$		0	0	0	-2	0	0	1	0	0	0	0	0.25-3.51	
$Fe[II](OH)_3^-$	0	0	0	-3	0	0	1	0	0	0	0	0	-31.000	
$Fe[III](OH)_4^-$	0	0	0	-3	0	0	1	0	0	0	0	0.25	-13.110	
$Fe[III](SO_4)_2^-$	0	0	0	1	0	0	1	0	0	2	0	0.25	11.704	
$Fe[III]HSO_4^{2+}$	0	0	0	2	0	0	1	0	0	1	0	0.25	10.030	
$Fe[II]SO_{4\,(aq)}$	0	0	0	0	0	0	1	0	0	1	0	0	2.2	
$Fe[III]SO_4^+$	0	0	0	1	0	0	1	0	0	1	0	0.25	10.418	
$H2SO_{4\,(aq)}$	0	0	0	2	0	0	0	0	0	1	0	0	-1.0209	

HSO_4^-	0	0	0	1	0	0	0	0	0	1	0	0	1.9791
$Cu[II]Cl^+$	0	0	0	0	1	0	0	0	0	0	1	0	0.437
$Cu[II]Cl_{2\,(aq)}$	0	0	0	0	1	0	0	0	0	0	2	0	0.1585
$Cu[II]Cl_4^{2-}$	0	0	0	0	1	0	0	0	0	0	4	0	-4.5681
Cu^+	0	0	0	-1	1	0	0	0	0	0	0	-0.25	-18.77
$Cu[I]Cl_2^-$	0	0	0	-1	1	0	0	0	0	0	2	-0.25	-13.949
$Cu[I]Cl_3^{-2}$	0	0	0	-1	1	0	0	0	0	0	3	-0.25	-13.141
$Cu[IIO_2^{-2}$	0	0	0	-4	1	0	0	0	0	0	0	0	-39.45

Table 6.11. Total Concentration of Components Initially in the Matrix Fluid and in the Injection Fluid.

Component	Initial Concentration (mol/dm^3 ~~liquid~~)	Injection Fluid Concentration (~~mol/dm^3~~ liquid)
Na^+	5.00250E-3	5.2600E-3
K^+	2.57809E-5	1.3305E-4
Ca^{2+}	6.86031E-4	1.6086E-2
H^+	1.54064E-5	3.4649E-1
Cu^{2+}	3.23586E-8	1.0520E-8
Al^{3+}	2.04237E-8	2.6300E-2
Fe^{2+}	3.59984E-12	4.5694E-2
$SiO_{2\,(aq)}$	1.87124E-4	2.0243E-3
HCO_3^-	1.74271E-3	3.5737E-4
SO_4^{2-}	5.00246E-4	2.7435E-1
Cl^-	3.67274E-3	5.2600E-3
$O_{2\,(aq)}$	2.52896E-4	1.1689E-2
pH	8.0	1.0

The injection fluid has a pH of 1.0 and density of 1.0520 kg/dm^3. Its composition remains constant throughout the simulation. The total concentration of the aqueous components in the injection fluid is detailed in Table 6.11. The dissolution of the copper ore is pH dependent; as can be seen from reaction **(6.7.1)**, the dissolution rate is proportional to the activity of H^+ to the 0.39 power.

The simulation was run for a period of 0.25 years using a uniform time step of 1E-3 years. The same time step is used for both hydrologic transport and for the geochemical reactions. The operator splitting solution method was implemented. Figure 6.5 depicts the projected copper recovery and the pH and pe at the extraction well over time. Figures 6.6 and 6.7 show the spatial distribution of chrysocolla and the five secondary minerals at the end of the 0.25 year simulation. The results compare well with those provided by Lichtner (1997). The input data sets for this example are given in Table 6.12.

Table 6.12 Input Data Sets for Problem 7

```
   1  Copper Leaching from 5 Well Pattern (P. Lichtner Benchmark) (kg,dm,years)
 1 0 0 0 1
C ******* DATA SET 2: BASIC INTEGER PARAMTERS
 961 900 1 0 25   1 4 -1 1 0   0 0 40 1 50   0 1 0 1 11   1 1 1
C ******* DATA SET 3: BASIC REAL PARAMETERS
 1.0D-2 0.0D0 1.0D-2 0.25D0 1.0D0   1.0D0 1.0D0 1.0D00 1.0D-6 1.0D0
C ******* DATA SET 4: PRINT AND AUXILIARY STORGE CONTROL
44000000004000000000400004
11111111111111111111111111
1.0D38
C ******* DATA SET 5: CHEMICAL OUTPUT AND CHEMICAL PROPERTY TYPE INDICATOR
 3
 1 481 961 NODEP

C ******* DATA SET 6: MATERIAL PROPERTIES
 0.0D0 0.0D0 0.0D0 2.56D0 AL AT AM RHOB
C ******* DATA SET 7: NODE COORDINATES
    1   30     1       0.0D0   0.0D0  0.0
   32   30     1       5.0D0   0.0D0  0.0
   63   30     1      10.0D0   0.0D0  0.0
   94   30     1      15.0D0   0.0D0  0.0
  125   30     1      20.0D0   0.0D0  0.0
  156   30     1      25.0D0   0.0D0  0.0
  187   30     1      30.0D0   0.0D0  0.0
  218   30     1      35.0D0   0.0D0  0.0
  249   30     1      40.0D0   0.0D0  0.0
  280   30     1      45.0D0   0.0D0  0.0
  311   30     1      50.0D0   0.0D0  0.0
  342   30     1      55.0D0   0.0D0  0.0
  373   30     1      60.0D0   0.0D0  0.0
  404   30     1      65.0D0   0.0D0  0.0
  435   30     1      70.0D0   0.0D0  0.0
  466   30     1      75.0D0   0.0D0  0.0
  497   30     1      80.0D0   0.0D0  0.0
  528   30     1      85.0D0   0.0D0  0.0
  559   30     1      90.0D0   0.0D0  0.0
  590   30     1      95.0D0   0.0D0  0.0
  621   30     1     100.0D0   0.0D0  0.0
  652   30     1     105.0D0   0.0D0  0.0
  683   30     1     110.0D0   0.0D0  0.0
  714   30     1     115.0D0   0.0D0  0.0
  745   30     1     120.0D0   0.0D0  0.0
  776   30     1     125.0D0   0.0D0  0.0
  807   30     1     130.0D0   0.0D0  0.0
  838   30     1     135.0D0   0.0D0  0.0
  869   30     1     140.0D0   0.0D0  0.0
  900   30     1     145.0D0   0.0D0  0.0
  931   30     1     150.0D0   0.0D0  0.0
    0    0     0       0.0     0.0    0.0            END OF X-COORD
    1   30     1       0.0D0   5.0D0  0.0
   32   30     1       0.0D0   5.0D0  0.0
   63   30     1       0.0D0   5.0D0  0.0
   94   30     1       0.0D0   5.0D0  0.0
```

Table 6.12 Input Data Sets for Problem 7 (continued)

```
  125   30     1       0.0D0   5.0D0  0.0
  156   30     1       0.0D0   5.0D0  0.0
```

```
  187   30     1      0.0D0   5.0D0  0.0
  218   30     1      0.0D0   5.0D0  0.0
  249   30     1      0.0D0   5.0D0  0.0
  280   30     1      0.0D0   5.0D0  0.0
  311   30     1      0.0D0   5.0D0  0.0
  342   30     1      0.0D0   5.0D0  0.0
  373   30     1      0.0D0   5.0D0  0.0
  404   30     1      0.0D0   5.0D0  0.0
  435   30     1      0.0D0   5.0D0  0.0
  466   30     1      0.0D0   5.0D0  0.0
  497   30     1      0.0D0   5.0D0  0.0
  528   30     1      0.0D0   5.0D0  0.0
  559   30     1      0.0D0   5.0D0  0.0
  590   30     1      0.0D0   5.0D0  0.0
  621   30     1      0.0D0   5.0D0  0.0
  652   30     1      0.0D0   5.0D0  0.0
  683   30     1      0.0D0   5.0D0  0.0
  714   30     1      0.0D0   5.0D0  0.0
  745   30     1      0.0D0   5.0D0  0.0
  776   30     1      0.0D0   5.0D0  0.0
  807   30     1      0.0D0   5.0D0  0.0
  838   30     1      0.0D0   5.0D0  0.0
  869   30     1      0.0D0   5.0D0  0.0
  900   30     1      0.0D0   5.0D0  0.0
  931   30     1      0.0D0   5.0D0  0.0
    0    0     0      0.0D0   0.0D0  0.0D0         END OF Z-COORD
C ******* DATA SET 8: ELEMENT CONNECTIVITY
    1    1   32   33    2    1   30   30           IE
C ******* DATA SET 10: CHEMICAL COMPONENT INFORMATION
 12 0   0 0 0 10   0 0   NOHA HS  NOKX KY KZ KP  NOMB MA
 Na +
  1   1
 K+
  2   1
 Ca +2
  3   1
 H+
  4   1
 Cu +2
  5   1
 Al +3
  6   1
 Fe +2
  7   1
 SiO2 (aq)
  8   1
 HCO3 -
  9   1
 SO4 -2
 10   1
 Cl -
 11   1
```

Table 6.12 Input Data Sets for Problem 7 (continued)

```
 O2 (aq)
 12   1
C ******* DATA SET 11:  INITIAL CONDITIONS (MASS/MEDIA VOLUME)
    1   960   1    2.50125D-4  0.0D0     0.0D0

    0    0    0    0.0         0.0       0.0          END OF I.C. Na+
```

```
1   960   1    1.28904D-6  0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. K+
1   960   1    3.43016D-5  0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. Ca+2
1   960   1    7.70319D-7  0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. H+
1   960   1    1.61793D-9  0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. Cu+2
1   960   1    1.02118D-9  0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. Al+3
1   960   1    1.79992D-13 0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. Fe+2
1   960   1    9.35618D-6  0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. SiO2(aq)
1   960   1    8.71354D-5  0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. HCO3-
1   960   1    2.50123D-5  0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. SO4 -2
1   960   1    1.83637D-4  0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. Cl -
1   960   1    1.26448D-5  0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. O2 (aq)
1   960   1    6.83153D-2  0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. Chrysocolla - P1
1   960   1    0.00000D00  0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. Jurbanite - P2
1   960   1    0.00000D00  0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. Alunite   - P3
1   960   1    1.20077D00  0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. Goethite  - P4
1   960   1    0.00000D00  0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. Gypsum    - P5
1   960   1    0.00000D00  0.0D0      0.0D0
```

Table 6.12 Input Data Sets for Problem 7 (continued)

```
0    0    0    0.0         0.0        0.0          END OF I.C. Jarosite  - P6
1   960   1    5.02412D-1  0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. Kaolinite - P7
1   960   1    3.55341D-1  0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. Muscovite - P8
1   960   1    3.61425D+1  0.0D0      0.0D0

0    0    0    0.0         0.0        0.0          END OF I.C. Quartz    - P9
```

```
    1   960   1    0.00000D00  0.0D0     0.0D0

    0    0    0    0.0         0.0       0.0          END OF I.C. SiO2 (am) - P10
C ******* DATA SET 12: CONTROL INTEGERS FOR TRANSIENT SOURCE/SINK AND B.C.
    0  0  0    2  2  2    0  0  0    0  0  0  0
C ******* DATA SET 13: WELL SOURCE/SINK (MASS/LIQUID VOLUME)
  1  961
  0.0D0   5.2600D-3   2.0D0   5.260D-3
  0.0D0   0.00D0      2.0D0   0.00D0
    1    1    1    1    1
    0    0    0    0    0                          END OF S/S Na+
  0.0D0   1.3305D-4   2.0D0   1.3305D-4
  0.0D0   0.00D0      2.0D0   0.00D0
    1    1    1    1    1
    0    0    0    0    0                          END OF S/S K+
  0.0D0   1.6086D-2   2.0D0   1.6086D-2
  0.0D0   0.00D0      2.0D0   0.00D0
    1    1    1    1    1
    0    0    0    0    0                          END OF S/S Ca+2
  0.0D0   3.4649D-1   2.0D0   3.4649D-1
  0.0D0   0.00D0      2.0D0   0.00D0
    1    1    1    1    1
    0    0    0    0    0                          END OF S/S H+
  0.0D0   1.0520D-8   2.0D0   1.0520D-8
  0.0D0   0.00D0      2.0D0   0.00D0
    1    1    1    1    1
    0    0    0    0    0                          END OF S/S Cu+2
  0.0D0   2.6300D-2   2.0D0   2.6300D-2
  0.0D0   0.00D0      2.0D0   0.00D0
    1    1    1    1    1
    0    0    0    0    0                          END OF S/S Al+3
  0.0D0   4.5694D-2   2.0D0   4.5694D-2
  0.0D0   0.00D0      2.0D0   0.00D0
    1    1    1    1    1
    0    0    0    0    0                          END OF S/S Fe+2
  0.0D0   2.0343D-3   2.0D0   2.0343D-3
  0.0D0   0.00D0      2.0D0   0.00D0
    1    1    1    1    1
    0    0    0    0    0                          END OF S/S SiO2(aq)
  0.0D0   3.5737D-4   2.0D0   3.5737D-4
  0.0D0   0.00D0      2.0D0   0.00D0
    1    1    1    1    1
    0    0    0    0    0                          END OF S/S HCO3-
  0.0D0   2.7435D-1   2.0D0   2.7435D-1
  0.0D0   0.00D0      2.0D0   0.00D0
```

Table 6.12 Input Data Sets for Problem 7 (continued)

```
    1    1    1    1    1
    0    0    0    0    0                          END OF S/S SO4 -2
  0.0D0   5.2600D-3   2.0D0   5.2600D-3
  0.0D0   0.00D0      2.0D0   0.00D0
    1    1    1    1    1
    0    0    0    0    0                          END OF S/S Cl-
  0.0D0   1.1689D-2   2.0D0   1.1689D-2
  0.0D0   0.00D0      2.0D0   0.00D0
    1    1    1    1    1
    0    0    0    0    0                          END OF S/S O2(aq)
  0.0D0   1.6556D4    2.0D0   1.6556D4
  0.0D0  -1.6556D4    2.0D0  -1.6556D4
    1    1    1    1    1
    0    0    0    0    0                          Q (dm^3/year per dm depth)
```

```
  0.0D0   1.0520D0    2.0D0   1.0520D0
  0.0D0   1.0005D0    2.0D0   1.0005D0
    1    1    1    1    1
    0    0    0    0    0                          END OF RHOL S/S
C ******* DATA SET 16: HYDROLOGICAL VARIABLES
    1    0    0   .4727141D+04   .4727141D+04   .00D+00   .00D+00
    2    0    0   .0000000D+00   .2159275D+04   .00D+00   .00D+00
    3    0    0   .0000000D+00   .1176175D+04   .00D+00   .00D+00
    4    0    0   .0000000D+00   .7639950D+03   .00D+00   .00D+00
    5    0    0   .0000000D+00   .5577350D+03   .00D+00   .00D+00
    6    0    0   .0000000D+00   .4381750D+03   .00D+00   .00D+00
    7    0    0   .0000000D+00   .3608200D+03   .00D+00   .00D+00
    8    0    0   .0000000D+00   .3066300D+03   .00D+00   .00D+00
    9    0    0   .0000000D+00   .2663950D+03   .00D+00   .00D+00
   10    0    0   .0000000D+00   .2351750D+03   .00D+00   .00D+00
   11    0    0   .0000000D+00   .2101000D+03   .00D+00   .00D+00
   12    0    0   .0000000D+00   .1893600D+03   .00D+00   .00D+00
   13    0    0   .0000000D+00   .1717950D+03   .00D+00   .00D+00
   14    0    0   .0000000D+00   .1565750D+03   .00D+00   .00D+00
   15    0    0   .0000000D+00   .1431200D+03   .00D+00   .00D+00
   16    0    0   .0000000D+00   .1310350D+03   .00D+00   .00D+00
   17    0    0   .0000000D+00   .1199650D+03   .00D+00   .00D+00
   18    0    0   .0000000D+00   .1097050D+03   .00D+00   .00D+00
   19    0    0   .0000000D+00   .1000525D+03   .00D+00   .00D+00
   20    0    0   .0000000D+00   .9086150D+02   .00D+00   .00D+00
   21    0    0   .0000000D+00   .8201650D+02   .00D+00   .00D+00
   22    0    0   .0000000D+00   .7342650D+02   .00D+00   .00D+00
   23    0    0   .0000000D+00   .6502000D+02   .00D+00   .00D+00
   24    0    0   .0000000D+00   .5674350D+02   .00D+00   .00D+00
   25    0    0   .0000000D+00   .4855300D+02   .00D+00   .00D+00
   26    0    0   .0000000D+00   .4041700D+02   .00D+00   .00D+00
   27    0    0   .0000000D+00   .3231400D+02   .00D+00   .00D+00
   28    0    0   .0000000D+00   .2422750D+02   .00D+00   .00D+00
   29    0    0   .0000000D+00   .1614950D+02   .00D+00   .00D+00
   30    0    0   .0000000D+00   .8074600D+01   .00D+00   .00D+00
   31    0    0   .0000000D+00   .0000000D+00   .00D+00   .00D+00
   32    0    0   .2159275D+04   .0000000D+00   .00D+00   .00D+00
   33    0    0   .1156725D+04   .1156725D+04   .00D+00   .00D+00
   34    0    0   .4818800D+03   .8290250D+03   .00D+00   .00D+00
   35    0    0   .2385950D+03   .6245650D+03   .00D+00   .00D+00
   36    0    0   .1365450D+03   .4930650D+03   .00D+00   .00D+00
```

Table 6.12 Input Data Sets for Problem 7 (continued)

```
   37    0    0   .8722150D+02   .4042050D+03   .00D+00   .00D+00
   38    0    0   .6037350D+02   .3411000D+03   .00D+00   .00D+00
   39    0    0   .4433700D+02   .2942700D+03   .00D+00   .00D+00
   40    0    0   .3405950D+02   .2581850D+03   .00D+00   .00D+00
   41    0    0   .2711500D+02   .2294850D+03   .00D+00   .00D+00
   42    0    0   .2223200D+02   .2060200D+03   .00D+00   .00D+00
   43    0    0   .1869450D+02   .1863600D+03   .00D+00   .00D+00
   44    0    0   .1607350D+02   .1695450D+03   .00D+00   .00D+00
   45    0    0   .1409900D+02   .1548650D+03   .00D+00   .00D+00
   46    0    0   .1259500D+02   .1418200D+03   .00D+00   .00D+00
   47    0    0   .1144250D+02   .1300250D+03   .00D+00   .00D+00
   48    0    0   .1055700D+02   .1191950D+03   .00D+00   .00D+00
   49    0    0   .9877400D+01   .1091150D+03   .00D+00   .00D+00
   50    0    0   .9359300D+01   .9960550D+02   .00D+00   .00D+00
   51    0    0   .8968350D+01   .9052650D+02   .00D+00   .00D+00
   52    0    0   .8677850D+01   .8176950D+02   .00D+00   .00D+00
   53    0    0   .8466600D+01   .7324950D+02   .00D+00   .00D+00
   54    0    0   .8317250D+01   .6489800D+02   .00D+00   .00D+00
```

55	0	0	.8215650D+01	.5666250D+02	.00D+00	.00D+00
56	0	0	.8150000D+01	.4850300D+02	.00D+00	.00D+00
57	0	0	.8110450D+01	.4038900D+02	.00D+00	.00D+00
58	0	0	.8088950D+01	.3230000D+02	.00D+00	.00D+00
59	0	0	.8078950D+01	.2422250D+02	.00D+00	.00D+00
60	0	0	.8075350D+01	.1614850D+02	.00D+00	.00D+00
61	0	0	.8074600D+01	.8074600D+01	.00D+00	.00D+00
62	0	0	.8074600D+01	.0000000D+00	.00D+00	.00D+00
63	0	0	.1176175D+04	.0000000D+00	.00D+00	.00D+00
64	0	0	.8290250D+03	.4818800D+03	.00D+00	.00D+00
65	0	0	.5321850D+03	.5321850D+03	.00D+00	.00D+00
66	0	0	.3359600D+03	.4818850D+03	.00D+00	.00D+00
67	0	0	.2203600D+03	.4180950D+03	.00D+00	.00D+00
68	0	0	.1519650D+03	.3614650D+03	.00D+00	.00D+00
69	0	0	.1099365D+03	.3149650D+03	.00D+00	.00D+00
70	0	0	.8291450D+02	.2773400D+03	.00D+00	.00D+00
71	0	0	.6478500D+02	.2467000D+03	.00D+00	.00D+00
72	0	0	.5216800D+02	.2214050D+03	.00D+00	.00D+00
73	0	0	.4311950D+02	.2001650D+03	.00D+00	.00D+00
74	0	0	.3647300D+02	.1820300D+03	.00D+00	.00D+00
75	0	0	.3149950D+02	.1662800D+03	.00D+00	.00D+00
76	0	0	.2772700D+02	.1523800D+03	.00D+00	.00D+00
77	0	0	.2483950D+02	.1399150D+03	.00D+00	.00D+00
78	0	0	.2261800D+02	.1285550D+03	.00D+00	.00D+00
79	0	0	.2090700D+02	.1180700D+03	.00D+00	.00D+00
80	0	0	.1959350D+02	.1082500D+03	.00D+00	.00D+00
81	0	0	.1859150D+02	.9895000D+02	.00D+00	.00D+00
82	0	0	.1783600D+02	.9003600D+02	.00D+00	.00D+00
83	0	0	.1727650D+02	.8140950D+02	.00D+00	.00D+00
84	0	0	.1687150D+02	.7299250D+02	.00D+00	.00D+00
85	0	0	.1658700D+02	.6472150D+02	.00D+00	.00D+00
86	0	0	.1639550D+02	.5654650D+02	.00D+00	.00D+00
87	0	0	.1627400D+02	.4843200D+02	.00D+00	.00D+00
88	0	0	.1620300D+02	.4034950D+02	.00D+00	.00D+00
89	0	0	.1616650D+02	.3228150D+02	.00D+00	.00D+00
90	0	0	.1615150D+02	.2421600D+02	.00D+00	.00D+00
91	0	0	.1614800D+02	.1614800D+02	.00D+00	.00D+00

Table 6.12 Input Data Sets for Problem 7 (continued)

92	0	0	.1614850D+02	.8075350D+01	.00D+00	.00D+00
93	0	0	.1614950D+02	.0000000D+00	.00D+00	.00D+00
94	0	0	.7639950D+03	.0000000D+00	.00D+00	.00D+00
95	0	0	.6245650D+03	.2385950D+03	.00D+00	.00D+00
96	0	0	.4818850D+03	.3359600D+03	.00D+00	.00D+00
97	0	0	.3526900D+03	.3526900D+03	.00D+00	.00D+00
98	0	0	.2569650D+03	.3359600D+03	.00D+00	.00D+00
99	0	0	.1903500D+03	.3085900D+03	.00D+00	.00D+00
100	0	0	.1444950D+03	.2799600D+03	.00D+00	.00D+00
101	0	0	.1125990D+03	.2534300D+03	.00D+00	.00D+00
102	0	0	.8999850D+02	.2298800D+03	.00D+00	.00D+00
103	0	0	.7365300D+02	.2092650D+03	.00D+00	.00D+00
104	0	0	.6160450D+02	.1912100D+03	.00D+00	.00D+00
105	0	0	.5257700D+02	.1753150D+03	.00D+00	.00D+00
106	0	0	.4572400D+02	.1611750D+03	.00D+00	.00D+00
107	0	0	.4047050D+02	.1484650D+03	.00D+00	.00D+00
108	0	0	.3641800D+02	.1368900D+03	.00D+00	.00D+00
109	0	0	.3328350D+02	.1262250D+03	.00D+00	.00D+00
110	0	0	.3086100D+02	.1162750D+03	.00D+00	.00D+00
111	0	0	.2899750D+02	.1068750D+03	.00D+00	.00D+00
112	0	0	.2757700D+02	.9790550D+02	.00D+00	.00D+00
113	0	0	.2650900D+02	.8925650D+02	.00D+00	.00D+00

114	0	0	.2572100D+02	.8084100D+02	.00D+00	.00D+00
115	0	0	.2515500D+02	.7259000D+02	.00D+00	.00D+00
116	0	0	.2476300D+02	.6444800D+02	.00D+00	.00D+00
117	0	0	.2450500D+02	.5637100D+02	.00D+00	.00D+00
118	0	0	.2434750D+02	.4832800D+02	.00D+00	.00D+00
119	0	0	.2426100D+02	.4029550D+02	.00D+00	.00D+00
120	0	0	.2422200D+02	.3226000D+02	.00D+00	.00D+00
121	0	0	.2421200D+02	.2421200D+02	.00D+00	.00D+00
122	0	0	.2421600D+02	.1615150D+02	.00D+00	.00D+00
123	0	0	.2422250D+02	.8078950D+01	.00D+00	.00D+00
124	0	0	.2422750D+02	.0000000D+00	.00D+00	.00D+00
125	0	0	.5577350D+03	.0000000D+00	.00D+00	.00D+00
126	0	0	.4930650D+03	.1365450D+03	.00D+00	.00D+00
127	0	0	.4180950D+03	.2203600D+03	.00D+00	.00D+00
128	0	0	.3359600D+03	.2569650D+03	.00D+00	.00D+00
129	0	0	.2644600D+03	.2644600D+03	.00D+00	.00D+00
130	0	0	.2079600D+03	.2569650D+03	.00D+00	.00D+00
131	0	0	.1650900D+03	.2428600D+03	.00D+00	.00D+00
132	0	0	.1329950D+03	.2265450D+03	.00D+00	.00D+00
133	0	0	.1089590D+03	.2101350D+03	.00D+00	.00D+00
134	0	0	.9084150D+02	.1945500D+03	.00D+00	.00D+00
135	0	0	.7706950D+02	.1801050D+03	.00D+00	.00D+00
136	0	0	.6650800D+02	.1668350D+03	.00D+00	.00D+00
137	0	0	.5834900D+02	.1546450D+03	.00D+00	.00D+00
138	0	0	.5201300D+02	.1434050D+03	.00D+00	.00D+00
139	0	0	.4707850D+02	.1329600D+03	.00D+00	.00D+00
140	0	0	.4323650D+02	.1231750D+03	.00D+00	.00D+00
141	0	0	.4025550D+02	.1139200D+03	.00D+00	.00D+00
142	0	0	.3795900D+02	.1050700D+03	.00D+00	.00D+00
143	0	0	.3621050D+02	.9654050D+02	.00D+00	.00D+00
144	0	0	.3490100D+02	.8824350D+02	.00D+00	.00D+00
145	0	0	.3394300D+02	.8010850D+02	.00D+00	.00D+00
146	0	0	.3326450D+02	.7207850D+02	.00D+00	.00D+00

Table 6.12 Input Data Sets for Problem 7 (continued)

147	0	0	.3280550D+02	.6410850D+02	.00D+00	.00D+00
148	0	0	.3251500D+02	.5616200D+02	.00D+00	.00D+00
149	0	0	.3234900D+02	.4821350D+02	.00D+00	.00D+00
150	0	0	.3227100D+02	.4024600D+02	.00D+00	.00D+00
151	0	0	.3225000D+02	.3225000D+02	.00D+00	.00D+00
152	0	0	.3226000D+02	.2422200D+02	.00D+00	.00D+00
153	0	0	.3228150D+02	.1616650D+02	.00D+00	.00D+00
154	0	0	.3230000D+02	.8088950D+01	.00D+00	.00D+00
155	0	0	.3231400D+02	.0000000D+00	.00D+00	.00D+00
156	0	0	.4381750D+03	.0000000D+00	.00D+00	.00D+00
157	0	0	.4042050D+03	.8722150D+02	.00D+00	.00D+00
158	0	0	.3614650D+03	.1519650D+03	.00D+00	.00D+00
159	0	0	.3085900D+03	.1903500D+03	.00D+00	.00D+00
160	0	0	.2569650D+03	.2079600D+03	.00D+00	.00D+00
161	0	0	.2119500D+03	.2119500D+03	.00D+00	.00D+00
162	0	0	.1749150D+03	.2079650D+03	.00D+00	.00D+00
163	0	0	.1453200D+03	.1997500D+03	.00D+00	.00D+00
164	0	0	.1219900D+03	.1895650D+03	.00D+00	.00D+00
165	0	0	.1036850D+03	.1786950D+03	.00D+00	.00D+00
166	0	0	.8932250D+02	.1678200D+03	.00D+00	.00D+00
167	0	0	.7803550D+02	.1572700D+03	.00D+00	.00D+00
168	0	0	.6915150D+02	.1471650D+03	.00D+00	.00D+00
169	0	0	.6215350D+02	.1375450D+03	.00D+00	.00D+00
170	0	0	.5664650D+02	.1283750D+03	.00D+00	.00D+00
171	0	0	.5232850D+02	.1195950D+03	.00D+00	.00D+00
172	0	0	.4896500D+02	.1111500D+03	.00D+00	.00D+00

173	0	0	.4637250D+02	.1029500D+03	.00D+00	.00D+00
174	0	0	.4440400D+02	.9494350D+02	.00D+00	.00D+00
175	0	0	.4294050D+02	.8706800D+02	.00D+00	.00D+00
176	0	0	.4188500D+02	.7927100D+02	.00D+00	.00D+00
177	0	0	.4115500D+02	.7150800D+02	.00D+00	.00D+00
178	0	0	.4068000D+02	.6374500D+02	.00D+00	.00D+00
179	0	0	.4040000D+02	.5595450D+02	.00D+00	.00D+00
180	0	0	.4026350D+02	.4811800D+02	.00D+00	.00D+00
181	0	0	.4022500D+02	.4022500D+02	.00D+00	.00D+00
182	0	0	.4024600D+02	.3227100D+02	.00D+00	.00D+00
183	0	0	.4029550D+02	.2426100D+02	.00D+00	.00D+00
184	0	0	.4034950D+02	.1620300D+02	.00D+00	.00D+00
185	0	0	.4038900D+02	.8110450D+01	.00D+00	.00D+00
186	0	0	.4041700D+02	.0000000D+00	.00D+00	.00D+00
187	0	0	.3608200D+03	.0000000D+00	.00D+00	.00D+00
188	0	0	.3411000D+03	.6037350D+02	.00D+00	.00D+00
189	0	0	.3149650D+03	.1099365D+03	.00D+00	.00D+00
190	0	0	.2799600D+03	.1444950D+03	.00D+00	.00D+00
191	0	0	.2428600D+03	.1650900D+03	.00D+00	.00D+00
192	0	0	.2079650D+03	.1749150D+03	.00D+00	.00D+00
193	0	0	.1772950D+03	.1772950D+03	.00D+00	.00D+00
194	0	0	.1513900D+03	.1749150D+03	.00D+00	.00D+00
195	0	0	.1300050D+03	.1696800D+03	.00D+00	.00D+00
196	0	0	.1125850D+03	.1628500D+03	.00D+00	.00D+00
197	0	0	.9850100D+02	.1552150D+03	.00D+00	.00D+00
198	0	0	.8716150D+02	.1472500D+03	.00D+00	.00D+00
199	0	0	.7806800D+02	.1392050D+03	.00D+00	.00D+00
200	0	0	.7080200D+02	.1312400D+03	.00D+00	.00D+00
201	0	0	.6502550D+02	.1234000D+03	.00D+00	.00D+00

Table 6.12 Input Data Sets for Problem 7 (continued)

202	0	0	.6046600D+02	.1156950D+03	.00D+00	.00D+00
203	0	0	.5690400D+02	.1081250D+03	.00D+00	.00D+00
204	0	0	.5416200D+02	.1006420D+03	.00D+00	.00D+00
205	0	0	.5209250D+02	.9321600D+02	.00D+00	.00D+00
206	0	0	.5057350D+02	.8581350D+02	.00D+00	.00D+00
207	0	0	.4950250D+02	.7839850D+02	.00D+00	.00D+00
208	0	0	.4879000D+02	.7093800D+02	.00D+00	.00D+00
209	0	0	.4835900D+02	.6340900D+02	.00D+00	.00D+00
210	0	0	.4814200D+02	.5579300D+02	.00D+00	.00D+00
211	0	0	.4807900D+02	.4807900D+02	.00D+00	.00D+00
212	0	0	.4811800D+02	.4026350D+02	.00D+00	.00D+00
213	0	0	.4821350D+02	.3234900D+02	.00D+00	.00D+00
214	0	0	.4832800D+02	.2434750D+02	.00D+00	.00D+00
215	0	0	.4843200D+02	.1627400D+02	.00D+00	.00D+00
216	0	0	.4850300D+02	.8150000D+01	.00D+00	.00D+00
217	0	0	.4855300D+02	.0000000D+00	.00D+00	.00D+00
218	0	0	.3066300D+03	.0000000D+00	.00D+00	.00D+00
219	0	0	.2942700D+03	.4433700D+02	.00D+00	.00D+00
220	0	0	.2773400D+03	.8291450D+02	.00D+00	.00D+00
221	0	0	.2534300D+03	.1125990D+03	.00D+00	.00D+00
222	0	0	.2265450D+03	.1329950D+03	.00D+00	.00D+00
223	0	0	.1997500D+03	.1453200D+03	.00D+00	.00D+00
224	0	0	.1749150D+03	.1513900D+03	.00D+00	.00D+00
225	0	0	.1529350D+03	.1529350D+03	.00D+00	.00D+00
226	0	0	.1340550D+03	.1513900D+03	.00D+00	.00D+00
227	0	0	.1181500D+03	.1478100D+03	.00D+00	.00D+00
228	0	0	.1049275D+03	.1429450D+03	.00D+00	.00D+00
229	0	0	.9404350D+02	.1372950D+03	.00D+00	.00D+00
230	0	0	.8515750D+02	.1311800D+03	.00D+00	.00D+00
231	0	0	.7796150D+02	.1248050D+03	.00D+00	.00D+00

232	0	0	.7218750D+02	.1182850D+03	.00D+00	.00D+00
233	0	0	.6760600D+02	.1116750D+03	.00D+00	.00D+00
234	0	0	.6402400D+02	.1050050D+03	.00D+00	.00D+00
235	0	0	.6127850D+02	.9827150D+02	.00D+00	.00D+00
236	0	0	.5923000D+02	.9146700D+02	.00D+00	.00D+00
237	0	0	.5775900D+02	.8457300D+02	.00D+00	.00D+00
238	0	0	.5676100D+02	.7757000D+02	.00D+00	.00D+00
239	0	0	.5614400D+02	.7043700D+02	.00D+00	.00D+00
240	0	0	.5582500D+02	.6316050D+02	.00D+00	.00D+00
241	0	0	.5573000D+02	.5573000D+02	.00D+00	.00D+00
242	0	0	.5579300D+02	.4814200D+02	.00D+00	.00D+00
243	0	0	.5595450D+02	.4040000D+02	.00D+00	.00D+00
244	0	0	.5616200D+02	.3251500D+02	.00D+00	.00D+00
245	0	0	.5637100D+02	.2450500D+02	.00D+00	.00D+00
246	0	0	.5654650D+02	.1639550D+02	.00D+00	.00D+00
247	0	0	.5666250D+02	.8215650D+01	.00D+00	.00D+00
248	0	0	.5674350D+02	.0000000D+00	.00D+00	.00D+00
249	0	0	.2663950D+03	.0000000D+00	.00D+00	.00D+00
250	0	0	.2581850D+03	.3405950D+02	.00D+00	.00D+00
251	0	0	.2467000D+03	.6478500D+02	.00D+00	.00D+00
252	0	0	.2298800D+03	.8999850D+02	.00D+00	.00D+00
253	0	0	.2101350D+03	.1089590D+03	.00D+00	.00D+00
254	0	0	.1895650D+03	.1219900D+03	.00D+00	.00D+00
255	0	0	.1696800D+03	.1300050D+03	.00D+00	.00D+00
256	0	0	.1513900D+03	.1340550D+03	.00D+00	.00D+00

Table 6.12 Input Data Sets for Problem 7 (continued)

257	0	0	.1351350D+03	.1351350D+03	.00D+00	.00D+00
258	0	0	.1210350D+03	.1340600D+03	.00D+00	.00D+00
259	0	0	.1090150D+03	.1314600D+03	.00D+00	.00D+00
260	0	0	.9892400D+02	.1278000D+03	.00D+00	.00D+00
261	0	0	.9055700D+02	.1234150D+03	.00D+00	.00D+00
262	0	0	.8369950D+02	.1185150D+03	.00D+00	.00D+00
263	0	0	.7815600D+02	.1132550D+03	.00D+00	.00D+00
264	0	0	.7374600D+02	.1077150D+03	.00D+00	.00D+00
265	0	0	.7030750D+02	.1019450D+03	.00D+00	.00D+00
266	0	0	.6769800D+02	.9597450D+02	.00D+00	.00D+00
267	0	0	.6579050D+02	.8980800D+02	.00D+00	.00D+00
268	0	0	.6447150D+02	.8344250D+02	.00D+00	.00D+00
269	0	0	.6363900D+02	.7687000D+02	.00D+00	.00D+00
270	0	0	.6319900D+02	.7008000D+02	.00D+00	.00D+00
271	0	0	.6306600D+02	.6306600D+02	.00D+00	.00D+00
272	0	0	.6316050D+02	.5582500D+02	.00D+00	.00D+00
273	0	0	.6340900D+02	.4835900D+02	.00D+00	.00D+00
274	0	0	.6374500D+02	.4068000D+02	.00D+00	.00D+00
275	0	0	.6410850D+02	.3280550D+02	.00D+00	.00D+00
276	0	0	.6444800D+02	.2476300D+02	.00D+00	.00D+00
277	0	0	.6472150D+02	.1658700D+02	.00D+00	.00D+00
278	0	0	.6489800D+02	.8317250D+01	.00D+00	.00D+00
279	0	0	.6502000D+02	.0000000D+00	.00D+00	.00D+00
280	0	0	.2351750D+03	.0000000D+00	.00D+00	.00D+00
281	0	0	.2294850D+03	.2711500D+02	.00D+00	.00D+00
282	0	0	.2214050D+03	.5216800D+02	.00D+00	.00D+00
283	0	0	.2092650D+03	.7365300D+02	.00D+00	.00D+00
284	0	0	.1945500D+03	.9084150D+02	.00D+00	.00D+00
285	0	0	.1786950D+03	.1036850D+03	.00D+00	.00D+00
286	0	0	.1628500D+03	.1125850D+03	.00D+00	.00D+00
287	0	0	.1478100D+03	.1181500D+03	.00D+00	.00D+00
288	0	0	.1340600D+03	.1210350D+03	.00D+00	.00D+00
289	0	0	.1218300D+03	.1218300D+03	.00D+00	.00D+00
290	0	0	.1111850D+03	.1210350D+03	.00D+00	.00D+00

291	0	0	.1020890D+03	.1190400D+03	.00D+00	.00D+00
292	0	0	.9444350D+02	.1161600D+03	.00D+00	.00D+00
293	0	0	.8812350D+02	.1125950D+03	.00D+00	.00D+00
294	0	0	.8299250D+02	.1085050D+03	.00D+00	.00D+00
295	0	0	.7891500D+02	.1039800D+03	.00D+00	.00D+00
296	0	0	.7576250D+02	.9908950D+02	.00D+00	.00D+00
297	0	0	.7341550D+02	.9387300D+02	.00D+00	.00D+00
298	0	0	.7176200D+02	.8834800D+02	.00D+00	.00D+00
299	0	0	.7069750D+02	.8251900D+02	.00D+00	.00D+00
300	0	0	.7012350D+02	.7638650D+02	.00D+00	.00D+00
301	0	0	.6994700D+02	.6994700D+02	.00D+00	.00D+00
302	0	0	.7008000D+02	.6319900D+02	.00D+00	.00D+00
303	0	0	.7043700D+02	.5614400D+02	.00D+00	.00D+00
304	0	0	.7093800D+02	.4879000D+02	.00D+00	.00D+00
305	0	0	.7150800D+02	.4115500D+02	.00D+00	.00D+00
306	0	0	.7207850D+02	.3326450D+02	.00D+00	.00D+00
307	0	0	.7259000D+02	.2515500D+02	.00D+00	.00D+00
308	0	0	.7299250D+02	.1687150D+02	.00D+00	.00D+00
309	0	0	.7324950D+02	.8466600D+01	.00D+00	.00D+00
310	0	0	.7342650D+02	.0000000D+00	.00D+00	.00D+00
311	0	0	.2101000D+03	.0000000D+00	.00D+00	.00D+00

Table 6.12 Input Data Sets for Problem 7 (continued)

312	0	0	.2060200D+03	.2223200D+02	.00D+00	.00D+00
313	0	0	.2001650D+03	.4311950D+02	.00D+00	.00D+00
314	0	0	.1912100D+03	.6160450D+02	.00D+00	.00D+00
315	0	0	.1801050D+03	.7706950D+02	.00D+00	.00D+00
316	0	0	.1678200D+03	.8932250D+02	.00D+00	.00D+00
317	0	0	.1552150D+03	.9850100D+02	.00D+00	.00D+00
318	0	0	.1429450D+03	.1049275D+03	.00D+00	.00D+00
319	0	0	.1314600D+03	.1090150D+03	.00D+00	.00D+00
320	0	0	.1210350D+03	.1111850D+03	.00D+00	.00D+00
321	0	0	.1118000D+03	.1118000D+03	.00D+00	.00D+00
322	0	0	.1038000D+03	.1111800D+03	.00D+00	.00D+00
323	0	0	.9700800D+02	.1095900D+03	.00D+00	.00D+00
324	0	0	.9135950D+02	.1072050D+03	.00D+00	.00D+00
325	0	0	.8677450D+02	.1041800D+03	.00D+00	.00D+00
326	0	0	.8315750D+02	.1006095D+03	.00D+00	.00D+00
327	0	0	.8041150D+02	.9656150D+02	.00D+00	.00D+00
328	0	0	.7843950D+02	.9208150D+02	.00D+00	.00D+00
329	0	0	.7714450D+02	.8719100D+02	.00D+00	.00D+00
330	0	0	.7643200D+02	.8189900D+02	.00D+00	.00D+00
331	0	0	.7621000D+02	.7621000D+02	.00D+00	.00D+00
332	0	0	.7638650D+02	.7012350D+02	.00D+00	.00D+00
333	0	0	.7687000D+02	.6363900D+02	.00D+00	.00D+00
334	0	0	.7757000D+02	.5676100D+02	.00D+00	.00D+00
335	0	0	.7839850D+02	.4950250D+02	.00D+00	.00D+00
336	0	0	.7927100D+02	.4188500D+02	.00D+00	.00D+00
337	0	0	.8010850D+02	.3394300D+02	.00D+00	.00D+00
338	0	0	.8084100D+02	.2572100D+02	.00D+00	.00D+00
339	0	0	.8140950D+02	.1727650D+02	.00D+00	.00D+00
340	0	0	.8176950D+02	.8677850D+01	.00D+00	.00D+00
341	0	0	.8201650D+02	.0000000D+00	.00D+00	.00D+00
342	0	0	.1893600D+03	.0000000D+00	.00D+00	.00D+00
343	0	0	.1863600D+03	.1869450D+02	.00D+00	.00D+00
344	0	0	.1820300D+03	.3647300D+02	.00D+00	.00D+00
345	0	0	.1753150D+03	.5257700D+02	.00D+00	.00D+00
346	0	0	.1668350D+03	.6650800D+02	.00D+00	.00D+00
347	0	0	.1572700D+03	.7803550D+02	.00D+00	.00D+00
348	0	0	.1472500D+03	.8716150D+02	.00D+00	.00D+00
349	0	0	.1372950D+03	.9404350D+02	.00D+00	.00D+00

350	0	0	.1278000D+03	.9892400D+02	.00D+00	.00D+00
351	0	0	.1190400D+03	.1020890D+03	.00D+00	.00D+00
352	0	0	.1111800D+03	.1038000D+03	.00D+00	.00D+00
353	0	0	.1043000D+03	.1043000D+03	.00D+00	.00D+00
354	0	0	.9842250D+02	.1038000D+03	.00D+00	.00D+00
355	0	0	.9353300D+02	.1024550D+03	.00D+00	.00D+00
356	0	0	.8958850D+02	.1003970D+03	.00D+00	.00D+00
357	0	0	.8653000D+02	.9771300D+02	.00D+00	.00D+00
358	0	0	.8428800D+02	.9446800D+02	.00D+00	.00D+00
359	0	0	.8278600D+02	.9070100D+02	.00D+00	.00D+00
360	0	0	.8194350D+02	.8643450D+02	.00D+00	.00D+00
361	0	0	.8167700D+02	.8167700D+02	.00D+00	.00D+00
362	0	0	.8189900D+02	.7643200D+02	.00D+00	.00D+00
363	0	0	.8251900D+02	.7069750D+02	.00D+00	.00D+00
364	0	0	.8344250D+02	.6447150D+02	.00D+00	.00D+00
365	0	0	.8457300D+02	.5775900D+02	.00D+00	.00D+00
366	0	0	.8581350D+02	.5057350D+02	.00D+00	.00D+00

Table 6.12 Input Data Sets for Problem 7 (continued)

367	0	0	.8706800D+02	.4294050D+02	.00D+00	.00D+00
368	0	0	.8824350D+02	.3490100D+02	.00D+00	.00D+00
369	0	0	.8925650D+02	.2650900D+02	.00D+00	.00D+00
370	0	0	.9003600D+02	.1783600D+02	.00D+00	.00D+00
371	0	0	.9052650D+02	.8968350D+01	.00D+00	.00D+00
372	0	0	.9086150D+02	.0000000D+00	.00D+00	.00D+00
373	0	0	.1717950D+03	.0000000D+00	.00D+00	.00D+00
374	0	0	.1695450D+03	.1607350D+02	.00D+00	.00D+00
375	0	0	.1662800D+03	.3149950D+02	.00D+00	.00D+00
376	0	0	.1611750D+03	.4572400D+02	.00D+00	.00D+00
377	0	0	.1546450D+03	.5834900D+02	.00D+00	.00D+00
378	0	0	.1471650D+03	.6915150D+02	.00D+00	.00D+00
379	0	0	.1392050D+03	.7806800D+02	.00D+00	.00D+00
380	0	0	.1311800D+03	.8515750D+02	.00D+00	.00D+00
381	0	0	.1234150D+03	.9055700D+02	.00D+00	.00D+00
382	0	0	.1161600D+03	.9444350D+02	.00D+00	.00D+00
383	0	0	.1095900D+03	.9700800D+02	.00D+00	.00D+00
384	0	0	.1038000D+03	.9842250D+02	.00D+00	.00D+00
385	0	0	.9885100D+02	.9885100D+02	.00D+00	.00D+00
386	0	0	.9476100D+02	.9842100D+02	.00D+00	.00D+00
387	0	0	.9151650D+02	.9724000D+02	.00D+00	.00D+00
388	0	0	.8908650D+02	.9538050D+02	.00D+00	.00D+00
389	0	0	.8742400D+02	.9289600D+02	.00D+00	.00D+00
390	0	0	.8647300D+02	.8981950D+02	.00D+00	.00D+00
391	0	0	.8616800D+02	.8616800D+02	.00D+00	.00D+00
392	0	0	.8643450D+02	.8194350D+02	.00D+00	.00D+00
393	0	0	.8719100D+02	.7714450D+02	.00D+00	.00D+00
394	0	0	.8834800D+02	.7176200D+02	.00D+00	.00D+00
395	0	0	.8980800D+02	.6579050D+02	.00D+00	.00D+00
396	0	0	.9146700D+02	.5923000D+02	.00D+00	.00D+00
397	0	0	.9321600D+02	.5209250D+02	.00D+00	.00D+00
398	0	0	.9494350D+02	.4440400D+02	.00D+00	.00D+00
399	0	0	.9654050D+02	.3621050D+02	.00D+00	.00D+00
400	0	0	.9790550D+02	.2757700D+02	.00D+00	.00D+00
401	0	0	.9895000D+02	.1859150D+02	.00D+00	.00D+00
402	0	0	.9960550D+02	.9359300D+01	.00D+00	.00D+00
403	0	0	.1000525D+03	.0000000D+00	.00D+00	.00D+00
404	0	0	.1565750D+03	.0000000D+00	.00D+00	.00D+00
405	0	0	.1548650D+03	.1409900D+02	.00D+00	.00D+00
406	0	0	.1523800D+03	.2772700D+02	.00D+00	.00D+00
407	0	0	.1484650D+03	.4047050D+02	.00D+00	.00D+00
408	0	0	.1434050D+03	.5201300D+02	.00D+00	.00D+00

409	0	0	.1375450D+03	.6215350D+02	.00D+00	.00D+00
410	0	0	.1312400D+03	.7080200D+02	.00D+00	.00D+00
411	0	0	.1248050D+03	.7796150D+02	.00D+00	.00D+00
412	0	0	.1185150D+03	.8369950D+02	.00D+00	.00D+00
413	0	0	.1125950D+03	.8812350D+02	.00D+00	.00D+00
414	0	0	.1072050D+03	.9135950D+02	.00D+00	.00D+00
415	0	0	.1024550D+03	.9353300D+02	.00D+00	.00D+00
416	0	0	.9842100D+02	.9476100D+02	.00D+00	.00D+00
417	0	0	.9514400D+02	.9514400D+02	.00D+00	.00D+00
418	0	0	.9263100D+02	.9476100D+02	.00D+00	.00D+00
419	0	0	.9087450D+02	.9367250D+02	.00D+00	.00D+00
420	0	0	.8984850D+02	.9191600D+02	.00D+00	.00D+00
421	0	0	.8951400D+02	.8951400D+02	.00D+00	.00D+00

Table 6.12 Input Data Sets for Problem 7 (continued)

422	0	0	.8981950D+02	.8647300D+02	.00D+00	.00D+00
423	0	0	.9070100D+02	.8278600D+02	.00D+00	.00D+00
424	0	0	.9208150D+02	.7843950D+02	.00D+00	.00D+00
425	0	0	.9387300D+02	.7341550D+02	.00D+00	.00D+00
426	0	0	.9597450D+02	.6769800D+02	.00D+00	.00D+00
427	0	0	.9827150D+02	.6127850D+02	.00D+00	.00D+00
428	0	0	.1006420D+03	.5416200D+02	.00D+00	.00D+00
429	0	0	.1029500D+03	.4637250D+02	.00D+00	.00D+00
430	0	0	.1050700D+03	.3795900D+02	.00D+00	.00D+00
431	0	0	.1068750D+03	.2899750D+02	.00D+00	.00D+00
432	0	0	.1082500D+03	.1959350D+02	.00D+00	.00D+00
433	0	0	.1091150D+03	.9877400D+01	.00D+00	.00D+00
434	0	0	.1097050D+03	.0000000D+00	.00D+00	.00D+00
435	0	0	.1431200D+03	.0000000D+00	.00D+00	.00D+00
436	0	0	.1418200D+03	.1259500D+02	.00D+00	.00D+00
437	0	0	.1399150D+03	.2483950D+02	.00D+00	.00D+00
438	0	0	.1368900D+03	.3641800D+02	.00D+00	.00D+00
439	0	0	.1329600D+03	.4707850D+02	.00D+00	.00D+00
440	0	0	.1283750D+03	.5664650D+02	.00D+00	.00D+00
441	0	0	.1234000D+03	.6502550D+02	.00D+00	.00D+00
442	0	0	.1182850D+03	.7218750D+02	.00D+00	.00D+00
443	0	0	.1132550D+03	.7815600D+02	.00D+00	.00D+00
444	0	0	.1085050D+03	.8299250D+02	.00D+00	.00D+00
445	0	0	.1041800D+03	.8677450D+02	.00D+00	.00D+00
446	0	0	.1003970D+03	.8958850D+02	.00D+00	.00D+00
447	0	0	.9724000D+02	.9151650D+02	.00D+00	.00D+00
448	0	0	.9476100D+02	.9263100D+02	.00D+00	.00D+00
449	0	0	.9298850D+02	.9298850D+02	.00D+00	.00D+00
450	0	0	.9193150D+02	.9263100D+02	.00D+00	.00D+00
451	0	0	.9158200D+02	.9158200D+02	.00D+00	.00D+00
452	0	0	.9191600D+02	.8984850D+02	.00D+00	.00D+00
453	0	0	.9289600D+02	.8742400D+02	.00D+00	.00D+00
454	0	0	.9446800D+02	.8428800D+02	.00D+00	.00D+00
455	0	0	.9656150D+02	.8041150D+02	.00D+00	.00D+00
456	0	0	.9908950D+02	.7576250D+02	.00D+00	.00D+00
457	0	0	.1019450D+03	.7030750D+02	.00D+00	.00D+00
458	0	0	.1050050D+03	.6402400D+02	.00D+00	.00D+00
459	0	0	.1081250D+03	.5690400D+02	.00D+00	.00D+00
460	0	0	.1111500D+03	.4896500D+02	.00D+00	.00D+00
461	0	0	.1139200D+03	.4025550D+02	.00D+00	.00D+00
462	0	0	.1162750D+03	.3086100D+02	.00D+00	.00D+00
463	0	0	.1180700D+03	.2090700D+02	.00D+00	.00D+00
464	0	0	.1191950D+03	.1055700D+02	.00D+00	.00D+00
465	0	0	.1199650D+03	.0000000D+00	.00D+00	.00D+00
466	0	0	.1310350D+03	.0000000D+00	.00D+00	.00D+00
467	0	0	.1300250D+03	.1144250D+02	.00D+00	.00D+00

468	0	0	.1285550D+03	.2261800D+02	.00D+00	.00D+00
469	0	0	.1262250D+03	.3328350D+02	.00D+00	.00D+00
470	0	0	.1231750D+03	.4323650D+02	.00D+00	.00D+00
471	0	0	.1195950D+03	.5232850D+02	.00D+00	.00D+00
472	0	0	.1156950D+03	.6046600D+02	.00D+00	.00D+00
473	0	0	.1116750D+03	.6760600D+02	.00D+00	.00D+00
474	0	0	.1077150D+03	.7374600D+02	.00D+00	.00D+00
475	0	0	.1039800D+03	.7891500D+02	.00D+00	.00D+00
476	0	0	.1006095D+03	.8315750D+02	.00D+00	.00D+00

Table 6.12 Input Data Sets for Problem 7 (continued)

477	0	0	.9771300D+02	.8653000D+02	.00D+00	.00D+00
478	0	0	.9538050D+02	.8908650D+02	.00D+00	.00D+00
479	0	0	.9367250D+02	.9087450D+02	.00D+00	.00D+00
480	0	0	.9263100D+02	.9193150D+02	.00D+00	.00D+00
481	0	0	.9228100D+02	.9228100D+02	.00D+00	.00D+00
482	0	0	.9263100D+02	.9193150D+02	.00D+00	.00D+00
483	0	0	.9367250D+02	.9087450D+02	.00D+00	.00D+00
484	0	0	.9538050D+02	.8908650D+02	.00D+00	.00D+00
485	0	0	.9771300D+02	.8653000D+02	.00D+00	.00D+00
486	0	0	.1006095D+03	.8315750D+02	.00D+00	.00D+00
487	0	0	.1039800D+03	.7891500D+02	.00D+00	.00D+00
488	0	0	.1077150D+03	.7374600D+02	.00D+00	.00D+00
489	0	0	.1116750D+03	.6760600D+02	.00D+00	.00D+00
490	0	0	.1156950D+03	.6046600D+02	.00D+00	.00D+00
491	0	0	.1195950D+03	.5232850D+02	.00D+00	.00D+00
492	0	0	.1231750D+03	.4323650D+02	.00D+00	.00D+00
493	0	0	.1262250D+03	.3328350D+02	.00D+00	.00D+00
494	0	0	.1285550D+03	.2261800D+02	.00D+00	.00D+00
495	0	0	.1300250D+03	.1144250D+02	.00D+00	.00D+00
496	0	0	.1310350D+03	.0000000D+00	.00D+00	.00D+00
497	0	0	.1199650D+03	.0000000D+00	.00D+00	.00D+00
498	0	0	.1191950D+03	.1055700D+02	.00D+00	.00D+00
499	0	0	.1180700D+03	.2090700D+02	.00D+00	.00D+00
500	0	0	.1162750D+03	.3086100D+02	.00D+00	.00D+00
501	0	0	.1139200D+03	.4025550D+02	.00D+00	.00D+00
502	0	0	.1111500D+03	.4896500D+02	.00D+00	.00D+00
503	0	0	.1081250D+03	.5690400D+02	.00D+00	.00D+00
504	0	0	.1050050D+03	.6402400D+02	.00D+00	.00D+00
505	0	0	.1019450D+03	.7030750D+02	.00D+00	.00D+00
506	0	0	.9908950D+02	.7576250D+02	.00D+00	.00D+00
507	0	0	.9656150D+02	.8041150D+02	.00D+00	.00D+00
508	0	0	.9446800D+02	.8428800D+02	.00D+00	.00D+00
509	0	0	.9289600D+02	.8742400D+02	.00D+00	.00D+00
510	0	0	.9191600D+02	.8984850D+02	.00D+00	.00D+00
511	0	0	.9158200D+02	.9158200D+02	.00D+00	.00D+00
512	0	0	.9193150D+02	.9263100D+02	.00D+00	.00D+00
513	0	0	.9298850D+02	.9298850D+02	.00D+00	.00D+00
514	0	0	.9476100D+02	.9263100D+02	.00D+00	.00D+00
515	0	0	.9724000D+02	.9151650D+02	.00D+00	.00D+00
516	0	0	.1003970D+03	.8958850D+02	.00D+00	.00D+00
517	0	0	.1041800D+03	.8677450D+02	.00D+00	.00D+00
518	0	0	.1085050D+03	.8299250D+02	.00D+00	.00D+00
519	0	0	.1132550D+03	.7815600D+02	.00D+00	.00D+00
520	0	0	.1182850D+03	.7218750D+02	.00D+00	.00D+00
521	0	0	.1234000D+03	.6502550D+02	.00D+00	.00D+00
522	0	0	.1283750D+03	.5664650D+02	.00D+00	.00D+00
523	0	0	.1329600D+03	.4707850D+02	.00D+00	.00D+00
524	0	0	.1368900D+03	.3641800D+02	.00D+00	.00D+00
525	0	0	.1399150D+03	.2483950D+02	.00D+00	.00D+00
526	0	0	.1418200D+03	.1259500D+02	.00D+00	.00D+00

527	0	0	.1431200D+03	.0000000D+00	.00D+00	.00D+00
528	0	0	.1097050D+03	.0000000D+00	.00D+00	.00D+00
529	0	0	.1091150D+03	.9877400D+01	.00D+00	.00D+00
530	0	0	.1082500D+03	.1959350D+02	.00D+00	.00D+00
531	0	0	.1068750D+03	.2899750D+02	.00D+00	.00D+00

Table 6.12 Input Data Sets for Problem 7 (continued)

532	0	0	.1050700D+03	.3795900D+02	.00D+00	.00D+00
533	0	0	.1029500D+03	.4637250D+02	.00D+00	.00D+00
534	0	0	.1006420D+03	.5416200D+02	.00D+00	.00D+00
535	0	0	.9827150D+02	.6127850D+02	.00D+00	.00D+00
536	0	0	.9597450D+02	.6769800D+02	.00D+00	.00D+00
537	0	0	.9387300D+02	.7341550D+02	.00D+00	.00D+00
538	0	0	.9208150D+02	.7843950D+02	.00D+00	.00D+00
539	0	0	.9070100D+02	.8278600D+02	.00D+00	.00D+00
540	0	0	.8981950D+02	.8647300D+02	.00D+00	.00D+00
541	0	0	.8951400D+02	.8951400D+02	.00D+00	.00D+00
542	0	0	.8984850D+02	.9191600D+02	.00D+00	.00D+00
543	0	0	.9087450D+02	.9367250D+02	.00D+00	.00D+00
544	0	0	.9263100D+02	.9476100D+02	.00D+00	.00D+00
545	0	0	.9514400D+02	.9514400D+02	.00D+00	.00D+00
546	0	0	.9842100D+02	.9476100D+02	.00D+00	.00D+00
547	0	0	.1024550D+03	.9353300D+02	.00D+00	.00D+00
548	0	0	.1072050D+03	.9135950D+02	.00D+00	.00D+00
549	0	0	.1125950D+03	.8812350D+02	.00D+00	.00D+00
550	0	0	.1185150D+03	.8369950D+02	.00D+00	.00D+00
551	0	0	.1248050D+03	.7796150D+02	.00D+00	.00D+00
552	0	0	.1312400D+03	.7080200D+02	.00D+00	.00D+00
553	0	0	.1375450D+03	.6215350D+02	.00D+00	.00D+00
554	0	0	.1434050D+03	.5201300D+02	.00D+00	.00D+00
555	0	0	.1484650D+03	.4047050D+02	.00D+00	.00D+00
556	0	0	.1523800D+03	.2772700D+02	.00D+00	.00D+00
557	0	0	.1548650D+03	.1409900D+02	.00D+00	.00D+00
558	0	0	.1565750D+03	.0000000D+00	.00D+00	.00D+00
559	0	0	.1000525D+03	.0000000D+00	.00D+00	.00D+00
560	0	0	.9960550D+02	.9359300D+01	.00D+00	.00D+00
561	0	0	.9895000D+02	.1859150D+02	.00D+00	.00D+00
562	0	0	.9790550D+02	.2757700D+02	.00D+00	.00D+00
563	0	0	.9654050D+02	.3621050D+02	.00D+00	.00D+00
564	0	0	.9494350D+02	.4440400D+02	.00D+00	.00D+00
565	0	0	.9321600D+02	.5209250D+02	.00D+00	.00D+00
566	0	0	.9146700D+02	.5923000D+02	.00D+00	.00D+00
567	0	0	.8980800D+02	.6579050D+02	.00D+00	.00D+00
568	0	0	.8834800D+02	.7176200D+02	.00D+00	.00D+00
569	0	0	.8719100D+02	.7714450D+02	.00D+00	.00D+00
570	0	0	.8643450D+02	.8194350D+02	.00D+00	.00D+00
571	0	0	.8616800D+02	.8616800D+02	.00D+00	.00D+00
572	0	0	.8647300D+02	.8981950D+02	.00D+00	.00D+00
573	0	0	.8742400D+02	.9289600D+02	.00D+00	.00D+00
574	0	0	.8908650D+02	.9538050D+02	.00D+00	.00D+00
575	0	0	.9151650D+02	.9724000D+02	.00D+00	.00D+00
576	0	0	.9476100D+02	.9842100D+02	.00D+00	.00D+00
577	0	0	.9885100D+02	.9885100D+02	.00D+00	.00D+00
578	0	0	.1038000D+03	.9842250D+02	.00D+00	.00D+00
579	0	0	.1095900D+03	.9700800D+02	.00D+00	.00D+00
580	0	0	.1161600D+03	.9444350D+02	.00D+00	.00D+00
581	0	0	.1234150D+03	.9055700D+02	.00D+00	.00D+00
582	0	0	.1311800D+03	.8515750D+02	.00D+00	.00D+00
583	0	0	.1392050D+03	.7806800D+02	.00D+00	.00D+00
584	0	0	.1471650D+03	.6915150D+02	.00D+00	.00D+00
585	0	0	.1546450D+03	.5834900D+02	.00D+00	.00D+00

586	0	0	.1611750D+03	.4572400D+02	.00D+00	.00D+00

Table 6.12 Input Data Sets for Problem 7 (continued)

587	0	0	.1662800D+03	.3149950D+02	.00D+00	.00D+00
588	0	0	.1695450D+03	.1607350D+02	.00D+00	.00D+00
589	0	0	.1717950D+03	.0000000D+00	.00D+00	.00D+00
590	0	0	.9086150D+02	.0000000D+00	.00D+00	.00D+00
591	0	0	.9052650D+02	.8968350D+01	.00D+00	.00D+00
592	0	0	.9003600D+02	.1783600D+02	.00D+00	.00D+00
593	0	0	.8925650D+02	.2650900D+02	.00D+00	.00D+00
594	0	0	.8824350D+02	.3490100D+02	.00D+00	.00D+00
595	0	0	.8706800D+02	.4294050D+02	.00D+00	.00D+00
596	0	0	.8581350D+02	.5057350D+02	.00D+00	.00D+00
597	0	0	.8457300D+02	.5775900D+02	.00D+00	.00D+00
598	0	0	.8344250D+02	.6447150D+02	.00D+00	.00D+00
599	0	0	.8251900D+02	.7069750D+02	.00D+00	.00D+00
600	0	0	.8189900D+02	.7643200D+02	.00D+00	.00D+00
601	0	0	.8167700D+02	.8167700D+02	.00D+00	.00D+00
602	0	0	.8194350D+02	.8643450D+02	.00D+00	.00D+00
603	0	0	.8278600D+02	.9070100D+02	.00D+00	.00D+00
604	0	0	.8428800D+02	.9446800D+02	.00D+00	.00D+00
605	0	0	.8653000D+02	.9771300D+02	.00D+00	.00D+00
606	0	0	.8958850D+02	.1003970D+03	.00D+00	.00D+00
607	0	0	.9353300D+02	.1024550D+03	.00D+00	.00D+00
608	0	0	.9842250D+02	.1038000D+03	.00D+00	.00D+00
609	0	0	.1043000D+03	.1043000D+03	.00D+00	.00D+00
610	0	0	.1111800D+03	.1038000D+03	.00D+00	.00D+00
611	0	0	.1190400D+03	.1020890D+03	.00D+00	.00D+00
612	0	0	.1278000D+03	.9892400D+02	.00D+00	.00D+00
613	0	0	.1372950D+03	.9404350D+02	.00D+00	.00D+00
614	0	0	.1472500D+03	.8716150D+02	.00D+00	.00D+00
615	0	0	.1572700D+03	.7803550D+02	.00D+00	.00D+00
616	0	0	.1668350D+03	.6650800D+02	.00D+00	.00D+00
617	0	0	.1753150D+03	.5257700D+02	.00D+00	.00D+00
618	0	0	.1820300D+03	.3647300D+02	.00D+00	.00D+00
619	0	0	.1863600D+03	.1869450D+02	.00D+00	.00D+00
620	0	0	.1893600D+03	.0000000D+00	.00D+00	.00D+00
621	0	0	.8201650D+02	.0000000D+00	.00D+00	.00D+00
622	0	0	.8176950D+02	.8677850D+01	.00D+00	.00D+00
623	0	0	.8140950D+02	.1727650D+02	.00D+00	.00D+00
624	0	0	.8084100D+02	.2572100D+02	.00D+00	.00D+00
625	0	0	.8010850D+02	.3394300D+02	.00D+00	.00D+00
626	0	0	.7927100D+02	.4188500D+02	.00D+00	.00D+00
627	0	0	.7839850D+02	.4950250D+02	.00D+00	.00D+00
628	0	0	.7757000D+02	.5676100D+02	.00D+00	.00D+00
629	0	0	.7687000D+02	.6363900D+02	.00D+00	.00D+00
630	0	0	.7638650D+02	.7012350D+02	.00D+00	.00D+00
631	0	0	.7621000D+02	.7621000D+02	.00D+00	.00D+00
632	0	0	.7643200D+02	.8189900D+02	.00D+00	.00D+00
633	0	0	.7714450D+02	.8719100D+02	.00D+00	.00D+00
634	0	0	.7843950D+02	.9208150D+02	.00D+00	.00D+00
635	0	0	.8041150D+02	.9656150D+02	.00D+00	.00D+00
636	0	0	.8315750D+02	.1006095D+03	.00D+00	.00D+00
637	0	0	.8677450D+02	.1041800D+03	.00D+00	.00D+00
638	0	0	.9135950D+02	.1072050D+03	.00D+00	.00D+00
639	0	0	.9700800D+02	.1095900D+03	.00D+00	.00D+00
640	0	0	.1038000D+03	.1111800D+03	.00D+00	.00D+00
641	0	0	.1118000D+03	.1118000D+03	.00D+00	.00D+00

Table 6.12 Input Data Sets for Problem 7 (continued)

642	0	0	.1210350D+03	.1111850D+03	.00D+00	.00D+00
643	0	0	.1314600D+03	.1090150D+03	.00D+00	.00D+00
644	0	0	.1429450D+03	.1049275D+03	.00D+00	.00D+00
645	0	0	.1552150D+03	.9850100D+02	.00D+00	.00D+00
646	0	0	.1678200D+03	.8932250D+02	.00D+00	.00D+00
647	0	0	.1801050D+03	.7706950D+02	.00D+00	.00D+00
648	0	0	.1912100D+03	.6160450D+02	.00D+00	.00D+00
649	0	0	.2001650D+03	.4311950D+02	.00D+00	.00D+00
650	0	0	.2060200D+03	.2223200D+02	.00D+00	.00D+00
651	0	0	.2101000D+03	.0000000D+00	.00D+00	.00D+00
652	0	0	.7342650D+02	.0000000D+00	.00D+00	.00D+00
653	0	0	.7324950D+02	.8466600D+01	.00D+00	.00D+00
654	0	0	.7299250D+02	.1687150D+02	.00D+00	.00D+00
655	0	0	.7259000D+02	.2515500D+02	.00D+00	.00D+00
656	0	0	.7207850D+02	.3326450D+02	.00D+00	.00D+00
657	0	0	.7150800D+02	.4115500D+02	.00D+00	.00D+00
658	0	0	.7093800D+02	.4879000D+02	.00D+00	.00D+00
659	0	0	.7043700D+02	.5614400D+02	.00D+00	.00D+00
660	0	0	.7008000D+02	.6319900D+02	.00D+00	.00D+00
661	0	0	.6994700D+02	.6994700D+02	.00D+00	.00D+00
662	0	0	.7012350D+02	.7638650D+02	.00D+00	.00D+00
663	0	0	.7069750D+02	.8251900D+02	.00D+00	.00D+00
664	0	0	.7176200D+02	.8834800D+02	.00D+00	.00D+00
665	0	0	.7341550D+02	.9387300D+02	.00D+00	.00D+00
666	0	0	.7576250D+02	.9908950D+02	.00D+00	.00D+00
667	0	0	.7891500D+02	.1039800D+03	.00D+00	.00D+00
668	0	0	.8299250D+02	.1085050D+03	.00D+00	.00D+00
669	0	0	.8812350D+02	.1125950D+03	.00D+00	.00D+00
670	0	0	.9444350D+02	.1161600D+03	.00D+00	.00D+00
671	0	0	.1020890D+03	.1190400D+03	.00D+00	.00D+00
672	0	0	.1111850D+03	.1210350D+03	.00D+00	.00D+00
673	0	0	.1218300D+03	.1218300D+03	.00D+00	.00D+00
674	0	0	.1340600D+03	.1210350D+03	.00D+00	.00D+00
675	0	0	.1478100D+03	.1181500D+03	.00D+00	.00D+00
676	0	0	.1628500D+03	.1125850D+03	.00D+00	.00D+00
677	0	0	.1786950D+03	.1036850D+03	.00D+00	.00D+00
678	0	0	.1945500D+03	.9084150D+02	.00D+00	.00D+00
679	0	0	.2092650D+03	.7365300D+02	.00D+00	.00D+00
680	0	0	.2214050D+03	.5216800D+02	.00D+00	.00D+00
681	0	0	.2294850D+03	.2711500D+02	.00D+00	.00D+00
682	0	0	.2351750D+03	.0000000D+00	.00D+00	.00D+00
683	0	0	.6502000D+02	.0000000D+00	.00D+00	.00D+00
684	0	0	.6489800D+02	.8317250D+01	.00D+00	.00D+00
685	0	0	.6472150D+02	.1658700D+02	.00D+00	.00D+00
686	0	0	.6444800D+02	.2476300D+02	.00D+00	.00D+00
687	0	0	.6410850D+02	.3280550D+02	.00D+00	.00D+00
688	0	0	.6374500D+02	.4068000D+02	.00D+00	.00D+00
689	0	0	.6340900D+02	.4835900D+02	.00D+00	.00D+00
690	0	0	.6316050D+02	.5582500D+02	.00D+00	.00D+00
691	0	0	.6306600D+02	.6306600D+02	.00D+00	.00D+00
692	0	0	.6319900D+02	.7008000D+02	.00D+00	.00D+00
693	0	0	.6363900D+02	.7687000D+02	.00D+00	.00D+00
694	0	0	.6447150D+02	.8344250D+02	.00D+00	.00D+00
695	0	0	.6579050D+02	.8980800D+02	.00D+00	.00D+00
696	0	0	.6769800D+02	.9597450D+02	.00D+00	.00D+00

Table 6.12 Input Data Sets for Problem 7 (continued)

697	0	0	.7030750D+02	.1019450D+03	.00D+00	.00D+00
698	0	0	.7374600D+02	.1077150D+03	.00D+00	.00D+00
699	0	0	.7815600D+02	.1132550D+03	.00D+00	.00D+00
700	0	0	.8369950D+02	.1185150D+03	.00D+00	.00D+00

701	0	0	.9055700D+02	.1234150D+03	.00D+00	.00D+00
702	0	0	.9892400D+02	.1278000D+03	.00D+00	.00D+00
703	0	0	.1090150D+03	.1314600D+03	.00D+00	.00D+00
704	0	0	.1210350D+03	.1340600D+03	.00D+00	.00D+00
705	0	0	.1351350D+03	.1351350D+03	.00D+00	.00D+00
706	0	0	.1513900D+03	.1340550D+03	.00D+00	.00D+00
707	0	0	.1696800D+03	.1300050D+03	.00D+00	.00D+00
708	0	0	.1895650D+03	.1219900D+03	.00D+00	.00D+00
709	0	0	.2101350D+03	.1089590D+03	.00D+00	.00D+00
710	0	0	.2298800D+03	.8999850D+02	.00D+00	.00D+00
711	0	0	.2467000D+03	.6478500D+02	.00D+00	.00D+00
712	0	0	.2581850D+03	.3405950D+02	.00D+00	.00D+00
713	0	0	.2663950D+03	.0000000D+00	.00D+00	.00D+00
714	0	0	.5674350D+02	.0000000D+00	.00D+00	.00D+00
715	0	0	.5666250D+02	.8215650D+01	.00D+00	.00D+00
716	0	0	.5654650D+02	.1639550D+02	.00D+00	.00D+00
717	0	0	.5637100D+02	.2450500D+02	.00D+00	.00D+00
718	0	0	.5616200D+02	.3251500D+02	.00D+00	.00D+00
719	0	0	.5595450D+02	.4040000D+02	.00D+00	.00D+00
720	0	0	.5579300D+02	.4814200D+02	.00D+00	.00D+00
721	0	0	.5573000D+02	.5573000D+02	.00D+00	.00D+00
722	0	0	.5582500D+02	.6316050D+02	.00D+00	.00D+00
723	0	0	.5614400D+02	.7043700D+02	.00D+00	.00D+00
724	0	0	.5676100D+02	.7757000D+02	.00D+00	.00D+00
725	0	0	.5775900D+02	.8457300D+02	.00D+00	.00D+00
726	0	0	.5923000D+02	.9146700D+02	.00D+00	.00D+00
727	0	0	.6127850D+02	.9827150D+02	.00D+00	.00D+00
728	0	0	.6402400D+02	.1050050D+03	.00D+00	.00D+00
729	0	0	.6760600D+02	.1116750D+03	.00D+00	.00D+00
730	0	0	.7218750D+02	.1182850D+03	.00D+00	.00D+00
731	0	0	.7796150D+02	.1248050D+03	.00D+00	.00D+00
732	0	0	.8515750D+02	.1311800D+03	.00D+00	.00D+00
733	0	0	.9404350D+02	.1372950D+03	.00D+00	.00D+00
734	0	0	.1049275D+03	.1429450D+03	.00D+00	.00D+00
735	0	0	.1181500D+03	.1478100D+03	.00D+00	.00D+00
736	0	0	.1340550D+03	.1513900D+03	.00D+00	.00D+00
737	0	0	.1529350D+03	.1529350D+03	.00D+00	.00D+00
738	0	0	.1749150D+03	.1513900D+03	.00D+00	.00D+00
739	0	0	.1997500D+03	.1453200D+03	.00D+00	.00D+00
740	0	0	.2265450D+03	.1329950D+03	.00D+00	.00D+00
741	0	0	.2534300D+03	.1125990D+03	.00D+00	.00D+00
742	0	0	.2773400D+03	.8291450D+02	.00D+00	.00D+00
743	0	0	.2942700D+03	.4433700D+02	.00D+00	.00D+00
744	0	0	.3066300D+03	.0000000D+00	.00D+00	.00D+00
745	0	0	.4855300D+02	.0000000D+00	.00D+00	.00D+00
746	0	0	.4850300D+02	.8150000D+01	.00D+00	.00D+00
747	0	0	.4843200D+02	.1627400D+02	.00D+00	.00D+00
748	0	0	.4832800D+02	.2434750D+02	.00D+00	.00D+00
749	0	0	.4821350D+02	.3234900D+02	.00D+00	.00D+00
750	0	0	.4811800D+02	.4026350D+02	.00D+00	.00D+00
751	0	0	.4807900D+02	.4807900D+02	.00D+00	.00D+00

Table 6.12 Input Data Sets for Problem 7 (continued)

752	0	0	.4814200D+02	.5579300D+02	.00D+00	.00D+00
753	0	0	.4835900D+02	.6340900D+02	.00D+00	.00D+00
754	0	0	.4879000D+02	.7093800D+02	.00D+00	.00D+00
755	0	0	.4950250D+02	.7839850D+02	.00D+00	.00D+00
756	0	0	.5057350D+02	.8581350D+02	.00D+00	.00D+00
757	0	0	.5209250D+02	.9321600D+02	.00D+00	.00D+00
758	0	0	.5416200D+02	.1006420D+03	.00D+00	.00D+00
759	0	0	.5690400D+02	.1081250D+03	.00D+00	.00D+00

760	0	0	.6046600D+02	.1156950D+03	.00D+00	.00D+00
761	0	0	.6502550D+02	.1234000D+03	.00D+00	.00D+00
762	0	0	.7080200D+02	.1312400D+03	.00D+00	.00D+00
763	0	0	.7806800D+02	.1392050D+03	.00D+00	.00D+00
764	0	0	.8716150D+02	.1472500D+03	.00D+00	.00D+00
765	0	0	.9850100D+02	.1552150D+03	.00D+00	.00D+00
766	0	0	.1125850D+03	.1628500D+03	.00D+00	.00D+00
767	0	0	.1300050D+03	.1696800D+03	.00D+00	.00D+00
768	0	0	.1513900D+03	.1749150D+03	.00D+00	.00D+00
769	0	0	.1772950D+03	.1772950D+03	.00D+00	.00D+00
770	0	0	.2079650D+03	.1749150D+03	.00D+00	.00D+00
771	0	0	.2428600D+03	.1650900D+03	.00D+00	.00D+00
772	0	0	.2799600D+03	.1444950D+03	.00D+00	.00D+00
773	0	0	.3149650D+03	.1099365D+03	.00D+00	.00D+00
774	0	0	.3411000D+03	.6037350D+02	.00D+00	.00D+00
775	0	0	.3608200D+03	.0000000D+00	.00D+00	.00D+00
776	0	0	.4041700D+02	.0000000D+00	.00D+00	.00D+00
777	0	0	.4038900D+02	.8110450D+01	.00D+00	.00D+00
778	0	0	.4034950D+02	.1620300D+02	.00D+00	.00D+00
779	0	0	.4029550D+02	.2426100D+02	.00D+00	.00D+00
780	0	0	.4024600D+02	.3227100D+02	.00D+00	.00D+00
781	0	0	.4022500D+02	.4022500D+02	.00D+00	.00D+00
782	0	0	.4026350D+02	.4811800D+02	.00D+00	.00D+00
783	0	0	.4040000D+02	.5595450D+02	.00D+00	.00D+00
784	0	0	.4068000D+02	.6374500D+02	.00D+00	.00D+00
785	0	0	.4115500D+02	.7150800D+02	.00D+00	.00D+00
786	0	0	.4188500D+02	.7927100D+02	.00D+00	.00D+00
787	0	0	.4294050D+02	.8706800D+02	.00D+00	.00D+00
788	0	0	.4440400D+02	.9494350D+02	.00D+00	.00D+00
789	0	0	.4637250D+02	.1029500D+03	.00D+00	.00D+00
790	0	0	.4896500D+02	.1111500D+03	.00D+00	.00D+00
791	0	0	.5232850D+02	.1195950D+03	.00D+00	.00D+00
792	0	0	.5664650D+02	.1283750D+03	.00D+00	.00D+00
793	0	0	.6215350D+02	.1375450D+03	.00D+00	.00D+00
794	0	0	.6915150D+02	.1471650D+03	.00D+00	.00D+00
795	0	0	.7803550D+02	.1572700D+03	.00D+00	.00D+00
796	0	0	.8932250D+02	.1678200D+03	.00D+00	.00D+00
797	0	0	.1036850D+03	.1786950D+03	.00D+00	.00D+00
798	0	0	.1219900D+03	.1895650D+03	.00D+00	.00D+00
799	0	0	.1453200D+03	.1997500D+03	.00D+00	.00D+00
800	0	0	.1749150D+03	.2079650D+03	.00D+00	.00D+00
801	0	0	.2119500D+03	.2119500D+03	.00D+00	.00D+00
802	0	0	.2569650D+03	.2079600D+03	.00D+00	.00D+00
803	0	0	.3085900D+03	.1903500D+03	.00D+00	.00D+00
804	0	0	.3614650D+03	.1519650D+03	.00D+00	.00D+00
805	0	0	.4042050D+03	.8722150D+02	.00D+00	.00D+00
806	0	0	.4381750D+03	.0000000D+00	.00D+00	.00D+00

Table 6.12 Input Data Sets for Problem 7 (continued)

807	0	0	.3231400D+02	.0000000D+00	.00D+00	.00D+00
808	0	0	.3230000D+02	.8088950D+01	.00D+00	.00D+00
809	0	0	.3228150D+02	.1616650D+02	.00D+00	.00D+00
810	0	0	.3226000D+02	.2422200D+02	.00D+00	.00D+00
811	0	0	.3225000D+02	.3225000D+02	.00D+00	.00D+00
812	0	0	.3227100D+02	.4024600D+02	.00D+00	.00D+00
813	0	0	.3234900D+02	.4821350D+02	.00D+00	.00D+00
814	0	0	.3251500D+02	.5616200D+02	.00D+00	.00D+00
815	0	0	.3280550D+02	.6410850D+02	.00D+00	.00D+00
816	0	0	.3326450D+02	.7207850D+02	.00D+00	.00D+00
817	0	0	.3394300D+02	.8010850D+02	.00D+00	.00D+00
818	0	0	.3490100D+02	.8824350D+02	.00D+00	.00D+00

819	0	0	.3621050D+02	.9654050D+02	.00D+00	.00D+00
820	0	0	.3795900D+02	.1050700D+03	.00D+00	.00D+00
821	0	0	.4025550D+02	.1139200D+03	.00D+00	.00D+00
822	0	0	.4323650D+02	.1231750D+03	.00D+00	.00D+00
823	0	0	.4707850D+02	.1329600D+03	.00D+00	.00D+00
824	0	0	.5201300D+02	.1434050D+03	.00D+00	.00D+00
825	0	0	.5834900D+02	.1546450D+03	.00D+00	.00D+00
826	0	0	.6650800D+02	.1668350D+03	.00D+00	.00D+00
827	0	0	.7706950D+02	.1801050D+03	.00D+00	.00D+00
828	0	0	.9084150D+02	.1945500D+03	.00D+00	.00D+00
829	0	0	.1089590D+03	.2101350D+03	.00D+00	.00D+00
830	0	0	.1329950D+03	.2265450D+03	.00D+00	.00D+00
831	0	0	.1650900D+03	.2428600D+03	.00D+00	.00D+00
832	0	0	.2079600D+03	.2569650D+03	.00D+00	.00D+00
833	0	0	.2644600D+03	.2644600D+03	.00D+00	.00D+00
834	0	0	.3359600D+03	.2569650D+03	.00D+00	.00D+00
835	0	0	.4180950D+03	.2203600D+03	.00D+00	.00D+00
836	0	0	.4930650D+03	.1365450D+03	.00D+00	.00D+00
837	0	0	.5577350D+03	.0000000D+00	.00D+00	.00D+00
838	0	0	.2422750D+02	.0000000D+00	.00D+00	.00D+00
839	0	0	.2422250D+02	.8078950D+01	.00D+00	.00D+00
840	0	0	.2421600D+02	.1615150D+02	.00D+00	.00D+00
841	0	0	.2421200D+02	.2421200D+02	.00D+00	.00D+00
842	0	0	.2422200D+02	.3226000D+02	.00D+00	.00D+00
843	0	0	.2426100D+02	.4029550D+02	.00D+00	.00D+00
844	0	0	.2434750D+02	.4832800D+02	.00D+00	.00D+00
845	0	0	.2450500D+02	.5637100D+02	.00D+00	.00D+00
846	0	0	.2476300D+02	.6444800D+02	.00D+00	.00D+00
847	0	0	.2515500D+02	.7259000D+02	.00D+00	.00D+00
848	0	0	.2572100D+02	.8084100D+02	.00D+00	.00D+00
849	0	0	.2650900D+02	.8925650D+02	.00D+00	.00D+00
850	0	0	.2757700D+02	.9790550D+02	.00D+00	.00D+00
851	0	0	.2899750D+02	.1068750D+03	.00D+00	.00D+00
852	0	0	.3086100D+02	.1162750D+03	.00D+00	.00D+00
853	0	0	.3328350D+02	.1262250D+03	.00D+00	.00D+00
854	0	0	.3641800D+02	.1368900D+03	.00D+00	.00D+00
855	0	0	.4047050D+02	.1484650D+03	.00D+00	.00D+00
856	0	0	.4572400D+02	.1611750D+03	.00D+00	.00D+00
857	0	0	.5257700D+02	.1753150D+03	.00D+00	.00D+00
858	0	0	.6160450D+02	.1912100D+03	.00D+00	.00D+00
859	0	0	.7365300D+02	.2092650D+03	.00D+00	.00D+00
860	0	0	.8999850D+02	.2298800D+03	.00D+00	.00D+00
861	0	0	.1125990D+03	.2534300D+03	.00D+00	.00D+00

Table 6.12 Input Data Sets for Problem 7 (continued)

862	0	0	.1444950D+03	.2799600D+03	.00D+00	.00D+00
863	0	0	.1903500D+03	.3085900D+03	.00D+00	.00D+00
864	0	0	.2569650D+03	.3359600D+03	.00D+00	.00D+00
865	0	0	.3526900D+03	.3526900D+03	.00D+00	.00D+00
866	0	0	.4818850D+03	.3359600D+03	.00D+00	.00D+00
867	0	0	.6245650D+03	.2385950D+03	.00D+00	.00D+00
868	0	0	.7639950D+03	.0000000D+00	.00D+00	.00D+00
869	0	0	.1614950D+02	.0000000D+00	.00D+00	.00D+00
870	0	0	.1614850D+02	.8075350D+01	.00D+00	.00D+00
871	0	0	.1614800D+02	.1614800D+02	.00D+00	.00D+00
872	0	0	.1615150D+02	.2421600D+02	.00D+00	.00D+00
873	0	0	.1616650D+02	.3228150D+02	.00D+00	.00D+00
874	0	0	.1620300D+02	.4034950D+02	.00D+00	.00D+00
875	0	0	.1627400D+02	.4843200D+02	.00D+00	.00D+00
876	0	0	.1639550D+02	.5654650D+02	.00D+00	.00D+00
877	0	0	.1658700D+02	.6472150D+02	.00D+00	.00D+00

878	0	0	.1687150D+02	.7299250D+02	.00D+00	.00D+00
879	0	0	.1727650D+02	.8140950D+02	.00D+00	.00D+00
880	0	0	.1783600D+02	.9003600D+02	.00D+00	.00D+00
881	0	0	.1859150D+02	.9895000D+02	.00D+00	.00D+00
882	0	0	.1959350D+02	.1082500D+03	.00D+00	.00D+00
883	0	0	.2090700D+02	.1180700D+03	.00D+00	.00D+00
884	0	0	.2261800D+02	.1285550D+03	.00D+00	.00D+00
885	0	0	.2483950D+02	.1399150D+03	.00D+00	.00D+00
886	0	0	.2772700D+02	.1523800D+03	.00D+00	.00D+00
887	0	0	.3149950D+02	.1662800D+03	.00D+00	.00D+00
888	0	0	.3647300D+02	.1820300D+03	.00D+00	.00D+00
889	0	0	.4311950D+02	.2001650D+03	.00D+00	.00D+00
890	0	0	.5216800D+02	.2214050D+03	.00D+00	.00D+00
891	0	0	.6478500D+02	.2467000D+03	.00D+00	.00D+00
892	0	0	.8291450D+02	.2773400D+03	.00D+00	.00D+00
893	0	0	.1099365D+03	.3149650D+03	.00D+00	.00D+00
894	0	0	.1519650D+03	.3614650D+03	.00D+00	.00D+00
895	0	0	.2203600D+03	.4180950D+03	.00D+00	.00D+00
896	0	0	.3359600D+03	.4818850D+03	.00D+00	.00D+00
897	0	0	.5321850D+03	.5321850D+03	.00D+00	.00D+00
898	0	0	.8290250D+03	.4818800D+03	.00D+00	.00D+00
899	0	0	.1176175D+04	.0000000D+00	.00D+00	.00D+00
900	0	0	.8074600D+01	.0000000D+00	.00D+00	.00D+00
901	0	0	.8074600D+01	.8074600D+01	.00D+00	.00D+00
902	0	0	.8075350D+01	.1614850D+02	.00D+00	.00D+00
903	0	0	.8078950D+01	.2422250D+02	.00D+00	.00D+00
904	0	0	.8088950D+01	.3230000D+02	.00D+00	.00D+00
905	0	0	.8110450D+01	.4038900D+02	.00D+00	.00D+00
906	0	0	.8150000D+01	.4850300D+02	.00D+00	.00D+00
907	0	0	.8215650D+01	.5666250D+02	.00D+00	.00D+00
908	0	0	.8317250D+01	.6489800D+02	.00D+00	.00D+00
909	0	0	.8466600D+01	.7324950D+02	.00D+00	.00D+00
910	0	0	.8677850D+01	.8176950D+02	.00D+00	.00D+00
911	0	0	.8968350D+01	.9052650D+02	.00D+00	.00D+00
912	0	0	.9359300D+01	.9960550D+02	.00D+00	.00D+00
913	0	0	.9877400D+01	.1091150D+03	.00D+00	.00D+00
914	0	0	.1055700D+02	.1191950D+03	.00D+00	.00D+00
915	0	0	.1144250D+02	.1300250D+03	.00D+00	.00D+00
916	0	0	.1259500D+02	.1418200D+03	.00D+00	.00D+00

Table 6.12 Input Data Sets for Problem 7 (continued)

917	0	0	.1409900D+02	.1548650D+03	.00D+00	.00D+00
918	0	0	.1607350D+02	.1695450D+03	.00D+00	.00D+00
919	0	0	.1869450D+02	.1863600D+03	.00D+00	.00D+00
920	0	0	.2223200D+02	.2060200D+03	.00D+00	.00D+00
921	0	0	.2711500D+02	.2294850D+03	.00D+00	.00D+00
922	0	0	.3405950D+02	.2581850D+03	.00D+00	.00D+00
923	0	0	.4433700D+02	.2942700D+03	.00D+00	.00D+00
924	0	0	.6037350D+02	.3411000D+03	.00D+00	.00D+00
925	0	0	.8722150D+02	.4042050D+03	.00D+00	.00D+00
926	0	0	.1365450D+03	.4930650D+03	.00D+00	.00D+00
927	0	0	.2385950D+03	.6245650D+03	.00D+00	.00D+00
928	0	0	.4818800D+03	.8290250D+03	.00D+00	.00D+00
929	0	0	.1156725D+04	.1156725D+04	.00D+00	.00D+00
930	0	0	.2159275D+04	.0000000D+00	.00D+00	.00D+00
931	0	0	.0000000D+00	.0000000D+00	.00D+00	.00D+00
932	0	0	.0000000D+00	.8074600D+01	.00D+00	.00D+00
933	0	0	.0000000D+00	.1614950D+02	.00D+00	.00D+00
934	0	0	.0000000D+00	.2422750D+02	.00D+00	.00D+00
935	0	0	.0000000D+00	.3231400D+02	.00D+00	.00D+00
936	0	0	.0000000D+00	.4041700D+02	.00D+00	.00D+00

```
  937     0     0    .0000000D+00    .4855300D+02    .00D+00    .00D+00
  938     0     0    .0000000D+00    .5674350D+02    .00D+00    .00D+00
  939     0     0    .0000000D+00    .6502000D+02    .00D+00    .00D+00
  940     0     0    .0000000D+00    .7342650D+02    .00D+00    .00D+00
  941     0     0    .0000000D+00    .8201650D+02    .00D+00    .00D+00
  942     0     0    .0000000D+00    .9086150D+02    .00D+00    .00D+00
  943     0     0    .0000000D+00    .1000525D+03    .00D+00    .00D+00
  944     0     0    .0000000D+00    .1097050D+03    .00D+00    .00D+00
  945     0     0    .0000000D+00    .1199650D+03    .00D+00    .00D+00
  946     0     0    .0000000D+00    .1310350D+03    .00D+00    .00D+00
  947     0     0    .0000000D+00    .1431200D+03    .00D+00    .00D+00
  948     0     0    .0000000D+00    .1565750D+03    .00D+00    .00D+00
  949     0     0    .0000000D+00    .1717950D+03    .00D+00    .00D+00
  950     0     0    .0000000D+00    .1893600D+03    .00D+00    .00D+00
  951     0     0    .0000000D+00    .2101000D+03    .00D+00    .00D+00
  952     0     0    .0000000D+00    .2351750D+03    .00D+00    .00D+00
  953     0     0    .0000000D+00    .2663950D+03    .00D+00    .00D+00
  954     0     0    .0000000D+00    .3066300D+03    .00D+00    .00D+00
  955     0     0    .0000000D+00    .3608200D+03    .00D+00    .00D+00
  956     0     0    .0000000D+00    .4381750D+03    .00D+00    .00D+00
  957     0     0    .0000000D+00    .5577350D+03    .00D+00    .00D+00
  958     0     0    .0000000D+00    .7639950D+03    .00D+00    .00D+00
  959     0     0    .0000000D+00    .1176175D+04    .00D+00    .00D+00
  960     0     0    .0000000D+00    .2159275D+04    .00D+00    .00D+00
  961     0     0    .4727141D+04    .4727141D+04    .00D+00    .00D+00
    0     0     0      0.0    0.0     0.0    0.0      END OF VELOCITY
    1   899     1      0.05   0.0
    0     0     0      0.0    0.0     0.0              END OF TH
    1   960     1      1.0005 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
12 0 34 0 0 10                          NONA NONS NOMX NOMY NOMZ NOMP
C ******* DATA SET 18: H+, E-, IONIC STRENGTH correction INFORMATION
 0.0 2 4 0 0   SICOR ICOR LNH LNG LNE
```

Table 6.12 Input Data Sets for Problem 7 (continued)

```
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 10 500 1.0d-8 1.0d00 1.0d00 1 omegac npcyl niterc epsc cnstrx y ipiv
c ******* DATA SET 23: Component name and component species types
 Na +
  1 0     INDTC(J,2)  IFCS
 K +
  1 0     INDTC(J,2)  IFCS
 Ca +2
  1 0     INDTC(J,2)  IFCS
 H +
  1 0     INDTC(J,2)  IFCS
 Cu +2
  1 0     INDTC(J,2)  IFCS
 Al +3
  1 0     INDTC(J,2)  IFCS
 Fe +2
  1 0     INDTC(J,2)  IFCS
 SiO2(aq)
  1 0     INDTC(J,2)  IFCS
 HCO3 -
  1 0     INDTC(J,2)  IFCS
```

```
 SO4 -2
  1 0      INDTC(J,2)  IFCS
 Cl -
  1 0      INDTC(J,2)  IFCS
 O2(aq)
  1 0      INDTC(J,2)  IFCS
C ******* DATA SET 24: COMPONENT SPECIES AND THEIR ION-EXCHANGE INDEX
 Na +
  0  1 0  ISCN  VJ  IONEX
 K +
  0  1 0  ISCN  VJ  IONEX
 Ca +2
  0  2 0  ISCN  VJ  IONEX
 H +
  0  1 0  ISCN  VJ  IONEX
 Cu +2
  0  2 0  ISCN  VJ  IONEX
 Al +3
  0  3 0  ISCN  VJ  IONEX
 Fe +2
  0  2 0  ISCN  VJ  IONEX
 SiO2(aq)
  0  0 0  ISCN  VJ  IONEX
 HCO3 -
  0 -1 0  ISCN  VJ  IONEX
 SO4 -2
  0 -2 0  ISCN  VJ  IONEX
 Cl -
  0 -1 0  ISCN  VJ  IONEX
 O2(aq)
  0  0 0  ISCN  VJ  IONEX
```

Table 6.12 Input Data Sets for Problem 7 (continued)

```
C ******** DATA SET 25:  COMPLEXED SPECIES
OH-
0    0 0 0 -1 0 0 0 0 0 0 0 0 0    0    0 0 0 -1 0 0 0 0 0 0 0 0 0
Fe +3
0    0 0 0  1 0 0 1 0 0 0 0 0.25 0    0 0 0  1 0 0 1 0 0 0 0 0.25
Al(OH)2 +
0    0 0 0 -2 0 1 0 0 0 0 0 0 0    0    0 0 0 -2 0 1 0 0 0 0 0 0 0
Al(OH)3 (aq)
0    0 0 0 -3 0 1 0 0 0 0 0 0 0    0    0 0 0 -3 0 1 0 0 0 0 0 0 0
Al(OH)4 -
0    0 0 0 -4 0 1 0 0 0 0 0 0 0    0    0 0 0 -4 0 1 0 0 0 0 0 0 0
Al(SO4)2 -
0    0 0 0  0 0 1 0 0 0 2 0 0    0    0 0 0  0 0 1 0 0 0 2 0 0
AlOH +2
0    0 0 0 -1 0 1 0 0 0 0 0 0 0    0    0 0 0 -1 0 1 0 0 0 0 0 0 0
AlSO4 +
0    0 0 0  0 0 1 0 0 0 1 0 0    0    0 0 0  0 0 1 0 0 0 1 0 0
H2CO3*
0    0 0 0  1 0 0 0 0 1 0 0 0    0    0 0 0  1 0 0 0 0 1 0 0 0
CO3 -2
0    0 0 0 -1 0 0 0 0 1 0 0 0    0    0 0 0 -1 0 0 0 0 1 0 0 0
CaCO3 (aq)
0    0 0 1 -1 0 0 0 0 1 0 0 0    0    0 0 1 -1 0 0 0 0 1 0 0 0
CaHCO3 +
0    0 0 1  0 0 0 0 0 1 0 0 0    0    0 0 1  0 0 0 0 0 1 0 0 0
CaOH +
0    0 0 1 -1 0 0 0 0 0 0 0 0    0    0 0 1 -1 0 0 0 0 0 0 0 0
CaSO4(aq)
```

```
0    0 0 1  0 0 0 0 0 0 1 0 0    0    0 0 1  0 0 0 0 0 0 1 0 0
CuOH +
0    0 0 0 -1 1 0 0 0 0 0 0 0 0    0    0 0 0 -1 1 0 0 0 0 0 0 0 0
CuSO4(aq)
0    0 0 0  0 1 0 0 0 0 1 0 0    0    0 0 0  0 1 0 0 0 0 1 0 0
Fe[II](OH)2 (aq)
0    0 0 0 -2 0 0 1 0 0 0 0 0    0    0 0 0 -2 0 0 1 0 0 0 0 0
Fe[III](OH)2 +
0    0 0 0 -1 0 0 1 0 0 0 0 0.25 0    0 0 0 -1 0 0 1 0 0 0 0 0.25
Fe[III](OH)3 (aq)
0    0 0 0 -2 0 0 1 0 0 0 0 0.25 0    0 0 0 -2 0 0 1 0 0 0 0 0.25
Fe[II](OH)3 -
0    0 0 0 -3 0 0 1 0 0 0 0 0    0    0 0 0 -3 0 0 1 0 0 0 0 0
Fe[III](OH)4 -
0    0 0 0 -3 0 0 1 0 0 0 0 0.25 0    0 0 0 -3 0 0 1 0 0 0 0 0.25
Fe[III](SO4)2 -
0    0 0 0  1 0 0 1 0 0 2 0 0.25 0    0 0 0  1 0 0 1 0 0 2 0 0.25
Fe[III]HSO4 +2
0    0 0 0  2 0 0 1 0 0 1 0 0.25 0    0 0 0  2 0 0 1 0 0 1 0 0.25
Fe[II]SO4 (aq)
0    0 0 0  0 0 0 1 0 0 1 0 0    0    0 0 0  0 0 0 1 0 0 1 0 0
Fe[III]SO4 +
0    0 0 0  1 0 0 1 0 0 1 0 0.25 0    0 0 0  1 0 0 1 0 0 1 0 0.25
H2SO4 (aq)
0    0 0 0  2 0 0 0 0 0 1 0 0    0    0 0 0  2 0 0 0 0 0 1 0 0
HSO4 -
0    0 0 0  1 0 0 0 0 0 1 0 0    0    0 0 0  1 0 0 0 0 0 1 0 0
```

Table 6.12 Input Data Sets for Problem 7 (continued)

```
Cu[II]Cl +
0    0 0 0  0 1 0 0 0 0 0 1 0    0    0 0 0  0 1 0 0 0 0 0 1 0
Cu[II]Cl2 (aq)
0    0 0 0  0 1 0 0 0 0 0 2 0    0    0 0 0  0 1 0 0 0 0 0 2 0
Cu[II]Cl4 -2
0    0 0 0  0 1 0 0 0 0 0 4 0    0    0 0 0  0 1 0 0 0 0 0 4 0
Cu +
0    0 0 0 -1 1 0 0 0 0 0 0 -0.25 0   0 0 0 -1 1 0 0 0 0 0 0 -0.25
Cu[I]Cl2 -
0    0 0 0 -1 1 0 0 0 0 0 0 2 -0.25 0   0 0 0 -1 1 0 0 0 0 0 2 -0.25
Cu[I]Cl3 -2
0    0 0 0 -1 1 0 0 0 0 0 0 3 -0.25 0   0 0 0 -1 1 0 0 0 0 0 3 -0.25
Cu[IIO2 -2
0    0 0 0 -4 1 0 0 0 0 0 0 0 0    0    0 0 0 -4 1 0 0 0 0 0 0 0 0
C ******** DATA SET 27:  PRECIPITATED SPECIES
Chrysocolla
0  -3.928     0 0 0 -2 1 0 0 1 0 0 0 0    0 0 0 -2 1 0 0 1 0 0 0 0
Jurbanite
0   3.23      0 0 0 -1 0 1 0 0 0 1 0 0    0 0 0 -1 0 1 0 0 0 1 0 0
Alunite
0   0.3479    0 1 0 -6 0 3 0 0 0 2 0 0    0 1 0 -6 0 3 0 0 0 2 0 0
Goethite
0   7.955     0 0 0 -2 0 0 1 0 0 0 0 0.25 0 0 0 -2 0 0 1 0 0 0 0 0.25
Gypsum
0   4.482     0 0 1  0 0 0 0 0 0 1 0 0    0 0 1  0 0 0 0 0 0 1 0 0
Jarosite
0  34.84      0 1 0 -3 0 0 3 0 0 2 0 0.75 0 1 0 -3 0 0 3 0 0 2 0 0.75
Kaolinite
0  -6.810     0 0 0 -6 0 2 0 2 0 0 0 0    0 0 0 -6 0 2 0 2 0 0 0 0
Muscovite
0 -13.59      0 1 0 -10 0 3 0 3 0 0 0 0    0 1 0 -10 0 3 0 3 0 0 0 0
Quartz
```

```
0   3.999     0 0 0  0 0 0 0 1 0 0 0 0    0 0 0  0 0 0 0 1 0 0 0 0
SiO2 (am)
0   2.714     0 0 0  0 0 0 0 1 0 0 0 0    0 0 0  0 0 0 0 1 0 0 0 0
C ******** DATA SET 29:  reaction data
44
 1  1  0              NRTS NPDS KRTYP           RXN 1: OH -
-13.995              LOGKEQ
-1  1                 STOICHIOMETRY          (Reactants, Products)
 4  13                GLOBAL SPECIES NUMBERS (Reactants, Products)
 3  1  0              NRTS NPDS KRTYP           RXN 2: Fe +3
  8.490               LOGKEQ
 1  1  0.25 1         STOICHIOMETRY          (Reactants, Products)
 4  7  12   14        GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 3: Al(OH)2 +
-10.595               LOGKEQ
-2  1  1              STOICHIOMETRY          (Reactants, Products)
 4  6  15             GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 4: Al(OH)3 (aq)
-16.158               LOGKEQ
-3  1  1              STOICHIOMETRY          (Reactants, Products)
 4  6  16             GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 5:Al(OH)4 -
-22.883               LOGKEQ
```

Table 6.12 Input Data Sets for Problem 7 (continued)

```
-4  1  1              STOICHIOMETRY          (Reactants, Products)
 4  6  17             GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 6: Al(SO4)2 -
  4.9                 LOGKEQ
 1  2  1              STOICHIOMETRY          (Reactants, Products)
 6  10 18             GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 7: AlOH +
 -4.9571              LOGKEQ
-1  1  1              STOICHIOMETRY          (Reactants, Products)
 4  6  19             GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 8: AlSO4 +
  3.01                LOGKEQ
 1  1  1              STOICHIOMETRY          (Reactants, Products)
 6  10 20             GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 9: H2CO3*
  6.3447              LOGKEQ
 1  1  1              STOICHIOMETRY          (Reactants, Products)
 4  9  21             GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 10: CO3 -
-10.329               LOGKEQ
-1  1  1              STOICHIOMETRY          (Reactants, Products)
 4  9  22             GLOBAL SPECIES NUMBERS (Reactants, Products)
 3  1  0              NRTS NPDS KRTYP           RXN 11: CaCO3 (aq)
 -7.0017              LOGKEQ
 1 -1  1  1           STOICHIOMETRY          (Reactants, Products)
 3  4  9  23          GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 12: CaHCO3 +
  1.0467              LOGKEQ
 1  1  1              STOICHIOMETRY          (Reactants, Products)
 3  9  24             GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 13: CaOH +
-12.8500              LOGKEQ
 1 -1  1              STOICHIOMETRY          (Reactants, Products)
 3  4  25             GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 14: CaSO4(aq)
  2.1111              LOGKEQ
```

```
 1  1  1              STOICHIOMETRY          (Reactants, Products)
 3  10 26             GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 15: CuOH +
 -7.2875              LOGKEQ
-1  1  1              STOICHIOMETRY          (Reactants, Products)
 4  5  27             GLOBAL SPECIES NUMBERS (Reactants, Products)
 2 1 0                NRTS NPDS KRTYP           RXN 16: CuSO4(aq)
  2.31                LOGKEQ
 1  1  1              STOICHIOMETRY          (Reactants, Products)
 5  10 28             GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 17: Fe[II](OH)2 (aq)
-20.6000              LOGKEQ
-2  1  1              STOICHIOMETRY          (Reactants, Products)
 4  7  29             GLOBAL SPECIES NUMBERS (Reactants, Products)
 3  1  0              NRTS NPDS KRTYP           RXN 18: Fe[III](OH)2 +
  2.820               LOGKEQ
-1  1  0.25 1         STOICHIOMETRY          (Reactants, Products)
 4  7  12   30        GLOBAL SPECIES NUMBERS (Reactants, Products)
 3  1  0              NRTS NPDS KRTYP           RXN 19: Fe[III](OH)3 (aq)
```

Table 6.12 Input Data Sets for Problem 7 (continued)

```
 -3.51                LOGKEQ
-2  1  0.25 1         STOICHIOMETRY          (Reactants, Products)
 4  7  12   31              GLOBAL SPECIES NUMBERS (Reactants, Products)
 2 1 0                NRTS NPDS KRTYP           RXN 20: Fe[II](OH)3 -
-31.000               LOGKEQ
-3  1  1              STOICHIOMETRY          (Reactants, Products)
 4  7  32             GLOBAL SPECIES NUMBERS (Reactants, Products)
 3  1  0              NRTS NPDS KRTYP           RXN 21: Fe[III](OH)4 -
-13.110               LOGKEQ
-3  1  0.25 1         STOICHIOMETRY          (Reactants, Products)
 4  7  12   33        GLOBAL SPECIES NUMBERS (Reactants, Products)
 4  1  0              NRTS NPDS KRTYP        RXN 22: Fe[III](SO4)2 -
 11.704               LOGKEQ
 1  1  2  0.25 1      STOICHIOMETRY          (Reactants, Products)
 4  7  10 12   34     GLOBAL SPECIES NUMBERS (Reactants, Products)
 4  1  0              NRTS NPDS KRTYP        RXN 23: Fe[III]HSO4 +2
 10.030               LOGKEQ
 2  1  1  0.25 1      STOICHIOMETRY          (Reactants, Products)
 4  7  10 12   35     GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 24: Fe[II]SO4 (aq)
 2.2                  LOGKEQ
 1  1    1            STOICHIOMETRY          (Reactants, Products)
 7  10   36           GLOBAL SPECIES NUMBERS (Reactants, Products)
 4  1  0              NRTS NPDS KRTYP        RXN 25: Fe[III]SO4 +
 10.4180              LOGKEQ
 1  1  1  0.25 1      STOICHIOMETRY          (Reactants, Products)
 4  7  10 12   37     GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 26: H2SO4 (aq)
-1.0209               LOGKEQ
 2  1    1            STOICHIOMETRY          (Reactants, Products)
 4  10   38           GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 27: HSO4 -
 1.9791               LOGKEQ
 1  1    1            STOICHIOMETRY          (Reactants, Products)
 4  10   39           GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 28: Cu[II]Cl +
 0.437                LOGKEQ
 1  1    1            STOICHIOMETRY          (Reactants, Products)
 5  11   40           GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 29: Cu[II]Cl2 (aq)
```

```
 0.1585               LOGKEQ
 1  2    1            STOICHIOMETRY          (Reactants, Products)
 5  11   41           GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 30: Cu[II]Cl4 -2
-4.5681               LOGKEQ
 1  4    1            STOICHIOMETRY          (Reactants, Products)
 5  11   42           GLOBAL SPECIES NUMBERS (Reactants, Products)
 3  1  0              NRTS NPDS KRTYP           RXN 31: Cu +
-18.77                LOGKEQ
-1  1 -0.25 1         STOICHIOMETRY          (Reactants, Products)
 4  5 12    43        GLOBAL SPECIES NUMBERS (Reactants, Products)
 4  1  0              NRTS NPDS KRTYP           RXN 32: Cu[I]Cl2 -
-13.949                LOGKEQ
-1  1  2 -0.25 1      STOICHIOMETRY          (Reactants, Products)
 4  5  11 12   44     GLOBAL SPECIES NUMBERS (Reactants, Products)
```

Table 6.12 Input Data Sets for Problem 7 (concluded)

```
 4  1  0              NRTS NPDS KRTYP           RXN 33: Cu[I]Cl3 -2
-13.141               LOGKEQ
-1  1  3 -0.25 1      STOICHIOMETRY          (Reactants, Products)
 4  5  11 12   45     GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  0              NRTS NPDS KRTYP           RXN 34: Cu[IIO2 -2
-39.45                LOGKEQ
-4  1    1            STOICHIOMETRY          (Reactants, Products)
 4  5    46           GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  3  1              NRTS NPDS KRTYP ***dissol*** RXN 35: Chrysocolla
-3.42919  0.49881     LOG(kb) LOG(kf)
1  0.39 -1.61  1  1   STOICHIOMETRY          (Reactants, Products)
47 4    4      5  8   GLOBAL SPECIES NUMBERS (Reactants, Products)
 3  1  1              NRTS NPDS KRTYP           RXN 36: Jurbanite
-0.50119  2.72881     LOG(kb) LOG(kf)
-1  1  1  1           STOICHIOMETRY          (Reactants, Products)
 4  6  10 48          GLOBAL SPECIES NUMBERS (Reactants, Products)
 4  1  1              NRTS NPDS KRTYP           RXN 37: Alunite
-0.50119 -0.15329     LOG(kb) LOG(kf)
 1 -6  3  2  1        STOICHIOMETRY          (Reactants, Products)
 2  4  6  10 49       GLOBAL SPECIES NUMBERS (Reactants, Products)
 3  1  1              NRTS NPDS KRTYP           RXN 38: Goethite
-0.50119  7.45381     LOG(kb) LOG(kf)
-2  1  0.25 1         STOICHIOMETRY          (Reactants, Products)
 4  7  12   50        GLOBAL SPECIES NUMBERS (Reactants, Products)
 2  1  1              NRTS NPDS KRTYP           RXN 39: Gypsum
 0.49881   4.98081    LOG(kb) LOG(kf)
 1  1  1              STOICHIOMETRY          (Reactants, Products)
 3  10 51            GLOBAL SPECIES NUMBERS (Reactants, Products)
 5  1  1              NRTS NPDS KRTYP     RXN 40: Jarosite
-0.50119  34.33881    LOG(kb) LOG(kf)
 1 -3  3  2  0.75 1   STOICHIOMETRY          (Reactants, Products)
 2  4  7  10 12   52  GLOBAL SPECIES NUMBERS (Reactants, Products)
 3  1  1              NRTS NPDS KRTYP           RXN 41: Kaolinite
-2.50119  -9.31119    LOG(kb) LOG(kf)
-6  2  2  1           STOICHIOMETRY          (Reactants, Products)
 4  6  8  53          GLOBAL SPECIES NUMBERS (Reactants, Products)
 4  1  1              NRTS NPDS KRTYP           RXN 42: Muscovite
-2.50119 -16.09119    LOG(kb) LOG(kf)
 1 -10 3  3  1        STOICHIOMETRY          (Reactants, Products)
 2  4  6  8  54       GLOBAL SPECIES NUMBERS (Reactants, Products)
 1  1  1              NRTS NPDS KRTYP           RXN 43: Quartz
-3.50119  0.49781     LOG(kb) LOG(kf)
 1  1                 STOICHIOMETRY          (Reactants, Products)
 8  55                GLOBAL SPECIES NUMBERS (Reactants, Products)
```

```
 1  1  1              NRTS NPDS KRTYP           RXN 44: SiO2 (am)
-0.50119  2.21281     LOG(kb) LOG(kf)
 1  1                 STOICHIOMETRY          (Reactants, Products)
 8  56                GLOBAL SPECIES NUMBERS (Reactants, Products)
                                END OF JOB
```

6.8 Problem 8: Kinetic Adsorption and Biodegradation

This application simulates bioremediation of a contaminated soil through the supply of an appropriate microorganism at the injection well. The biogeochemical reaction system for this application is adapted from the one dimensional reactive transport benchmark problem developed by Valocchi and Tebes (1997), and simulated in Problem 6. The steady state flow field for this example is identical to the one used in Problem 7 (See Figure 6.4). The injection and extraction wells in this case serve as a means of bioremediating this hypothetical field site.

A 50 x 50 dm region adjacent to the injection well is assumed to be initially contaminated with cobalt and nitrilotriacetate (NTA), a chelating agent. The remainder of the region is initially free from these species. Seven components are used to characterize the system: H^+, $H_2CO_3^*$, NH_4^+, O_2, NTA^{3-}, Co^{2+}, and an adsorbent surface site >SOH. Table 6.13 summarizes the total concentrations of these components present initially in the region. The fluid composition is simulated using fourteen soluble complexed species. Formation of all are assumed to be equilibrium. Table 6.14 summarizes the reaction tableau for these aqueous species and the equilibrium constants for their formation.

Table 6.13. Total Concentration of Components and Kinetic Species Initially in the Matrix Fluid and in the Injection Fluid. All chemical species concentrations are expressed in mol/dm^3 of media. Biomass concentration is expressed in kg/dm^3 of media.

Species	Contaminated Zone Initially	Non-Contaminated Zone Initially	Injection Fluid ≤ 48 hours	Injection Fluid > 48 hours
pH	6.3	6.5	6	6
$H_2CO_3^*$	2.45E-8	2.45E-8	2.45E-8	2.45E-8
NH_4^+	0	0	0	0
O_2	1.5625E-6	1.5625E-6	1.5625E-6	1.5625E-6
NTA3-	2.6150E-7	0	0	0
Co2+	2.6150E-7	0	0	0
>SOH	1.4000E-3	1.4000E-3	NA	NA
>SOH_2-CoNTA	0	0	NA	NA
>$(SO)_2$-Co	0	0	NA	NA

Cells $_{(aq)}$	0	0	6.8000E-9	0
Cells $_{(ads)}$	0	0	NA	NA

Table 6.14. Tableau of Equilibrium Aqueous Speciation Reactions for Bioremediation Application.

	~~H^+~~	~~NTA^{3-}~~	~~Co^{2+}~~	~~$H_2CO_3^*$~~	~~NH_4^+~~	O_2	log K_{eq}	
H_3NTA	3	1	0	0	0	0	14.9	
H_2NTA^-	2	1	0	0	0	0	13.3	
$HNTA^{2-}$	1	1	0	0	0	0	10.3	
$CoNTA^-$	0	1	1	0	0	0	11.7	
$Co(NTA)_2^{4-}$	0	2	1	0	0	0	14.5	
$CoOHNTA^{2-}$	-1	1	1	0	0	0	0.5	
$CoOH^+$	-1	0	1	0	0	0	-9.7	
$Co(OH)_2$	-2	0	1	0	0	0	-22.9	
$Co(OH)_3$	-3	0	1	0	0	0	-31.5	
OH^-	-1	0	0	0	0	0	-14.0	
HCO_3^-	-1	0	0	1	0	0	-6.3	
CO_3^{2-}		-2	0	0	1	0	0	-16.5
NH_3	1	0	0	0	1	0	-9.3	

The mobility of two aqueous species, Co^{2+} and $CoNTA^-$, is retarded due to kinetic adsorption to an oxide coating on the porous media. The distribution and charge of the adsorption sites on the oxide coating is pH dependent as given by reactions **(6.8.1)** and **(6.8.2)**. The two kinetic chemical adsorption reactions are given by **(6.8.3)** and **(6.8.4)**.

$$>SOH + H^+ \rightleftharpoons >SOH_2^+ , \quad \log K_{eq} = 5.6 \qquad (6.8.1)$$

$$>SOH - H^+ \rightleftharpoons >SO^- , \quad \log K_{eq} = -11.6 \qquad (6.8.2)$$

$$>SOH_2^+ + CoNTA^-_{(aq)} \underset{k_{b1}}{\overset{k_{f1}}{\rightleftharpoons}} >SOH_2\text{-}CoNTA_{(ads)} \qquad (6.8.3)$$

$$2(>SO^-) + Co^{2+}_{(aq)} \underset{k_{b2}}{\overset{k_{f2}}{\rightleftharpoons}} (>SO)_2\text{-}Co_{(ads)} \qquad (6.8.4)$$

where k_{f1} = 0.8000 hr^{-1}, k_{b1} = 0.005260 hr^{-1}, and k_{f2} = 0.2667 hr^{-1}, k_{b2} = 0.05260 hr^{-1}. The adsorption parameters were selected to make this a significant kinetic process in the system; they do not necessarily represent the true adsorption behavior for Co^{2+} or $CoNTA^-$.

A preliminary simulation was performed without flow due to pumping to allow for this adsorption process to occur until a steady state distribution of Co^{2+} and NTA^{3-} between the aqueous and adsorbed phases occurred. The purpose was to approximate a preremediation condition in which some species' mobility is hindered by adsorption to the matrix. Figure 6.8 shows the results of this kinetic adsorption process. Because of the pH of the system, the reactive adsorbent sites are primarily positively charged, and $>SOH_2\text{-}CoNTA_{(ads)}$ is the primary surface species. Negligible amounts of $>(SO)_2\text{-}Co_{(ads)}$ are formed. By approximately 1000 hours, a steady state condition is reached with 40% of the total Co^{2+} and NTA^{3-} adsorbed to the media.

After the adsorption process was allowed to reach steady state, the pumping wells were activated. For a period of 48 hours, the injection fluid contains a microorganism capable of degrading NTA. After that initial period, injection of water continues to maintain flow through the region but supply of the microorganism is ceased. The simulation is run for a total of 2500 hours. Table 6.13 summarizes the chemical and microbial concentrations in the injection solution. Both the matrix fluid and the injection fluid are assumed to have a density of 1 kg/dm^3.

Biodegradation can alter the chemical distribution in this system. It is assumed that the microorganisms can use nitroltriacetate as a growth substrate but can degrade only one of the aqueous complexed forms, $HNTA^{2-}$. The biodegradation reaction is:

$$HNTA^{2-} + 1.620\ O_2 + 1.272\ H_2O + 2.424\ H^+ \rightarrow 17.3707\ \underset{(cells)}{C_5H_7O_2N} + 3.120\ H_2CO_3^* + 0.424\ NH_4^+ \qquad (6.8.5)$$

where K_S = 7.64E-7 mol/L, K_O = 6.25E-6 mol/L, μ_{max} = 0.0916519 hr^{-1}, b_0 = 5.44E-5 $gram/dm^3$ of media, and K_d = 0.00208 hr^{-1} (Valocchi and Tebes, 1997). It is assumed that the microorganisms are in the aqueous phase in the injection solution, but that they may adsorb to the porous media once in the matrix. A kinetic reaction is used to describe this adsorption process:

$$C_5H_7O_2N\ (aq) \rightleftharpoons C_5H_7O_2N\ (ads) \qquad (6.8.6)$$

where k_f = 0.2667 hr^{-1} and k_{b2} = 0.05260 hr^{-1}. Microorganisms both in solution and adsorbed to the media are assumed capable of degrading HNTA by reaction **(6.8.5)** and at the same rate.

Figure 6.9 depicts the total aqueous Co^{2+} and $>SOH_2$-$CoNTA_{(ads)}$ in the system after 44 hours and 304 hours of pumping. Transport of the aqueous species is apparent. A portion of the adsorbed species is removed from the originally contaminated zone, and some is formed in the initially clean region as aqueous Co^{2+} and NTA^{3-} are transported toward the extraction well. Figures 6.10 and 6.11 show the aqueous and adsorbed microbial species concentrations at these same times and contrasts them to a "no growth" condition. This "no growth condition" reflects a separate simulation performed with injection of the aqueous microorganism and its subsequent transport through and adsorption to the porous media; biodegradation reaction **(6.8.5)** was not included. Enhanced levels of biomass both in solution and adsorbed to the media result when reaction **(6.8.5)** is allowed to proceed.

Figure 6.12 shows the concentration of total aqueous Co^{2+} and NTA^{3-} over time at the recovery well. Three conditions are contrasted to allow the impact of different processes to be assessed: (1) recovery of a non-reactive tracer present initially in the same amount and spatial distribution as Co^{2+} and NTA^{3-}, (2) recovery of Co^{2+} and NTA^{3-} when flow is maintained through the region but microorganisms are not injected into the system, and (3) recovery of Co^{2+} and NTA^{3-} when microorganisms are injected into the contaminated zone and biodegradation can proceed. Contrasting conditions 1 and 2 shows the retardation of Co^{2+} and NTA^{3-} due to their adsorption to the oxide coating, and indicates that flushing of the contaminated zone with clean water will achieve cleanup under the conditions simulated. Contrasting conditions 2 and 3 helps make evident the slight acceleration of remediation that can be achieved with biodegradation in this system. NTA is removed from the system resulting in less recovered at the extraction well. Co^{2+} arrives slightly earlier as a result. Cobalt is retained in the media because of the combined effects of its equilibrium aqueous complexation with NTA^{3-} and its subsequent kinetic adsorption to the porous media surface as $>SOH_2$-$CoNTA_{(ads)}$. As biodegradation removes NTA from the system, less is available to complex with Co^{2+} and adsorb to the surface. Cobalt's mobility is enhanced as a result when biodegradation occurs. Though the impact is small for the particular parameters chosen for this example, this result helps to illustrate the value of the capability of simulating kinetic geochemical and microbiological effects simultaneously.

The input data sets for Problem 8 are prepared according to Appendix A and are given in Table 6.15.

Table 6.15 Input Data Sets for Problem 8

```
   1  MICROBIAL BENCHMARK PROBLEM (PART B) + 2D FLOW (KG,DM,HR)
 1 0 0 0 0
C ******* DATA SET 2: BASIC INTEGER PARAMTERS
 961 900 1 0 200   1 4 -1 1 0   0 0 40 1 50   0 1 0 1 11   1 1 1
C ******* DATA SET 3: BASIC REAL PARAMETERS
0.1 0.1D0 36.0 17520 1.0D0   1.0D0 1.0D0 1.0D00 1.0D-6 1.0D0
C ******* DATA SET 4: PRINT AND AUXILIARY STORGE CONTROL
4444444444400000000040000000004000000000400000000040000000004000000000400000000040000000000
4000000000400000000040000000004000000000400000000040000000004000000000400000000040000000000
4000000000400000000040000000004000000000400000000004
1010001010100000000010000000001000010000100001000010000100001000010000100001000010000
1000010000100001000010000000001000000000100000000010000000001000000000100000000010000000000
1000000000100000000010000000001000000000001
1.0D38
C ******* DATA SET 5: CHEMICAL OUTPUT AND CHEMICAL PROPERTY TYPE INDICATOR
 3
 1 481 961 NODEP

C ******* DATA SET 6: MATERIAL PROPERTIES
 0.0D0 0.0D0 0.0D0 2.56D0 AL AT AM RHOB
C ******* DATA SET 7: NODE COORDINATES
    1   30     1       0.0D0   0.0D0  0.0
   32   30     1       5.0D0   0.0D0  0.0
   63   30     1      10.0D0   0.0D0  0.0
   94   30     1      15.0D0   0.0D0  0.0
  125   30     1      20.0D0   0.0D0  0.0
  156   30     1      25.0D0   0.0D0  0.0
  187   30     1      30.0D0   0.0D0  0.0
  218   30     1      35.0D0   0.0D0  0.0
  249   30     1      40.0D0   0.0D0  0.0
  280   30     1      45.0D0   0.0D0  0.0
  311   30     1      50.0D0   0.0D0  0.0
  342   30     1      55.0D0   0.0D0  0.0
  373   30     1      60.0D0   0.0D0  0.0
  404   30     1      65.0D0   0.0D0  0.0
  435   30     1      70.0D0   0.0D0  0.0
  466   30     1      75.0D0   0.0D0  0.0
  497   30     1      80.0D0   0.0D0  0.0
  528   30     1      85.0D0   0.0D0  0.0
  559   30     1      90.0D0   0.0D0  0.0
  590   30     1      95.0D0   0.0D0  0.0
  621   30     1     100.0D0   0.0D0  0.0
  652   30     1     105.0D0   0.0D0  0.0
  683   30     1     110.0D0   0.0D0  0.0
  714   30     1     115.0D0   0.0D0  0.0
  745   30     1     120.0D0   0.0D0  0.0
  776   30     1     125.0D0   0.0D0  0.0
  807   30     1     130.0D0   0.0D0  0.0
  838   30     1     135.0D0   0.0D0  0.0
  869   30     1     140.0D0   0.0D0  0.0
  900   30     1     145.0D0   0.0D0  0.0
  931   30     1     150.0D0   0.0D0  0.0
    0    0     0      0.0     0.0    0.0           END OF X-COORD
```

Table 6.15 Input Data Sets for Problem 8 (continued)

```
    1   30     1      0.0D0   5.0D0  0.0
   32   30     1      0.0D0   5.0D0  0.0
```

```
   63   30      1       0.0D0    5.0D0  0.0
   94   30      1       0.0D0    5.0D0  0.0
  125   30      1       0.0D0    5.0D0  0.0
  156   30      1       0.0D0    5.0D0  0.0
  187   30      1       0.0D0    5.0D0  0.0
  218   30      1       0.0D0    5.0D0  0.0
  249   30      1       0.0D0    5.0D0  0.0
  280   30      1       0.0D0    5.0D0  0.0
  311   30      1       0.0D0    5.0D0  0.0
  342   30      1       0.0D0    5.0D0  0.0
  373   30      1       0.0D0    5.0D0  0.0
  404   30      1       0.0D0    5.0D0  0.0
  435   30      1       0.0D0    5.0D0  0.0
  466   30      1       0.0D0    5.0D0  0.0
  497   30      1       0.0D0    5.0D0  0.0
  528   30      1       0.0D0    5.0D0  0.0
  559   30      1       0.0D0    5.0D0  0.0
  590   30      1       0.0D0    5.0D0  0.0
  621   30      1       0.0D0    5.0D0  0.0
  652   30      1       0.0D0    5.0D0  0.0
  683   30      1       0.0D0    5.0D0  0.0
  714   30      1       0.0D0    5.0D0  0.0
  745   30      1       0.0D0    5.0D0  0.0
  776   30      1       0.0D0    5.0D0  0.0
  807   30      1       0.0D0    5.0D0  0.0
  838   30      1       0.0D0    5.0D0  0.0
  869   30      1       0.0D0    5.0D0  0.0
  900   30      1       0.0D0    5.0D0  0.0
  931   30      1       0.0D0    5.0D0  0.0
    0    0      0       0.0D0    0.0D0  0.0D0          END OF Z-COORD
C ******* DATA SET 8: ELEMENT CONNECTIVITY
    1    1   32   33    2    1   30   30           IE
C ******* DATA SET 10: CHEMICAL COMPONENT INFORMATION
 6 1 0 2 0 0 1 1   NOHA NOHS NOKX KY KZ KP MB MA
 H+
  1   1
 H2CO3*
  2   1
 NH4+
  3   1
 O2
  4   1
 NTA3-
  5   1
 Co 2+
  6   1
 >SOH
  7   2
C ******* DATA SET 11:  INITIAL CONDITIONS (MASS/MEDIA VOLUME)
    1    10   1    2.3289d-4 0.0D0     0.0D0
   32    10   1    2.3289d-4 0.0D0     0.0D0
   63    10   1    2.3289d-4 0.0D0     0.0D0
   94    10   1    2.3289d-4 0.0D0     0.0D0
```

Table 6.15 Input Data Sets for Problem 8 (continued)

```
  125    10   1    2.3289d-4 0.0D0     0.0D0
  156    10   1    2.3289d-4 0.0D0     0.0D0
  187    10   1    2.3289d-4 0.0D0     0.0D0
  218    10   1    2.3289d-4 0.0D0     0.0D0
  249    10   1    2.3289d-4 0.0D0     0.0D0
  280    10   1    2.3289d-4 0.0D0     0.0D0
```

```
311    10   1    2.3289d-4 0.0D0     0.0D0
 12    19   1    1.5653d-4 0.0D0     0.0D0
 43    19   1    1.5653d-4 0.0D0     0.0D0
 74    19   1    1.5653d-4 0.0D0     0.0D0
105    19   1    1.5653d-4 0.0D0     0.0D0
136    19   1    1.5653d-4 0.0D0     0.0D0
167    19   1    1.5653d-4 0.0D0     0.0D0
198    19   1    1.5653d-4 0.0D0     0.0D0
229    19   1    1.5653d-4 0.0D0     0.0D0
260    19   1    1.5653d-4 0.0D0     0.0D0
291    19   1    1.5653d-4 0.0D0     0.0D0
322    639  1    1.5653d-4 0.0D0     0.0D0
  0    0    0    0.0       0.0       0.0          END OF I.C. H+ - variable PH
  1    960  1    2.45d-8   0.0D0     0.0D0
  0    0    0.0  0.0       0.0       0.0D0        END OF I.C. H2CO3(g)
  1    960  1    0.00d-14  0.0D0     0.0D0
  0    0    0    0.0       0.0       0.0          END OF I.C. NH4+
  1    960  1    1.5625d-6 0.0D0     0.0D0
  0    0    0    0.0       0.0       0.0          END OF I.C. O2
  1    10   1    1.5810d-7 0.0D0     0.0D0
 32    10   1    1.5810d-7 0.0D0     0.0D0
 63    10   1    1.5810d-7 0.0D0     0.0D0
 94    10   1    1.5810d-7 0.0D0     0.0D0
125    10   1    1.5810d-7 0.0D0     0.0D0
156    10   1    1.5810d-7 0.0D0     0.0D0
187    10   1    1.5810d-7 0.0D0     0.0D0
218    10   1    1.5810d-7 0.0D0     0.0D0
249    10   1    1.5810d-7 0.0D0     0.0D0
280    10   1    1.5810d-7 0.0D0     0.0D0
311    10   1    1.5810d-7 0.0D0     0.0D0
 12    19   1    0.0000d-7 0.0D0     0.0D0
 43    19   1    0.0000d-7 0.0D0     0.0D0
 74    19   1    0.0000d-7 0.0D0     0.0D0
105    19   1    0.0000d-7 0.0D0     0.0D0
136    19   1    0.0000d-7 0.0D0     0.0D0
167    19   1    0.0000d-7 0.0D0     0.0D0
198    19   1    0.0000d-7 0.0D0     0.0D0
229    19   1    0.0000d-7 0.0D0     0.0D0
260    19   1    0.0000d-7 0.0D0     0.0D0
291    19   1    0.0000d-7 0.0D0     0.0D0
322    639  1    0.0000d-7 0.0D0     0.0D0
  0    0    0    0.0       0.0       0.0          END OF I.C. NTA3-
  1    10   1    1.5810d-7 0.0D0     0.0D0
 32    10   1    1.5810d-7 0.0D0     0.0D0
 63    10   1    1.5810d-7 0.0D0     0.0D0
 94    10   1    1.5810d-7 0.0D0     0.0D0
125    10   1    1.5810d-7 0.0D0     0.0D0
156    10   1    1.5810d-7 0.0D0     0.0D0
187    10   1    1.5810d-7 0.0D0     0.0D0
```

Table 6.15 Input Data Sets for Problem 8 (continued)

```
218    10   1    1.5810d-7 0.0D0     0.0D0
249    10   1    1.5810d-7 0.0D0     0.0D0
280    10   1    1.5810d-7 0.0D0     0.0D0
311    10   1    1.5810d-7 0.0D0     0.0D0
 12    19   1    0.0000d-7 0.0D0     0.0D0
 43    19   1    0.0000d-7 0.0D0     0.0D0
 74    19   1    0.0000d-7 0.0D0     0.0D0
105    19   1    0.0000d-7 0.0D0     0.0D0
136    19   1    0.0000d-7 0.0D0     0.0D0
167    19   1    0.0000d-7 0.0D0     0.0D0
```

```
  198    19   1    0.0000d-7 0.0D0     0.0D0
  229    19   1    0.0000d-7 0.0D0     0.0D0
  260    19   1    0.0000d-7 0.0D0     0.0D0
  291    19   1    0.0000d-7 0.0D0     0.0D0
  322    639  1    0.0000d-7 0.0D0     0.0D0
    0    0    0    0.0       0.0       0.0          END OF I.C. Co2+
    1    960  1    1.40d-3   0.0D0     0.0D0
    0    0    0    0.0       0.0       0.0          END OF I.C. >SOH
    1    960  1    0.00d-5   0.0D0     0.0D0
    0    0    0    0.0       0.0       0.0          END OF I.C. Cells (aq)
    1    10   1    1.0340d-7 0.0D0     0.0D0
   32    10   1    1.0340d-7 0.0D0     0.0D0
   63    10   1    1.0340d-7 0.0D0     0.0D0
   94    10   1    1.0340d-7 0.0D0     0.0D0
  125    10   1    1.0340d-7 0.0D0     0.0D0
  156    10   1    1.0340d-7 0.0D0     0.0D0
  187    10   1    1.0340d-7 0.0D0     0.0D0
  218    10   1    1.0340d-7 0.0D0     0.0D0
  249    10   1    1.0340d-7 0.0D0     0.0D0
  280    10   1    1.0340d-7 0.0D0     0.0D0
  311    10   1    1.0340d-7 0.0D0     0.0D0
   12    19   1    0.0000d-7 0.0D0     0.0D0
   43    19   1    0.0000d-7 0.0D0     0.0D0
   74    19   1    0.0000d-7 0.0D0     0.0D0
  105    19   1    0.0000d-7 0.0D0     0.0D0
  136    19   1    0.0000d-7 0.0D0     0.0D0
  167    19   1    0.0000d-7 0.0D0     0.0D0
  198    19   1    0.0000d-7 0.0D0     0.0D0
  229    19   1    0.0000d-7 0.0D0     0.0D0
  260    19   1    0.0000d-7 0.0D0     0.0D0
  291    19   1    0.0000d-7 0.0D0     0.0D0
  322    639  1    0.0000d-7 0.0D0     0.0D0
    0    0    0    0.0       0.0       0.0          END OF I.C. CoNTA(ads) = Ky1
    1    960  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    960  1    0.00d-5   0.0D0     0.0D0
    0    0    0    0.0       0.0       0.0          END OF I.C. Cells (ads)
C ******* DATA SET 12: CONTROL INTEGERS FOR TRANSIENT SOURCE/SINK AND B.C.
    0  0  0    2  2  4    0  0  0    0  0  0  0
C ******* DATA SET 13: WELL SOURCE/SINK (MASS/LIQUID VOLUME)
  1  961
0.0D0 8.387D-7  48.0D0 8.387D-7  48.01D0 8.387D-7 17520.0D0 8.387d-7
0.0D0 0.00D0    48.0D0 0.00D0    48.01D0 0.00D0   17520.0D0 0.00D0
    1    1    1    1    1
    0    0    0    0    0                        END OF B.C. H+
```

Table 6.15 Input Data Sets for Problem 8 (continued)

```
0.0D0 4.90D-7   48.0D0 4.90D-7   48.01D0 4.90D-7  17520.0D0 4.90d-7
0.0D0 0.00D0    48.0D0 0.00D0    48.01D0 0.00D0   17520.0D0 0.00D0
    1    1    1    1    1
    0    0    0    0    0                        END OF B.C. H2CO3(g)
0.0D0 0.00D0    48.0D0 0.00D0    48.01D0 0.00D0   17520.0D0 0.00D0
0.0D0 0.00D0    48.0D0 0.00D0    48.01D0 0.00D0   17520.0D0 0.00D0
    1    1    1    1    1
    0    0    0    0    0                        END OF B.C. NH4+
0.0D0 3.125D-5  48.0D0 3.125D-5  48.01D0 3.125D-5 17520.0D0 3.125D-5
0.0D0 0.00D0    48.0D0 0.00D0    48.01D0 0.00D0   17520.0D0 0.00D0
    1    1    1    1    1
    0    0    0    0    0                        END OF B.C. O2
0.0D0 0.00D-6   48.0D0 0.00D-6   48.01D0 0.00D0   17520.0D0 0.00D0
0.0D0 0.00D0    48.0D0 0.00D0    48.01D0 0.00D0   17520.0D0 0.00D0
```

```
    1    1    1    1    1
    0    0    0    0    0                              END OF B.C. NTA3-
0.0D0 0.00D-6   48.0D0 0.00D-6   48.01D0 0.00D0   17520.0D0 0.00D0
0.0D0 0.00D0    48.0D0 0.00D0    48.01D0 0.00D0   17520.0D0 0.00D0
    1    1    1    1    1
    0    0    0    0    0                              END OF B.C. Co2+
0.0D0 1.36D-6   48.0D0 1.36D-6   48.01D0 0.00D0   17520.0D0 0.00D0
0.0D0 0.00D0    48.0D0 0.00D0    48.01D0 0.00D0   17520.0D0 0.00D0
    1    1    1    1    1
    0    0    0    0    0              Cells(aq) kg/dm^3 liq *** rev
0.0D0  1.9D0  48.0D0  1.9D0  48.01D0  1.90D0  17520.0D0  1.90D0
0.0D0 -1.9D0  48.0D0 -1.9D0  48.01D0 -1.90D0  17520.0D0 -1.90D0
    1    1    1    1    1
    0    0    0    0    0                              Q (dm^3/hr per dm depth)
0.0D0 1.0000D0  48.0D0 1.0000D0  48.01D0 1.00D0   17520.0D0 1.00D0
0.0D0 1.0000D0  48.0D0 1.0000D0  48.01D0 1.00D0   17520.0D0 1.00D0
    1    1    1    1    1
    0    0    0    0    0                              END OF RHOL S/S
C ******* DATA SET 16: HYDROLOGICAL VARIABLES
    1    0    0   .5396279D+00   .5396279D+00   .00D+00   .00D+00
    2    0    0   .0000000D+00   .2464926D+00   .00D+00   .00D+00
    3    0    0   .0000000D+00   .1342666D+00   .00D+00   .00D+00
    4    0    0   .0000000D+00   .8721404D-01   .00D+00   .00D+00
    5    0    0   .0000000D+00   .6366838D-01   .00D+00   .00D+00
    6    0    0   .0000000D+00   .5001998D-01   .00D+00   .00D+00
    7    0    0   .0000000D+00   .4118950D-01   .00D+00   .00D+00
    8    0    0   .0000000D+00   .3500342D-01   .00D+00   .00D+00
    9    0    0   .0000000D+00   .3041039D-01   .00D+00   .00D+00
   10    0    0   .0000000D+00   .2684646D-01   .00D+00   .00D+00
   11    0    0   .0000000D+00   .2398402D-01   .00D+00   .00D+00
   12    0    0   .0000000D+00   .2161644D-01   .00D+00   .00D+00
   13    0    0   .0000000D+00   .1961130D-01   .00D+00   .00D+00
   14    0    0   .0000000D+00   .1787386D-01   .00D+00   .00D+00
   15    0    0   .0000000D+00   .1633790D-01   .00D+00   .00D+00
   16    0    0   .0000000D+00   .1495833D-01   .00D+00   .00D+00
   17    0    0   .0000000D+00   .1369463D-01   .00D+00   .00D+00
   18    0    0   .0000000D+00   .1252340D-01   .00D+00   .00D+00
   19    0    0   .0000000D+00   .1142152D-01   .00D+00   .00D+00
   20    0    0   .0000000D+00   .1037232D-01   .00D+00   .00D+00
   21    0    0   .0000000D+00   .9362614D-02   .00D+00   .00D+00
   22    0    0   .0000000D+00   .8382021D-02   .00D+00   .00D+00
```

Table 6.15 Input Data Sets for Problem 8 (continued)

```
   23    0    0   .0000000D+00   .7422374D-02   .00D+00   .00D+00
   24    0    0   .0000000D+00   .6477568D-02   .00D+00   .00D+00
   25    0    0   .0000000D+00   .5542580D-02   .00D+00   .00D+00
   26    0    0   .0000000D+00   .4613813D-02   .00D+00   .00D+00
   27    0    0   .0000000D+00   .3688813D-02   .00D+00   .00D+00
   28    0    0   .0000000D+00   .2765696D-02   .00D+00   .00D+00
   29    0    0   .0000000D+00   .1843550D-02   .00D+00   .00D+00
   30    0    0   .0000000D+00   .9217580D-03   .00D+00   .00D+00
   31    0    0   .0000000D+00   .0000000D+00   .00D+00   .00D+00
   32    0    0   .2464926D+00   .0000000D+00   .00D+00   .00D+00
   33    0    0   .1320462D+00   .1320462D+00   .00D+00   .00D+00
   34    0    0   .5500913D-01   .9463756D-01   .00D+00   .00D+00
   35    0    0   .2723687D-01   .7129737D-01   .00D+00   .00D+00
   36    0    0   .1558733D-01   .5628596D-01   .00D+00   .00D+00
   37    0    0   .9956792D-02   .4614212D-01   .00D+00   .00D+00
   38    0    0   .6891952D-02   .3893836D-01   .00D+00   .00D+00
   39    0    0   .5061301D-02   .3359247D-01   .00D+00   .00D+00
   40    0    0   .3888071D-02   .2947317D-01   .00D+00   .00D+00
```

41	0	0	.3095320D-02	.2619692D-01	.00D+00	.00D+00
42	0	0	.2537900D-02	.2351826D-01	.00D+00	.00D+00
43	0	0	.2134075D-02	.2127397D-01	.00D+00	.00D+00
44	0	0	.1834874D-02	.1935445D-01	.00D+00	.00D+00
45	0	0	.1609475D-02	.1767865D-01	.00D+00	.00D+00
46	0	0	.1437785D-02	.1618950D-01	.00D+00	.00D+00
47	0	0	.1306221D-02	.1484304D-01	.00D+00	.00D+00
48	0	0	.1205137D-02	.1360674D-01	.00D+00	.00D+00
49	0	0	.1127557D-02	.1245605D-01	.00D+00	.00D+00
50	0	0	.1068413D-02	.1137049D-01	.00D+00	.00D+00
51	0	0	.1023784D-02	.1033408D-01	.00D+00	.00D+00
52	0	0	.9906221D-03	.9334418D-02	.00D+00	.00D+00
53	0	0	.9665068D-03	.8361815D-02	.00D+00	.00D+00
54	0	0	.9494578D-03	.7408447D-02	.00D+00	.00D+00
55	0	0	.9378596D-03	.6468322D-02	.00D+00	.00D+00
56	0	0	.9303653D-03	.5536872D-02	.00D+00	.00D+00
57	0	0	.9258505D-03	.4610616D-02	.00D+00	.00D+00
58	0	0	.9233961D-03	.3687215D-02	.00D+00	.00D+00
59	0	0	.9222546D-03	.2765126D-02	.00D+00	.00D+00
60	0	0	.9218436D-03	.1843436D-02	.00D+00	.00D+00
61	0	0	.9217580D-03	.9217580D-03	.00D+00	.00D+00
62	0	0	.9217580D-03	.0000000D+00	.00D+00	.00D+00
63	0	0	.1342666D+00	.0000000D+00	.00D+00	.00D+00
64	0	0	.9463756D-01	.5500913D-01	.00D+00	.00D+00
65	0	0	.6075171D-01	.6075171D-01	.00D+00	.00D+00
66	0	0	.3835160D-01	.5500970D-01	.00D+00	.00D+00
67	0	0	.2515525D-01	.4772774D-01	.00D+00	.00D+00
68	0	0	.1734760D-01	.4126313D-01	.00D+00	.00D+00
69	0	0	.1254983D-01	.3595491D-01	.00D+00	.00D+00
70	0	0	.9465126D-02	.3165982D-01	.00D+00	.00D+00
71	0	0	.7395548D-02	.2816210D-01	.00D+00	.00D+00
72	0	0	.5955251D-02	.2527454D-01	.00D+00	.00D+00
73	0	0	.4922317D-02	.2284989D-01	.00D+00	.00D+00
74	0	0	.4163584D-02	.2077968D-01	.00D+00	.00D+00
75	0	0	.3595833D-02	.1898174D-01	.00D+00	.00D+00
76	0	0	.3165183D-02	.1739498D-01	.00D+00	.00D+00
77	0	0	.2835559D-02	.1597203D-01	.00D+00	.00D+00

Table 6.15 Input Data Sets for Problem 8 (continued)

78	0	0	.2581963D-02	.1467523D-01	.00D+00	.00D+00
79	0	0	.2386644D-02	.1347831D-01	.00D+00	.00D+00
80	0	0	.2236701D-02	.1235731D-01	.00D+00	.00D+00
81	0	0	.2122317D-02	.1129566D-01	.00D+00	.00D+00
82	0	0	.2036073D-02	.1027808D-01	.00D+00	.00D+00
83	0	0	.1972203D-02	.9293322D-02	.00D+00	.00D+00
84	0	0	.1925970D-02	.8332477D-02	.00D+00	.00D+00
85	0	0	.1893493D-02	.7388299D-02	.00D+00	.00D+00
86	0	0	.1871632D-02	.6455080D-02	.00D+00	.00D+00
87	0	0	.1857763D-02	.5528767D-02	.00D+00	.00D+00
88	0	0	.1849658D-02	.4606107D-02	.00D+00	.00D+00
89	0	0	.1845491D-02	.3685103D-02	.00D+00	.00D+00
90	0	0	.1843779D-02	.2764384D-02	.00D+00	.00D+00
91	0	0	.1843379D-02	.1843379D-02	.00D+00	.00D+00
92	0	0	.1843436D-02	.9218436D-03	.00D+00	.00D+00
93	0	0	.1843550D-02	.0000000D+00	.00D+00	.00D+00
94	0	0	.8721404D-01	.0000000D+00	.00D+00	.00D+00
95	0	0	.7129737D-01	.2723687D-01	.00D+00	.00D+00
96	0	0	.5500970D-01	.3835160D-01	.00D+00	.00D+00
97	0	0	.4026142D-01	.4026142D-01	.00D+00	.00D+00
98	0	0	.2933390D-01	.3835160D-01	.00D+00	.00D+00
99	0	0	.2172945D-01	.3522717D-01	.00D+00	.00D+00

100	0	0	.1649486D-01	.3195890D-01	.00D+00	.00D+00
101	0	0	.1285377D-01	.2893037D-01	.00D+00	.00D+00
102	0	0	.1027380D-01	.2624201D-01	.00D+00	.00D+00
103	0	0	.8407877D-02	.2388870D-01	.00D+00	.00D+00
104	0	0	.7032477D-02	.2182763D-01	.00D+00	.00D+00
105	0	0	.6001941D-02	.2001313D-01	.00D+00	.00D+00
106	0	0	.5219635D-02	.1839897D-01	.00D+00	.00D+00
107	0	0	.4619920D-02	.1694806D-01	.00D+00	.00D+00
108	0	0	.4157306D-02	.1562671D-01	.00D+00	.00D+00
109	0	0	.3799486D-02	.1440925D-01	.00D+00	.00D+00
110	0	0	.3522945D-02	.1327340D-01	.00D+00	.00D+00
111	0	0	.3310217D-02	.1220034D-01	.00D+00	.00D+00
112	0	0	.3148059D-02	.1117643D-01	.00D+00	.00D+00
113	0	0	.3026142D-02	.1018910D-01	.00D+00	.00D+00
114	0	0	.2936187D-02	.9228425D-02	.00D+00	.00D+00
115	0	0	.2871575D-02	.8286530D-02	.00D+00	.00D+00
116	0	0	.2826826D-02	.7357078D-02	.00D+00	.00D+00
117	0	0	.2797374D-02	.6435046D-02	.00D+00	.00D+00
118	0	0	.2779395D-02	.5516895D-02	.00D+00	.00D+00
119	0	0	.2769521D-02	.4599943D-02	.00D+00	.00D+00
120	0	0	.2765068D-02	.3682648D-02	.00D+00	.00D+00
121	0	0	.2763927D-02	.2763927D-02	.00D+00	.00D+00
122	0	0	.2764384D-02	.1843779D-02	.00D+00	.00D+00
123	0	0	.2765126D-02	.9222546D-03	.00D+00	.00D+00
124	0	0	.2765696D-02	.0000000D+00	.00D+00	.00D+00
125	0	0	.6366838D-01	.0000000D+00	.00D+00	.00D+00
126	0	0	.5628596D-01	.1558733D-01	.00D+00	.00D+00
127	0	0	.4772774D-01	.2515525D-01	.00D+00	.00D+00
128	0	0	.3835160D-01	.2933390D-01	.00D+00	.00D+00
129	0	0	.3018950D-01	.3018950D-01	.00D+00	.00D+00
130	0	0	.2373973D-01	.2933390D-01	.00D+00	.00D+00
131	0	0	.1884589D-01	.2772374D-01	.00D+00	.00D+00
132	0	0	.1518208D-01	.2586130D-01	.00D+00	.00D+00

Table 6.15 Input Data Sets for Problem 8 (continued)

133	0	0	.1243824D-01	.2398801D-01	.00D+00	.00D+00
134	0	0	.1037003D-01	.2220890D-01	.00D+00	.00D+00
135	0	0	.8797888D-02	.2055993D-01	.00D+00	.00D+00
136	0	0	.7592237D-02	.1904509D-01	.00D+00	.00D+00
137	0	0	.6660845D-02	.1765354D-01	.00D+00	.00D+00
138	0	0	.5937557D-02	.1637043D-01	.00D+00	.00D+00
139	0	0	.5374258D-02	.1517808D-01	.00D+00	.00D+00
140	0	0	.4935674D-02	.1406107D-01	.00D+00	.00D+00
141	0	0	.4595377D-02	.1300457D-01	.00D+00	.00D+00
142	0	0	.4333219D-02	.1199429D-01	.00D+00	.00D+00
143	0	0	.4133619D-02	.1102061D-01	.00D+00	.00D+00
144	0	0	.3984132D-02	.1007346D-01	.00D+00	.00D+00
145	0	0	.3874772D-02	.9144806D-02	.00D+00	.00D+00
146	0	0	.3797317D-02	.8228139D-02	.00D+00	.00D+00
147	0	0	.3744920D-02	.7318322D-02	.00D+00	.00D+00
148	0	0	.3711758D-02	.6411187D-02	.00D+00	.00D+00
149	0	0	.3692808D-02	.5503824D-02	.00D+00	.00D+00
150	0	0	.3683904D-02	.4594292D-02	.00D+00	.00D+00
151	0	0	.3681507D-02	.3681507D-02	.00D+00	.00D+00
152	0	0	.3682648D-02	.2765068D-02	.00D+00	.00D+00
153	0	0	.3685103D-02	.1845491D-02	.00D+00	.00D+00
154	0	0	.3687215D-02	.9233961D-03	.00D+00	.00D+00
155	0	0	.3688813D-02	.0000000D+00	.00D+00	.00D+00
156	0	0	.5001998D-01	.0000000D+00	.00D+00	.00D+00
157	0	0	.4614212D-01	.9956792D-02	.00D+00	.00D+00
158	0	0	.4126313D-01	.1734760D-01	.00D+00	.00D+00

159	0	0	.3522717D-01	.2172945D-01	.00D+00	.00D+00
160	0	0	.2933390D-01	.2373973D-01	.00D+00	.00D+00
161	0	0	.2419521D-01	.2419521D-01	.00D+00	.00D+00
162	0	0	.1996747D-01	.2374030D-01	.00D+00	.00D+00
163	0	0	.1658904D-01	.2280251D-01	.00D+00	.00D+00
164	0	0	.1392580D-01	.2163984D-01	.00D+00	.00D+00
165	0	0	.1183619D-01	.2039897D-01	.00D+00	.00D+00
166	0	0	.1019663D-01	.1915753D-01	.00D+00	.00D+00
167	0	0	.8908162D-02	.1795320D-01	.00D+00	.00D+00
168	0	0	.7894007D-02	.1679966D-01	.00D+00	.00D+00
169	0	0	.7095148D-02	.1570148D-01	.00D+00	.00D+00
170	0	0	.6466495D-02	.1465468D-01	.00D+00	.00D+00
171	0	0	.5973573D-02	.1365240D-01	.00D+00	.00D+00
172	0	0	.5589612D-02	.1268836D-01	.00D+00	.00D+00
173	0	0	.5293664D-02	.1175228D-01	.00D+00	.00D+00
174	0	0	.5068950D-02	.1083830D-01	.00D+00	.00D+00
175	0	0	.4901884D-02	.9939269D-02	.00D+00	.00D+00
176	0	0	.4781393D-02	.9049201D-02	.00D+00	.00D+00
177	0	0	.4698059D-02	.8163014D-02	.00D+00	.00D+00
178	0	0	.4643836D-02	.7276826D-02	.00D+00	.00D+00
179	0	0	.4611872D-02	.6387500D-02	.00D+00	.00D+00
180	0	0	.4596290D-02	.5492922D-02	.00D+00	.00D+00
181	0	0	.4591895D-02	.4591895D-02	.00D+00	.00D+00
182	0	0	.4594292D-02	.3683904D-02	.00D+00	.00D+00
183	0	0	.4599943D-02	.2769521D-02	.00D+00	.00D+00
184	0	0	.4606107D-02	.1849658D-02	.00D+00	.00D+00
185	0	0	.4610616D-02	.9258505D-03	.00D+00	.00D+00
186	0	0	.4613813D-02	.0000000D+00	.00D+00	.00D+00
187	0	0	.4118950D-01	.0000000D+00	.00D+00	.00D+00

Table 6.15 Input Data Sets for Problem 8 (continued)

188	0	0	.3893836D-01	.6891952D-02	.00D+00	.00D+00
189	0	0	.3595491D-01	.1254983D-01	.00D+00	.00D+00
190	0	0	.3195890D-01	.1649486D-01	.00D+00	.00D+00
191	0	0	.2772374D-01	.1884589D-01	.00D+00	.00D+00
192	0	0	.2374030D-01	.1996747D-01	.00D+00	.00D+00
193	0	0	.2023916D-01	.2023916D-01	.00D+00	.00D+00
194	0	0	.1728196D-01	.1996747D-01	.00D+00	.00D+00
195	0	0	.1484075D-01	.1936986D-01	.00D+00	.00D+00
196	0	0	.1285217D-01	.1859018D-01	.00D+00	.00D+00
197	0	0	.1124441D-01	.1771861D-01	.00D+00	.00D+00
198	0	0	.9949943D-02	.1680936D-01	.00D+00	.00D+00
199	0	0	.8911872D-02	.1589098D-01	.00D+00	.00D+00
200	0	0	.8082420D-02	.1498174D-01	.00D+00	.00D+00
201	0	0	.7423002D-02	.1408676D-01	.00D+00	.00D+00
202	0	0	.6902511D-02	.1320719D-01	.00D+00	.00D+00
203	0	0	.6495890D-02	.1234304D-01	.00D+00	.00D+00
204	0	0	.6182877D-02	.1148881D-01	.00D+00	.00D+00
205	0	0	.5946632D-02	.1064110D-01	.00D+00	.00D+00
206	0	0	.5773231D-02	.9796062D-02	.00D+00	.00D+00
207	0	0	.5650970D-02	.8949600D-02	.00D+00	.00D+00
208	0	0	.5569635D-02	.8097945D-02	.00D+00	.00D+00
209	0	0	.5520434D-02	.7238470D-02	.00D+00	.00D+00
210	0	0	.5495662D-02	.6369064D-02	.00D+00	.00D+00
211	0	0	.5488470D-02	.5488470D-02	.00D+00	.00D+00
212	0	0	.5492922D-02	.4596290D-02	.00D+00	.00D+00
213	0	0	.5503824D-02	.3692808D-02	.00D+00	.00D+00
214	0	0	.5516895D-02	.2779395D-02	.00D+00	.00D+00
215	0	0	.5528767D-02	.1857763D-02	.00D+00	.00D+00
216	0	0	.5536872D-02	.9303653D-03	.00D+00	.00D+00
217	0	0	.5542580D-02	.0000000D+00	.00D+00	.00D+00

218	0	0	.3500342D-01	.0000000D+00	.00D+00	.00D+00
219	0	0	.3359247D-01	.5061301D-02	.00D+00	.00D+00
220	0	0	.3165982D-01	.9465126D-02	.00D+00	.00D+00
221	0	0	.2893037D-01	.1285377D-01	.00D+00	.00D+00
222	0	0	.2586130D-01	.1518208D-01	.00D+00	.00D+00
223	0	0	.2280251D-01	.1658904D-01	.00D+00	.00D+00
224	0	0	.1996747D-01	.1728196D-01	.00D+00	.00D+00
225	0	0	.1745833D-01	.1745833D-01	.00D+00	.00D+00
226	0	0	.1530308D-01	.1728196D-01	.00D+00	.00D+00
227	0	0	.1348744D-01	.1687329D-01	.00D+00	.00D+00
228	0	0	.1197803D-01	.1631792D-01	.00D+00	.00D+00
229	0	0	.1073556D-01	.1567295D-01	.00D+00	.00D+00
230	0	0	.9721176D-02	.1497489D-01	.00D+00	.00D+00
231	0	0	.8899715D-02	.1424715D-01	.00D+00	.00D+00
232	0	0	.8240582D-02	.1350285D-01	.00D+00	.00D+00
233	0	0	.7717580D-02	.1274829D-01	.00D+00	.00D+00
234	0	0	.7308676D-02	.1198687D-01	.00D+00	.00D+00
235	0	0	.6995263D-02	.1121821D-01	.00D+00	.00D+00
236	0	0	.6761416D-02	.1044144D-01	.00D+00	.00D+00
237	0	0	.6593493D-02	.9654452D-02	.00D+00	.00D+00
238	0	0	.6479566D-02	.8855023D-02	.00D+00	.00D+00
239	0	0	.6409132D-02	.8040753D-02	.00D+00	.00D+00
240	0	0	.6372717D-02	.7210103D-02	.00D+00	.00D+00
241	0	0	.6361872D-02	.6361872D-02	.00D+00	.00D+00
242	0	0	.6369064D-02	.5495662D-02	.00D+00	.00D+00

Table 6.15 Input Data Sets for Problem 8 (continued)

243	0	0	.6387500D-02	.4611872D-02	.00D+00	.00D+00
244	0	0	.6411187D-02	.3711758D-02	.00D+00	.00D+00
245	0	0	.6435046D-02	.2797374D-02	.00D+00	.00D+00
246	0	0	.6455080D-02	.1871632D-02	.00D+00	.00D+00
247	0	0	.6468322D-02	.9378596D-03	.00D+00	.00D+00
248	0	0	.6477568D-02	.0000000D+00	.00D+00	.00D+00
249	0	0	.3041039D-01	.0000000D+00	.00D+00	.00D+00
250	0	0	.2947317D-01	.3888071D-02	.00D+00	.00D+00
251	0	0	.2816210D-01	.7395548D-02	.00D+00	.00D+00
252	0	0	.2624201D-01	.1027380D-01	.00D+00	.00D+00
253	0	0	.2398801D-01	.1243824D-01	.00D+00	.00D+00
254	0	0	.2163984D-01	.1392580D-01	.00D+00	.00D+00
255	0	0	.1936986D-01	.1484075D-01	.00D+00	.00D+00
256	0	0	.1728196D-01	.1530308D-01	.00D+00	.00D+00
257	0	0	.1542637D-01	.1542637D-01	.00D+00	.00D+00
258	0	0	.1381678D-01	.1530365D-01	.00D+00	.00D+00
259	0	0	.1244463D-01	.1500685D-01	.00D+00	.00D+00
260	0	0	.1129269D-01	.1458904D-01	.00D+00	.00D+00
261	0	0	.1033756D-01	.1408847D-01	.00D+00	.00D+00
262	0	0	.9554737D-02	.1352911D-01	.00D+00	.00D+00
263	0	0	.8921918D-02	.1292865D-01	.00D+00	.00D+00
264	0	0	.8418493D-02	.1229623D-01	.00D+00	.00D+00
265	0	0	.8025970D-02	.1163756D-01	.00D+00	.00D+00
266	0	0	.7728082D-02	.1095599D-01	.00D+00	.00D+00
267	0	0	.7510331D-02	.1025205D-01	.00D+00	.00D+00
268	0	0	.7359760D-02	.9525400D-02	.00D+00	.00D+00
269	0	0	.7264726D-02	.8775114D-02	.00D+00	.00D+00
270	0	0	.7214498D-02	.8000000D-02	.00D+00	.00D+00
271	0	0	.7199315D-02	.7199315D-02	.00D+00	.00D+00
272	0	0	.7210103D-02	.6372717D-02	.00D+00	.00D+00
273	0	0	.7238470D-02	.5520434D-02	.00D+00	.00D+00
274	0	0	.7276826D-02	.4643836D-02	.00D+00	.00D+00
275	0	0	.7318322D-02	.3744920D-02	.00D+00	.00D+00
276	0	0	.7357078D-02	.2826826D-02	.00D+00	.00D+00

277	0	0	.7388299D-02	.1893493D-02	.00D+00	.00D+00
278	0	0	.7408447D-02	.9494578D-03	.00D+00	.00D+00
279	0	0	.7422374D-02	.0000000D+00	.00D+00	.00D+00
280	0	0	.2684646D-01	.0000000D+00	.00D+00	.00D+00
281	0	0	.2619692D-01	.3095320D-02	.00D+00	.00D+00
282	0	0	.2527454D-01	.5955251D-02	.00D+00	.00D+00
283	0	0	.2388870D-01	.8407877D-02	.00D+00	.00D+00
284	0	0	.2220890D-01	.1037003D-01	.00D+00	.00D+00
285	0	0	.2039897D-01	.1183619D-01	.00D+00	.00D+00
286	0	0	.1859018D-01	.1285217D-01	.00D+00	.00D+00
287	0	0	.1687329D-01	.1348744D-01	.00D+00	.00D+00
288	0	0	.1530365D-01	.1381678D-01	.00D+00	.00D+00
289	0	0	.1390753D-01	.1390753D-01	.00D+00	.00D+00
290	0	0	.1269235D-01	.1381678D-01	.00D+00	.00D+00
291	0	0	.1165400D-01	.1358904D-01	.00D+00	.00D+00
292	0	0	.1078122D-01	.1326027D-01	.00D+00	.00D+00
293	0	0	.1005976D-01	.1285331D-01	.00D+00	.00D+00
294	0	0	.9474030D-02	.1238642D-01	.00D+00	.00D+00
295	0	0	.9008562D-02	.1186986D-01	.00D+00	.00D+00
296	0	0	.8648687D-02	.1131159D-01	.00D+00	.00D+00
297	0	0	.8380765D-02	.1071610D-01	.00D+00	.00D+00

Table 6.15 Input Data Sets for Problem 8 (continued)

298	0	0	.8192009D-02	.1008539D-01	.00D+00	.00D+00
299	0	0	.8070491D-02	.9419977D-02	.00D+00	.00D+00
300	0	0	.8004966D-02	.8719920D-02	.00D+00	.00D+00
301	0	0	.7984817D-02	.7984817D-02	.00D+00	.00D+00
302	0	0	.8000000D-02	.7214498D-02	.00D+00	.00D+00
303	0	0	.8040753D-02	.6409132D-02	.00D+00	.00D+00
304	0	0	.8097945D-02	.5569635D-02	.00D+00	.00D+00
305	0	0	.8163014D-02	.4698059D-02	.00D+00	.00D+00
306	0	0	.8228139D-02	.3797317D-02	.00D+00	.00D+00
307	0	0	.8286530D-02	.2871575D-02	.00D+00	.00D+00
308	0	0	.8332477D-02	.1925970D-02	.00D+00	.00D+00
309	0	0	.8361815D-02	.9665068D-03	.00D+00	.00D+00
310	0	0	.8382021D-02	.0000000D+00	.00D+00	.00D+00
311	0	0	.2398402D-01	.0000000D+00	.00D+00	.00D+00
312	0	0	.2351826D-01	.2537900D-02	.00D+00	.00D+00
313	0	0	.2284989D-01	.4922317D-02	.00D+00	.00D+00
314	0	0	.2182763D-01	.7032477D-02	.00D+00	.00D+00
315	0	0	.2055993D-01	.8797888D-02	.00D+00	.00D+00
316	0	0	.1915753D-01	.1019663D-01	.00D+00	.00D+00
317	0	0	.1771861D-01	.1124441D-01	.00D+00	.00D+00
318	0	0	.1631792D-01	.1197803D-01	.00D+00	.00D+00
319	0	0	.1500685D-01	.1244463D-01	.00D+00	.00D+00
320	0	0	.1381678D-01	.1269235D-01	.00D+00	.00D+00
321	0	0	.1276256D-01	.1276256D-01	.00D+00	.00D+00
322	0	0	.1184932D-01	.1269178D-01	.00D+00	.00D+00
323	0	0	.1107397D-01	.1251027D-01	.00D+00	.00D+00
324	0	0	.1042917D-01	.1223801D-01	.00D+00	.00D+00
325	0	0	.9905765D-02	.1189269D-01	.00D+00	.00D+00
326	0	0	.9492865D-02	.1148510D-01	.00D+00	.00D+00
327	0	0	.9179395D-02	.1102300D-01	.00D+00	.00D+00
328	0	0	.8954281D-02	.1051159D-01	.00D+00	.00D+00
329	0	0	.8806450D-02	.9953311D-02	.00D+00	.00D+00
330	0	0	.8725114D-02	.9349201D-02	.00D+00	.00D+00
331	0	0	.8699772D-02	.8699772D-02	.00D+00	.00D+00
332	0	0	.8719920D-02	.8004966D-02	.00D+00	.00D+00
333	0	0	.8775114D-02	.7264726D-02	.00D+00	.00D+00
334	0	0	.8855023D-02	.6479566D-02	.00D+00	.00D+00
335	0	0	.8949600D-02	.5650970D-02	.00D+00	.00D+00

336	0	0	.9049201D-02	.4781393D-02	.00D+00	.00D+00
337	0	0	.9144806D-02	.3874772D-02	.00D+00	.00D+00
338	0	0	.9228425D-02	.2936187D-02	.00D+00	.00D+00
339	0	0	.9293322D-02	.1972203D-02	.00D+00	.00D+00
340	0	0	.9334418D-02	.9906221D-03	.00D+00	.00D+00
341	0	0	.9362614D-02	.0000000D+00	.00D+00	.00D+00
342	0	0	.2161644D-01	.0000000D+00	.00D+00	.00D+00
343	0	0	.2127397D-01	.2134075D-02	.00D+00	.00D+00
344	0	0	.2077968D-01	.4163584D-02	.00D+00	.00D+00
345	0	0	.2001313D-01	.6001941D-02	.00D+00	.00D+00
346	0	0	.1904509D-01	.7592237D-02	.00D+00	.00D+00
347	0	0	.1795320D-01	.8908162D-02	.00D+00	.00D+00
348	0	0	.1680936D-01	.9949943D-02	.00D+00	.00D+00
349	0	0	.1567295D-01	.1073556D-01	.00D+00	.00D+00
350	0	0	.1458904D-01	.1129269D-01	.00D+00	.00D+00
351	0	0	.1358904D-01	.1165400D-01	.00D+00	.00D+00
352	0	0	.1269178D-01	.1184932D-01	.00D+00	.00D+00

Table 6.15 Input Data Sets for Problem 8 (continued)

353	0	0	.1190639D-01	.1190639D-01	.00D+00	.00D+00
354	0	0	.1123545D-01	.1184932D-01	.00D+00	.00D+00
355	0	0	.1067728D-01	.1169578D-01	.00D+00	.00D+00
356	0	0	.1022700D-01	.1146084D-01	.00D+00	.00D+00
357	0	0	.9877854D-02	.1115445D-01	.00D+00	.00D+00
358	0	0	.9621918D-02	.1078402D-01	.00D+00	.00D+00
359	0	0	.9450457D-02	.1035400D-01	.00D+00	.00D+00
360	0	0	.9354281D-02	.9866952D-02	.00D+00	.00D+00
361	0	0	.9323858D-02	.9323858D-02	.00D+00	.00D+00
362	0	0	.9349201D-02	.8725114D-02	.00D+00	.00D+00
363	0	0	.9419977D-02	.8070491D-02	.00D+00	.00D+00
364	0	0	.9525400D-02	.7359760D-02	.00D+00	.00D+00
365	0	0	.9654452D-02	.6593493D-02	.00D+00	.00D+00
366	0	0	.9796062D-02	.5773231D-02	.00D+00	.00D+00
367	0	0	.9939269D-02	.4901884D-02	.00D+00	.00D+00
368	0	0	.1007346D-01	.3984132D-02	.00D+00	.00D+00
369	0	0	.1018910D-01	.3026142D-02	.00D+00	.00D+00
370	0	0	.1027808D-01	.2036073D-02	.00D+00	.00D+00
371	0	0	.1033408D-01	.1023784D-02	.00D+00	.00D+00
372	0	0	.1037232D-01	.0000000D+00	.00D+00	.00D+00
373	0	0	.1961130D-01	.0000000D+00	.00D+00	.00D+00
374	0	0	.1935445D-01	.1834874D-02	.00D+00	.00D+00
375	0	0	.1898174D-01	.3595833D-02	.00D+00	.00D+00
376	0	0	.1839897D-01	.5219635D-02	.00D+00	.00D+00
377	0	0	.1765354D-01	.6660845D-02	.00D+00	.00D+00
378	0	0	.1679966D-01	.7894007D-02	.00D+00	.00D+00
379	0	0	.1589098D-01	.8911872D-02	.00D+00	.00D+00
380	0	0	.1497489D-01	.9721176D-02	.00D+00	.00D+00
381	0	0	.1408847D-01	.1033756D-01	.00D+00	.00D+00
382	0	0	.1326027D-01	.1078122D-01	.00D+00	.00D+00
383	0	0	.1251027D-01	.1107397D-01	.00D+00	.00D+00
384	0	0	.1184932D-01	.1123545D-01	.00D+00	.00D+00
385	0	0	.1128436D-01	.1128436D-01	.00D+00	.00D+00
386	0	0	.1081747D-01	.1123527D-01	.00D+00	.00D+00
387	0	0	.1044709D-01	.1110046D-01	.00D+00	.00D+00
388	0	0	.1016969D-01	.1088818D-01	.00D+00	.00D+00
389	0	0	.9979909D-02	.1060457D-01	.00D+00	.00D+00
390	0	0	.9871347D-02	.1025337D-01	.00D+00	.00D+00
391	0	0	.9836530D-02	.9836530D-02	.00D+00	.00D+00
392	0	0	.9866952D-02	.9354281D-02	.00D+00	.00D+00
393	0	0	.9953311D-02	.8806450D-02	.00D+00	.00D+00
394	0	0	.1008539D-01	.8192009D-02	.00D+00	.00D+00

395	0	0	.1025205D-01	.7510331D-02	.00D+00	.00D+00
396	0	0	.1044144D-01	.6761416D-02	.00D+00	.00D+00
397	0	0	.1064110D-01	.5946632D-02	.00D+00	.00D+00
398	0	0	.1083830D-01	.5068950D-02	.00D+00	.00D+00
399	0	0	.1102061D-01	.4133619D-02	.00D+00	.00D+00
400	0	0	.1117643D-01	.3148059D-02	.00D+00	.00D+00
401	0	0	.1129566D-01	.2122317D-02	.00D+00	.00D+00
402	0	0	.1137049D-01	.1068413D-02	.00D+00	.00D+00
403	0	0	.1142152D-01	.0000000D+00	.00D+00	.00D+00
404	0	0	.1787386D-01	.0000000D+00	.00D+00	.00D+00
405	0	0	.1767865D-01	.1609475D-02	.00D+00	.00D+00
406	0	0	.1739498D-01	.3165183D-02	.00D+00	.00D+00
407	0	0	.1694806D-01	.4619920D-02	.00D+00	.00D+00

Table 6.15 Input Data Sets for Problem 8 (continued)

408	0	0	.1637043D-01	.5937557D-02	.00D+00	.00D+00
409	0	0	.1570148D-01	.7095148D-02	.00D+00	.00D+00
410	0	0	.1498174D-01	.8082420D-02	.00D+00	.00D+00
411	0	0	.1424715D-01	.8899715D-02	.00D+00	.00D+00
412	0	0	.1352911D-01	.9554737D-02	.00D+00	.00D+00
413	0	0	.1285331D-01	.1005976D-01	.00D+00	.00D+00
414	0	0	.1223801D-01	.1042917D-01	.00D+00	.00D+00
415	0	0	.1169578D-01	.1067728D-01	.00D+00	.00D+00
416	0	0	.1123527D-01	.1081747D-01	.00D+00	.00D+00
417	0	0	.1086119D-01	.1086119D-01	.00D+00	.00D+00
418	0	0	.1057432D-01	.1081747D-01	.00D+00	.00D+00
419	0	0	.1037380D-01	.1069321D-01	.00D+00	.00D+00
420	0	0	.1025668D-01	.1049269D-01	.00D+00	.00D+00
421	0	0	.1021849D-01	.1021849D-01	.00D+00	.00D+00
422	0	0	.1025337D-01	.9871347D-02	.00D+00	.00D+00
423	0	0	.1035400D-01	.9450457D-02	.00D+00	.00D+00
424	0	0	.1051159D-01	.8954281D-02	.00D+00	.00D+00
425	0	0	.1071610D-01	.8380765D-02	.00D+00	.00D+00
426	0	0	.1095599D-01	.7728082D-02	.00D+00	.00D+00
427	0	0	.1121821D-01	.6995263D-02	.00D+00	.00D+00
428	0	0	.1148881D-01	.6182877D-02	.00D+00	.00D+00
429	0	0	.1175228D-01	.5293664D-02	.00D+00	.00D+00
430	0	0	.1199429D-01	.4333219D-02	.00D+00	.00D+00
431	0	0	.1220034D-01	.3310217D-02	.00D+00	.00D+00
432	0	0	.1235731D-01	.2236701D-02	.00D+00	.00D+00
433	0	0	.1245605D-01	.1127557D-02	.00D+00	.00D+00
434	0	0	.1252340D-01	.0000000D+00	.00D+00	.00D+00
435	0	0	.1633790D-01	.0000000D+00	.00D+00	.00D+00
436	0	0	.1618950D-01	.1437785D-02	.00D+00	.00D+00
437	0	0	.1597203D-01	.2835559D-02	.00D+00	.00D+00
438	0	0	.1562671D-01	.4157306D-02	.00D+00	.00D+00
439	0	0	.1517808D-01	.5374258D-02	.00D+00	.00D+00
440	0	0	.1465468D-01	.6466495D-02	.00D+00	.00D+00
441	0	0	.1408676D-01	.7423002D-02	.00D+00	.00D+00
442	0	0	.1350285D-01	.8240582D-02	.00D+00	.00D+00
443	0	0	.1292865D-01	.8921918D-02	.00D+00	.00D+00
444	0	0	.1238642D-01	.9474030D-02	.00D+00	.00D+00
445	0	0	.1189269D-01	.9905765D-02	.00D+00	.00D+00
446	0	0	.1146084D-01	.1022700D-01	.00D+00	.00D+00
447	0	0	.1110046D-01	.1044709D-01	.00D+00	.00D+00
448	0	0	.1081747D-01	.1057432D-01	.00D+00	.00D+00
449	0	0	.1061513D-01	.1061513D-01	.00D+00	.00D+00
450	0	0	.1049446D-01	.1057432D-01	.00D+00	.00D+00
451	0	0	.1045457D-01	.1045457D-01	.00D+00	.00D+00
452	0	0	.1049269D-01	.1025668D-01	.00D+00	.00D+00
453	0	0	.1060457D-01	.9979909D-02	.00D+00	.00D+00

454	0	0	.1078402D-01	.9621918D-02	.00D+00	.00D+00
455	0	0	.1102300D-01	.9179395D-02	.00D+00	.00D+00
456	0	0	.1131159D-01	.8648687D-02	.00D+00	.00D+00
457	0	0	.1163756D-01	.8025970D-02	.00D+00	.00D+00
458	0	0	.1198687D-01	.7308676D-02	.00D+00	.00D+00
459	0	0	.1234304D-01	.6495890D-02	.00D+00	.00D+00
460	0	0	.1268836D-01	.5589612D-02	.00D+00	.00D+00
461	0	0	.1300457D-01	.4595377D-02	.00D+00	.00D+00
462	0	0	.1327340D-01	.3522945D-02	.00D+00	.00D+00

Table 6.15 Input Data Sets for Problem 8 (continued)

463	0	0	.1347831D-01	.2386644D-02	.00D+00	.00D+00
464	0	0	.1360674D-01	.1205137D-02	.00D+00	.00D+00
465	0	0	.1369463D-01	.0000000D+00	.00D+00	.00D+00
466	0	0	.1495833D-01	.0000000D+00	.00D+00	.00D+00
467	0	0	.1484304D-01	.1306221D-02	.00D+00	.00D+00
468	0	0	.1467523D-01	.2581963D-02	.00D+00	.00D+00
469	0	0	.1440925D-01	.3799486D-02	.00D+00	.00D+00
470	0	0	.1406107D-01	.4935674D-02	.00D+00	.00D+00
471	0	0	.1365240D-01	.5973573D-02	.00D+00	.00D+00
472	0	0	.1320719D-01	.6902511D-02	.00D+00	.00D+00
473	0	0	.1274829D-01	.7717580D-02	.00D+00	.00D+00
474	0	0	.1229623D-01	.8418493D-02	.00D+00	.00D+00
475	0	0	.1186986D-01	.9008562D-02	.00D+00	.00D+00
476	0	0	.1148510D-01	.9492865D-02	.00D+00	.00D+00
477	0	0	.1115445D-01	.9877854D-02	.00D+00	.00D+00
478	0	0	.1088818D-01	.1016969D-01	.00D+00	.00D+00
479	0	0	.1069321D-01	.1037380D-01	.00D+00	.00D+00
480	0	0	.1057432D-01	.1049446D-01	.00D+00	.00D+00
481	0	0	.1053436D-01	.1053436D-01	.00D+00	.00D+00
482	0	0	.1057432D-01	.1049446D-01	.00D+00	.00D+00
483	0	0	.1069321D-01	.1037380D-01	.00D+00	.00D+00
484	0	0	.1088818D-01	.1016969D-01	.00D+00	.00D+00
485	0	0	.1115445D-01	.9877854D-02	.00D+00	.00D+00
486	0	0	.1148510D-01	.9492865D-02	.00D+00	.00D+00
487	0	0	.1186986D-01	.9008562D-02	.00D+00	.00D+00
488	0	0	.1229623D-01	.8418493D-02	.00D+00	.00D+00
489	0	0	.1274829D-01	.7717580D-02	.00D+00	.00D+00
490	0	0	.1320719D-01	.6902511D-02	.00D+00	.00D+00
491	0	0	.1365240D-01	.5973573D-02	.00D+00	.00D+00
492	0	0	.1406107D-01	.4935674D-02	.00D+00	.00D+00
493	0	0	.1440925D-01	.3799486D-02	.00D+00	.00D+00
494	0	0	.1467523D-01	.2581963D-02	.00D+00	.00D+00
495	0	0	.1484304D-01	.1306221D-02	.00D+00	.00D+00
496	0	0	.1495833D-01	.0000000D+00	.00D+00	.00D+00
497	0	0	.1369463D-01	.0000000D+00	.00D+00	.00D+00
498	0	0	.1360674D-01	.1205137D-02	.00D+00	.00D+00
499	0	0	.1347831D-01	.2386644D-02	.00D+00	.00D+00
500	0	0	.1327340D-01	.3522945D-02	.00D+00	.00D+00
501	0	0	.1300457D-01	.4595377D-02	.00D+00	.00D+00
502	0	0	.1268836D-01	.5589612D-02	.00D+00	.00D+00
503	0	0	.1234304D-01	.6495890D-02	.00D+00	.00D+00
504	0	0	.1198687D-01	.7308676D-02	.00D+00	.00D+00
505	0	0	.1163756D-01	.8025970D-02	.00D+00	.00D+00
506	0	0	.1131159D-01	.8648687D-02	.00D+00	.00D+00
507	0	0	.1102300D-01	.9179395D-02	.00D+00	.00D+00
508	0	0	.1078402D-01	.9621918D-02	.00D+00	.00D+00
509	0	0	.1060457D-01	.9979909D-02	.00D+00	.00D+00
510	0	0	.1049269D-01	.1025668D-01	.00D+00	.00D+00
511	0	0	.1045457D-01	.1045457D-01	.00D+00	.00D+00
512	0	0	.1049446D-01	.1057432D-01	.00D+00	.00D+00

513	0	0	.1061513D-01	.1061513D-01	.00D+00	.00D+00
514	0	0	.1081747D-01	.1057432D-01	.00D+00	.00D+00
515	0	0	.1110046D-01	.1044709D-01	.00D+00	.00D+00
516	0	0	.1146084D-01	.1022700D-01	.00D+00	.00D+00
517	0	0	.1189269D-01	.9905765D-02	.00D+00	.00D+00

Table 6.15 Input Data Sets for Problem 8 (continued)

518	0	0	.1238642D-01	.9474030D-02	.00D+00	.00D+00
519	0	0	.1292865D-01	.8921918D-02	.00D+00	.00D+00
520	0	0	.1350285D-01	.8240582D-02	.00D+00	.00D+00
521	0	0	.1408676D-01	.7423002D-02	.00D+00	.00D+00
522	0	0	.1465468D-01	.6466495D-02	.00D+00	.00D+00
523	0	0	.1517808D-01	.5374258D-02	.00D+00	.00D+00
524	0	0	.1562671D-01	.4157306D-02	.00D+00	.00D+00
525	0	0	.1597203D-01	.2835559D-02	.00D+00	.00D+00
526	0	0	.1618950D-01	.1437785D-02	.00D+00	.00D+00
527	0	0	.1633790D-01	.0000000D+00	.00D+00	.00D+00
528	0	0	.1252340D-01	.0000000D+00	.00D+00	.00D+00
529	0	0	.1245605D-01	.1127557D-02	.00D+00	.00D+00
530	0	0	.1235731D-01	.2236701D-02	.00D+00	.00D+00
531	0	0	.1220034D-01	.3310217D-02	.00D+00	.00D+00
532	0	0	.1199429D-01	.4333219D-02	.00D+00	.00D+00
533	0	0	.1175228D-01	.5293664D-02	.00D+00	.00D+00
534	0	0	.1148881D-01	.6182877D-02	.00D+00	.00D+00
535	0	0	.1121821D-01	.6995263D-02	.00D+00	.00D+00
536	0	0	.1095599D-01	.7728082D-02	.00D+00	.00D+00
537	0	0	.1071610D-01	.8380765D-02	.00D+00	.00D+00
538	0	0	.1051159D-01	.8954281D-02	.00D+00	.00D+00
539	0	0	.1035400D-01	.9450457D-02	.00D+00	.00D+00
540	0	0	.1025337D-01	.9871347D-02	.00D+00	.00D+00
541	0	0	.1021849D-01	.1021849D-01	.00D+00	.00D+00
542	0	0	.1025668D-01	.1049269D-01	.00D+00	.00D+00
543	0	0	.1037380D-01	.1069321D-01	.00D+00	.00D+00
544	0	0	.1057432D-01	.1081747D-01	.00D+00	.00D+00
545	0	0	.1086119D-01	.1086119D-01	.00D+00	.00D+00
546	0	0	.1123527D-01	.1081747D-01	.00D+00	.00D+00
547	0	0	.1169578D-01	.1067728D-01	.00D+00	.00D+00
548	0	0	.1223801D-01	.1042917D-01	.00D+00	.00D+00
549	0	0	.1285331D-01	.1005976D-01	.00D+00	.00D+00
550	0	0	.1352911D-01	.9554737D-02	.00D+00	.00D+00
551	0	0	.1424715D-01	.8899715D-02	.00D+00	.00D+00
552	0	0	.1498174D-01	.8082420D-02	.00D+00	.00D+00
553	0	0	.1570148D-01	.7095148D-02	.00D+00	.00D+00
554	0	0	.1637043D-01	.5937557D-02	.00D+00	.00D+00
555	0	0	.1694806D-01	.4619920D-02	.00D+00	.00D+00
556	0	0	.1739498D-01	.3165183D-02	.00D+00	.00D+00
557	0	0	.1767865D-01	.1609475D-02	.00D+00	.00D+00
558	0	0	.1787386D-01	.0000000D+00	.00D+00	.00D+00
559	0	0	.1142152D-01	.0000000D+00	.00D+00	.00D+00
560	0	0	.1137049D-01	.1068413D-02	.00D+00	.00D+00
561	0	0	.1129566D-01	.2122317D-02	.00D+00	.00D+00
562	0	0	.1117643D-01	.3148059D-02	.00D+00	.00D+00
563	0	0	.1102061D-01	.4133619D-02	.00D+00	.00D+00
564	0	0	.1083830D-01	.5068950D-02	.00D+00	.00D+00
565	0	0	.1064110D-01	.5946632D-02	.00D+00	.00D+00
566	0	0	.1044144D-01	.6761416D-02	.00D+00	.00D+00
567	0	0	.1025205D-01	.7510331D-02	.00D+00	.00D+00
568	0	0	.1008539D-01	.8192009D-02	.00D+00	.00D+00
569	0	0	.9953311D-02	.8806450D-02	.00D+00	.00D+00
570	0	0	.9866952D-02	.9354281D-02	.00D+00	.00D+00
571	0	0	.9836530D-02	.9836530D-02	.00D+00	.00D+00

572	0	0	.9871347D-02	.1025337D-01	.00D+00	.00D+00

Table 6.15 Input Data Sets for Problem 8 (continued)

573	0	0	.9979909D-02	.1060457D-01	.00D+00	.00D+00
574	0	0	.1016969D-01	.1088818D-01	.00D+00	.00D+00
575	0	0	.1044709D-01	.1110046D-01	.00D+00	.00D+00
576	0	0	.1081747D-01	.1123527D-01	.00D+00	.00D+00
577	0	0	.1128436D-01	.1128436D-01	.00D+00	.00D+00
578	0	0	.1184932D-01	.1123545D-01	.00D+00	.00D+00
579	0	0	.1251027D-01	.1107397D-01	.00D+00	.00D+00
580	0	0	.1326027D-01	.1078122D-01	.00D+00	.00D+00
581	0	0	.1408847D-01	.1033756D-01	.00D+00	.00D+00
582	0	0	.1497489D-01	.9721176D-02	.00D+00	.00D+00
583	0	0	.1589098D-01	.8911872D-02	.00D+00	.00D+00
584	0	0	.1679966D-01	.7894007D-02	.00D+00	.00D+00
585	0	0	.1765354D-01	.6660845D-02	.00D+00	.00D+00
586	0	0	.1839897D-01	.5219635D-02	.00D+00	.00D+00
587	0	0	.1898174D-01	.3595833D-02	.00D+00	.00D+00
588	0	0	.1935445D-01	.1834874D-02	.00D+00	.00D+00
589	0	0	.1961130D-01	.0000000D+00	.00D+00	.00D+00
590	0	0	.1037232D-01	.0000000D+00	.00D+00	.00D+00
591	0	0	.1033408D-01	.1023784D-02	.00D+00	.00D+00
592	0	0	.1027808D-01	.2036073D-02	.00D+00	.00D+00
593	0	0	.1018910D-01	.3026142D-02	.00D+00	.00D+00
594	0	0	.1007346D-01	.3984132D-02	.00D+00	.00D+00
595	0	0	.9939269D-02	.4901884D-02	.00D+00	.00D+00
596	0	0	.9796062D-02	.5773231D-02	.00D+00	.00D+00
597	0	0	.9654452D-02	.6593493D-02	.00D+00	.00D+00
598	0	0	.9525400D-02	.7359760D-02	.00D+00	.00D+00
599	0	0	.9419977D-02	.8070491D-02	.00D+00	.00D+00
600	0	0	.9349201D-02	.8725114D-02	.00D+00	.00D+00
601	0	0	.9323858D-02	.9323858D-02	.00D+00	.00D+00
602	0	0	.9354281D-02	.9866952D-02	.00D+00	.00D+00
603	0	0	.9450457D-02	.1035400D-01	.00D+00	.00D+00
604	0	0	.9621918D-02	.1078402D-01	.00D+00	.00D+00
605	0	0	.9877854D-02	.1115445D-01	.00D+00	.00D+00
606	0	0	.1022700D-01	.1146084D-01	.00D+00	.00D+00
607	0	0	.1067728D-01	.1169578D-01	.00D+00	.00D+00
608	0	0	.1123545D-01	.1184932D-01	.00D+00	.00D+00
609	0	0	.1190639D-01	.1190639D-01	.00D+00	.00D+00
610	0	0	.1269178D-01	.1184932D-01	.00D+00	.00D+00
611	0	0	.1358904D-01	.1165400D-01	.00D+00	.00D+00
612	0	0	.1458904D-01	.1129269D-01	.00D+00	.00D+00
613	0	0	.1567295D-01	.1073556D-01	.00D+00	.00D+00
614	0	0	.1680936D-01	.9949943D-02	.00D+00	.00D+00
615	0	0	.1795320D-01	.8908162D-02	.00D+00	.00D+00
616	0	0	.1904509D-01	.7592237D-02	.00D+00	.00D+00
617	0	0	.2001313D-01	.6001941D-02	.00D+00	.00D+00
618	0	0	.2077968D-01	.4163584D-02	.00D+00	.00D+00
619	0	0	.2127397D-01	.2134075D-02	.00D+00	.00D+00
620	0	0	.2161644D-01	.0000000D+00	.00D+00	.00D+00
621	0	0	.9362614D-02	.0000000D+00	.00D+00	.00D+00
622	0	0	.9334418D-02	.9906221D-03	.00D+00	.00D+00
623	0	0	.9293322D-02	.1972203D-02	.00D+00	.00D+00
624	0	0	.9228425D-02	.2936187D-02	.00D+00	.00D+00
625	0	0	.9144806D-02	.3874772D-02	.00D+00	.00D+00
626	0	0	.9049201D-02	.4781393D-02	.00D+00	.00D+00
627	0	0	.8949600D-02	.5650970D-02	.00D+00	.00D+00

Table 6.15 Input Data Sets for Problem 8 (continued)

628	0	0	.8855023D-02	.6479566D-02	.00D+00	.00D+00
629	0	0	.8775114D-02	.7264726D-02	.00D+00	.00D+00
630	0	0	.8719920D-02	.8004966D-02	.00D+00	.00D+00
631	0	0	.8699772D-02	.8699772D-02	.00D+00	.00D+00
632	0	0	.8725114D-02	.9349201D-02	.00D+00	.00D+00
633	0	0	.8806450D-02	.9953311D-02	.00D+00	.00D+00
634	0	0	.8954281D-02	.1051159D-01	.00D+00	.00D+00
635	0	0	.9179395D-02	.1102300D-01	.00D+00	.00D+00
636	0	0	.9492865D-02	.1148510D-01	.00D+00	.00D+00
637	0	0	.9905765D-02	.1189269D-01	.00D+00	.00D+00
638	0	0	.1042917D-01	.1223801D-01	.00D+00	.00D+00
639	0	0	.1107397D-01	.1251027D-01	.00D+00	.00D+00
640	0	0	.1184932D-01	.1269178D-01	.00D+00	.00D+00
641	0	0	.1276256D-01	.1276256D-01	.00D+00	.00D+00
642	0	0	.1381678D-01	.1269235D-01	.00D+00	.00D+00
643	0	0	.1500685D-01	.1244463D-01	.00D+00	.00D+00
644	0	0	.1631792D-01	.1197803D-01	.00D+00	.00D+00
645	0	0	.1771861D-01	.1124441D-01	.00D+00	.00D+00
646	0	0	.1915753D-01	.1019663D-01	.00D+00	.00D+00
647	0	0	.2055993D-01	.8797888D-02	.00D+00	.00D+00
648	0	0	.2182763D-01	.7032477D-02	.00D+00	.00D+00
649	0	0	.2284989D-01	.4922317D-02	.00D+00	.00D+00
650	0	0	.2351826D-01	.2537900D-02	.00D+00	.00D+00
651	0	0	.2398402D-01	.0000000D+00	.00D+00	.00D+00
652	0	0	.8382021D-02	.0000000D+00	.00D+00	.00D+00
653	0	0	.8361815D-02	.9665068D-03	.00D+00	.00D+00
654	0	0	.8332477D-02	.1925970D-02	.00D+00	.00D+00
655	0	0	.8286530D-02	.2871575D-02	.00D+00	.00D+00
656	0	0	.8228139D-02	.3797317D-02	.00D+00	.00D+00
657	0	0	.8163014D-02	.4698059D-02	.00D+00	.00D+00
658	0	0	.8097945D-02	.5569635D-02	.00D+00	.00D+00
659	0	0	.8040753D-02	.6409132D-02	.00D+00	.00D+00
660	0	0	.8000000D-02	.7214498D-02	.00D+00	.00D+00
661	0	0	.7984817D-02	.7984817D-02	.00D+00	.00D+00
662	0	0	.8004966D-02	.8719920D-02	.00D+00	.00D+00
663	0	0	.8070491D-02	.9419977D-02	.00D+00	.00D+00
664	0	0	.8192009D-02	.1008539D-01	.00D+00	.00D+00
665	0	0	.8380765D-02	.1071610D-01	.00D+00	.00D+00
666	0	0	.8648687D-02	.1131159D-01	.00D+00	.00D+00
667	0	0	.9008562D-02	.1186986D-01	.00D+00	.00D+00
668	0	0	.9474030D-02	.1238642D-01	.00D+00	.00D+00
669	0	0	.1005976D-01	.1285331D-01	.00D+00	.00D+00
670	0	0	.1078122D-01	.1326027D-01	.00D+00	.00D+00
671	0	0	.1165400D-01	.1358904D-01	.00D+00	.00D+00
672	0	0	.1269235D-01	.1381678D-01	.00D+00	.00D+00
673	0	0	.1390753D-01	.1390753D-01	.00D+00	.00D+00
674	0	0	.1530365D-01	.1381678D-01	.00D+00	.00D+00
675	0	0	.1687329D-01	.1348744D-01	.00D+00	.00D+00
676	0	0	.1859018D-01	.1285217D-01	.00D+00	.00D+00
677	0	0	.2039897D-01	.1183619D-01	.00D+00	.00D+00
678	0	0	.2220890D-01	.1037003D-01	.00D+00	.00D+00
679	0	0	.2388870D-01	.8407877D-02	.00D+00	.00D+00
680	0	0	.2527454D-01	.5955251D-02	.00D+00	.00D+00
681	0	0	.2619692D-01	.3095320D-02	.00D+00	.00D+00
682	0	0	.2684646D-01	.0000000D+00	.00D+00	.00D+00

Table 6.15 Input Data Sets for Problem 8 (continued)

683	0	0	.7422374D-02	.0000000D+00	.00D+00	.00D+00
684	0	0	.7408447D-02	.9494578D-03	.00D+00	.00D+00
685	0	0	.7388299D-02	.1893493D-02	.00D+00	.00D+00
686	0	0	.7357078D-02	.2826826D-02	.00D+00	.00D+00

687	0	0	.7318322D-02	.3744920D-02	.00D+00	.00D+00
688	0	0	.7276826D-02	.4643836D-02	.00D+00	.00D+00
689	0	0	.7238470D-02	.5520434D-02	.00D+00	.00D+00
690	0	0	.7210103D-02	.6372717D-02	.00D+00	.00D+00
691	0	0	.7199315D-02	.7199315D-02	.00D+00	.00D+00
692	0	0	.7214498D-02	.8000000D-02	.00D+00	.00D+00
693	0	0	.7264726D-02	.8775114D-02	.00D+00	.00D+00
694	0	0	.7359760D-02	.9525400D-02	.00D+00	.00D+00
695	0	0	.7510331D-02	.1025205D-01	.00D+00	.00D+00
696	0	0	.7728082D-02	.1095599D-01	.00D+00	.00D+00
697	0	0	.8025970D-02	.1163756D-01	.00D+00	.00D+00
698	0	0	.8418493D-02	.1229623D-01	.00D+00	.00D+00
699	0	0	.8921918D-02	.1292865D-01	.00D+00	.00D+00
700	0	0	.9554737D-02	.1352911D-01	.00D+00	.00D+00
701	0	0	.1033756D-01	.1408847D-01	.00D+00	.00D+00
702	0	0	.1129269D-01	.1458904D-01	.00D+00	.00D+00
703	0	0	.1244463D-01	.1500685D-01	.00D+00	.00D+00
704	0	0	.1381678D-01	.1530365D-01	.00D+00	.00D+00
705	0	0	.1542637D-01	.1542637D-01	.00D+00	.00D+00
706	0	0	.1728196D-01	.1530308D-01	.00D+00	.00D+00
707	0	0	.1936986D-01	.1484075D-01	.00D+00	.00D+00
708	0	0	.2163984D-01	.1392580D-01	.00D+00	.00D+00
709	0	0	.2398801D-01	.1243824D-01	.00D+00	.00D+00
710	0	0	.2624201D-01	.1027380D-01	.00D+00	.00D+00
711	0	0	.2816210D-01	.7395548D-02	.00D+00	.00D+00
712	0	0	.2947317D-01	.3888071D-02	.00D+00	.00D+00
713	0	0	.3041039D-01	.0000000D+00	.00D+00	.00D+00
714	0	0	.6477568D-02	.0000000D+00	.00D+00	.00D+00
715	0	0	.6468322D-02	.9378596D-03	.00D+00	.00D+00
716	0	0	.6455080D-02	.1871632D-02	.00D+00	.00D+00
717	0	0	.6435046D-02	.2797374D-02	.00D+00	.00D+00
718	0	0	.6411187D-02	.3711758D-02	.00D+00	.00D+00
719	0	0	.6387500D-02	.4611872D-02	.00D+00	.00D+00
720	0	0	.6369064D-02	.5495662D-02	.00D+00	.00D+00
721	0	0	.6361872D-02	.6361872D-02	.00D+00	.00D+00
722	0	0	.6372717D-02	.7210103D-02	.00D+00	.00D+00
723	0	0	.6409132D-02	.8040753D-02	.00D+00	.00D+00
724	0	0	.6479566D-02	.8855023D-02	.00D+00	.00D+00
725	0	0	.6593493D-02	.9654452D-02	.00D+00	.00D+00
726	0	0	.6761416D-02	.1044144D-01	.00D+00	.00D+00
727	0	0	.6995263D-02	.1121821D-01	.00D+00	.00D+00
728	0	0	.7308676D-02	.1198687D-01	.00D+00	.00D+00
729	0	0	.7717580D-02	.1274829D-01	.00D+00	.00D+00
730	0	0	.8240582D-02	.1350285D-01	.00D+00	.00D+00
731	0	0	.8899715D-02	.1424715D-01	.00D+00	.00D+00
732	0	0	.9721176D-02	.1497489D-01	.00D+00	.00D+00
733	0	0	.1073556D-01	.1567295D-01	.00D+00	.00D+00
734	0	0	.1197803D-01	.1631792D-01	.00D+00	.00D+00
735	0	0	.1348744D-01	.1687329D-01	.00D+00	.00D+00
736	0	0	.1530308D-01	.1728196D-01	.00D+00	.00D+00
737	0	0	.1745833D-01	.1745833D-01	.00D+00	.00D+00

Table 6.15 Input Data Sets for Problem 8 (continued)

738	0	0	.1996747D-01	.1728196D-01	.00D+00	.00D+00
739	0	0	.2280251D-01	.1658904D-01	.00D+00	.00D+00
740	0	0	.2586130D-01	.1518208D-01	.00D+00	.00D+00
741	0	0	.2893037D-01	.1285377D-01	.00D+00	.00D+00
742	0	0	.3165982D-01	.9465126D-02	.00D+00	.00D+00
743	0	0	.3359247D-01	.5061301D-02	.00D+00	.00D+00
744	0	0	.3500342D-01	.0000000D+00	.00D+00	.00D+00
745	0	0	.5542580D-02	.0000000D+00	.00D+00	.00D+00

746	0	0	.5536872D-02	.9303653D-03	.00D+00	.00D+00
747	0	0	.5528767D-02	.1857763D-02	.00D+00	.00D+00
748	0	0	.5516895D-02	.2779395D-02	.00D+00	.00D+00
749	0	0	.5503824D-02	.3692808D-02	.00D+00	.00D+00
750	0	0	.5492922D-02	.4596290D-02	.00D+00	.00D+00
751	0	0	.5488470D-02	.5488470D-02	.00D+00	.00D+00
752	0	0	.5495662D-02	.6369064D-02	.00D+00	.00D+00
753	0	0	.5520434D-02	.7238470D-02	.00D+00	.00D+00
754	0	0	.5569635D-02	.8097945D-02	.00D+00	.00D+00
755	0	0	.5650970D-02	.8949600D-02	.00D+00	.00D+00
756	0	0	.5773231D-02	.9796062D-02	.00D+00	.00D+00
757	0	0	.5946632D-02	.1064110D-01	.00D+00	.00D+00
758	0	0	.6182877D-02	.1148881D-01	.00D+00	.00D+00
759	0	0	.6495890D-02	.1234304D-01	.00D+00	.00D+00
760	0	0	.6902511D-02	.1320719D-01	.00D+00	.00D+00
761	0	0	.7423002D-02	.1408676D-01	.00D+00	.00D+00
762	0	0	.8082420D-02	.1498174D-01	.00D+00	.00D+00
763	0	0	.8911872D-02	.1589098D-01	.00D+00	.00D+00
764	0	0	.9949943D-02	.1680936D-01	.00D+00	.00D+00
765	0	0	.1124441D-01	.1771861D-01	.00D+00	.00D+00
766	0	0	.1285217D-01	.1859018D-01	.00D+00	.00D+00
767	0	0	.1484075D-01	.1936986D-01	.00D+00	.00D+00
768	0	0	.1728196D-01	.1996747D-01	.00D+00	.00D+00
769	0	0	.2023916D-01	.2023916D-01	.00D+00	.00D+00
770	0	0	.2374030D-01	.1996747D-01	.00D+00	.00D+00
771	0	0	.2772374D-01	.1884589D-01	.00D+00	.00D+00
772	0	0	.3195890D-01	.1649486D-01	.00D+00	.00D+00
773	0	0	.3595491D-01	.1254983D-01	.00D+00	.00D+00
774	0	0	.3893836D-01	.6891952D-02	.00D+00	.00D+00
775	0	0	.4118950D-01	.0000000D+00	.00D+00	.00D+00
776	0	0	.4613813D-02	.0000000D+00	.00D+00	.00D+00
777	0	0	.4610616D-02	.9258505D-03	.00D+00	.00D+00
778	0	0	.4606107D-02	.1849658D-02	.00D+00	.00D+00
779	0	0	.4599943D-02	.2769521D-02	.00D+00	.00D+00
780	0	0	.4594292D-02	.3683904D-02	.00D+00	.00D+00
781	0	0	.4591895D-02	.4591895D-02	.00D+00	.00D+00
782	0	0	.4596290D-02	.5492922D-02	.00D+00	.00D+00
783	0	0	.4611872D-02	.6387500D-02	.00D+00	.00D+00
784	0	0	.4643836D-02	.7276826D-02	.00D+00	.00D+00
785	0	0	.4698059D-02	.8163014D-02	.00D+00	.00D+00
786	0	0	.4781393D-02	.9049201D-02	.00D+00	.00D+00
787	0	0	.4901884D-02	.9939269D-02	.00D+00	.00D+00
788	0	0	.5068950D-02	.1083830D-01	.00D+00	.00D+00
789	0	0	.5293664D-02	.1175228D-01	.00D+00	.00D+00
790	0	0	.5589612D-02	.1268836D-01	.00D+00	.00D+00
791	0	0	.5973573D-02	.1365240D-01	.00D+00	.00D+00
792	0	0	.6466495D-02	.1465468D-01	.00D+00	.00D+00

Table 6.15 Input Data Sets for Problem 8 (continued)

793	0	0	.7095148D-02	.1570148D-01	.00D+00	.00D+00
794	0	0	.7894007D-02	.1679966D-01	.00D+00	.00D+00
795	0	0	.8908162D-02	.1795320D-01	.00D+00	.00D+00
796	0	0	.1019663D-01	.1915753D-01	.00D+00	.00D+00
797	0	0	.1183619D-01	.2039897D-01	.00D+00	.00D+00
798	0	0	.1392580D-01	.2163984D-01	.00D+00	.00D+00
799	0	0	.1658904D-01	.2280251D-01	.00D+00	.00D+00
800	0	0	.1996747D-01	.2374030D-01	.00D+00	.00D+00
801	0	0	.2419521D-01	.2419521D-01	.00D+00	.00D+00
802	0	0	.2933390D-01	.2373973D-01	.00D+00	.00D+00
803	0	0	.3522717D-01	.2172945D-01	.00D+00	.00D+00
804	0	0	.4126313D-01	.1734760D-01	.00D+00	.00D+00

805	0	0	.4614212D-01	.9956792D-02	.00D+00	.00D+00
806	0	0	.5001998D-01	.0000000D+00	.00D+00	.00D+00
807	0	0	.3688813D-02	.0000000D+00	.00D+00	.00D+00
808	0	0	.3687215D-02	.9233961D-03	.00D+00	.00D+00
809	0	0	.3685103D-02	.1845491D-02	.00D+00	.00D+00
810	0	0	.3682648D-02	.2765068D-02	.00D+00	.00D+00
811	0	0	.3681507D-02	.3681507D-02	.00D+00	.00D+00
812	0	0	.3683904D-02	.4594292D-02	.00D+00	.00D+00
813	0	0	.3692808D-02	.5503824D-02	.00D+00	.00D+00
814	0	0	.3711758D-02	.6411187D-02	.00D+00	.00D+00
815	0	0	.3744920D-02	.7318322D-02	.00D+00	.00D+00
816	0	0	.3797317D-02	.8228139D-02	.00D+00	.00D+00
817	0	0	.3874772D-02	.9144806D-02	.00D+00	.00D+00
818	0	0	.3984132D-02	.1007346D-01	.00D+00	.00D+00
819	0	0	.4133619D-02	.1102061D-01	.00D+00	.00D+00
820	0	0	.4333219D-02	.1199429D-01	.00D+00	.00D+00
821	0	0	.4595377D-02	.1300457D-01	.00D+00	.00D+00
822	0	0	.4935674D-02	.1406107D-01	.00D+00	.00D+00
823	0	0	.5374258D-02	.1517808D-01	.00D+00	.00D+00
824	0	0	.5937557D-02	.1637043D-01	.00D+00	.00D+00
825	0	0	.6660845D-02	.1765354D-01	.00D+00	.00D+00
826	0	0	.7592237D-02	.1904509D-01	.00D+00	.00D+00
827	0	0	.8797888D-02	.2055993D-01	.00D+00	.00D+00
828	0	0	.1037003D-01	.2220890D-01	.00D+00	.00D+00
829	0	0	.1243824D-01	.2398801D-01	.00D+00	.00D+00
830	0	0	.1518208D-01	.2586130D-01	.00D+00	.00D+00
831	0	0	.1884589D-01	.2772374D-01	.00D+00	.00D+00
832	0	0	.2373973D-01	.2933390D-01	.00D+00	.00D+00
833	0	0	.3018950D-01	.3018950D-01	.00D+00	.00D+00
834	0	0	.3835160D-01	.2933390D-01	.00D+00	.00D+00
835	0	0	.4772774D-01	.2515525D-01	.00D+00	.00D+00
836	0	0	.5628596D-01	.1558733D-01	.00D+00	.00D+00
837	0	0	.6366838D-01	.0000000D+00	.00D+00	.00D+00
838	0	0	.2765696D-02	.0000000D+00	.00D+00	.00D+00
839	0	0	.2765126D-02	.9222546D-03	.00D+00	.00D+00
840	0	0	.2764384D-02	.1843779D-02	.00D+00	.00D+00
841	0	0	.2763927D-02	.2763927D-02	.00D+00	.00D+00
842	0	0	.2765068D-02	.3682648D-02	.00D+00	.00D+00
843	0	0	.2769521D-02	.4599943D-02	.00D+00	.00D+00
844	0	0	.2779395D-02	.5516895D-02	.00D+00	.00D+00
845	0	0	.2797374D-02	.6435046D-02	.00D+00	.00D+00
846	0	0	.2826826D-02	.7357078D-02	.00D+00	.00D+00
847	0	0	.2871575D-02	.8286530D-02	.00D+00	.00D+00

Table 6.15 Input Data Sets for Problem 8 (continued)

848	0	0	.2936187D-02	.9228425D-02	.00D+00	.00D+00
849	0	0	.3026142D-02	.1018910D-01	.00D+00	.00D+00
850	0	0	.3148059D-02	.1117643D-01	.00D+00	.00D+00
851	0	0	.3310217D-02	.1220034D-01	.00D+00	.00D+00
852	0	0	.3522945D-02	.1327340D-01	.00D+00	.00D+00
853	0	0	.3799486D-02	.1440925D-01	.00D+00	.00D+00
854	0	0	.4157306D-02	.1562671D-01	.00D+00	.00D+00
855	0	0	.4619920D-02	.1694806D-01	.00D+00	.00D+00
856	0	0	.5219635D-02	.1839897D-01	.00D+00	.00D+00
857	0	0	.6001941D-02	.2001313D-01	.00D+00	.00D+00
858	0	0	.7032477D-02	.2182763D-01	.00D+00	.00D+00
859	0	0	.8407877D-02	.2388870D-01	.00D+00	.00D+00
860	0	0	.1027380D-01	.2624201D-01	.00D+00	.00D+00
861	0	0	.1285377D-01	.2893037D-01	.00D+00	.00D+00
862	0	0	.1649486D-01	.3195890D-01	.00D+00	.00D+00
863	0	0	.2172945D-01	.3522717D-01	.00D+00	.00D+00

864	0	0	.2933390D-01	.3835160D-01	.00D+00	.00D+00
865	0	0	.4026142D-01	.4026142D-01	.00D+00	.00D+00
866	0	0	.5500970D-01	.3835160D-01	.00D+00	.00D+00
867	0	0	.7129737D-01	.2723687D-01	.00D+00	.00D+00
868	0	0	.8721404D-01	.0000000D+00	.00D+00	.00D+00
869	0	0	.1843550D-02	.0000000D+00	.00D+00	.00D+00
870	0	0	.1843436D-02	.9218436D-03	.00D+00	.00D+00
871	0	0	.1843379D-02	.1843379D-02	.00D+00	.00D+00
872	0	0	.1843779D-02	.2764384D-02	.00D+00	.00D+00
873	0	0	.1845491D-02	.3685103D-02	.00D+00	.00D+00
874	0	0	.1849658D-02	.4606107D-02	.00D+00	.00D+00
875	0	0	.1857763D-02	.5528767D-02	.00D+00	.00D+00
876	0	0	.1871632D-02	.6455080D-02	.00D+00	.00D+00
877	0	0	.1893493D-02	.7388299D-02	.00D+00	.00D+00
878	0	0	.1925970D-02	.8332477D-02	.00D+00	.00D+00
879	0	0	.1972203D-02	.9293322D-02	.00D+00	.00D+00
880	0	0	.2036073D-02	.1027808D-01	.00D+00	.00D+00
881	0	0	.2122317D-02	.1129566D-01	.00D+00	.00D+00
882	0	0	.2236701D-02	.1235731D-01	.00D+00	.00D+00
883	0	0	.2386644D-02	.1347831D-01	.00D+00	.00D+00
884	0	0	.2581963D-02	.1467523D-01	.00D+00	.00D+00
885	0	0	.2835559D-02	.1597203D-01	.00D+00	.00D+00
886	0	0	.3165183D-02	.1739498D-01	.00D+00	.00D+00
887	0	0	.3595833D-02	.1898174D-01	.00D+00	.00D+00
888	0	0	.4163584D-02	.2077968D-01	.00D+00	.00D+00
889	0	0	.4922317D-02	.2284989D-01	.00D+00	.00D+00
890	0	0	.5955251D-02	.2527454D-01	.00D+00	.00D+00
891	0	0	.7395548D-02	.2816210D-01	.00D+00	.00D+00
892	0	0	.9465126D-02	.3165982D-01	.00D+00	.00D+00
893	0	0	.1254983D-01	.3595491D-01	.00D+00	.00D+00
894	0	0	.1734760D-01	.4126313D-01	.00D+00	.00D+00
895	0	0	.2515525D-01	.4772774D-01	.00D+00	.00D+00
896	0	0	.3835160D-01	.5500970D-01	.00D+00	.00D+00
897	0	0	.6075171D-01	.6075171D-01	.00D+00	.00D+00
898	0	0	.9463756D-01	.5500913D-01	.00D+00	.00D+00
899	0	0	.1342666D+00	.0000000D+00	.00D+00	.00D+00
900	0	0	.9217580D-03	.0000000D+00	.00D+00	.00D+00
901	0	0	.9217580D-03	.9217580D-03	.00D+00	.00D+00
902	0	0	.9218436D-03	.1843436D-02	.00D+00	.00D+00

Table 6.15 Input Data Sets for Problem 8 (continued)

903	0	0	.9222546D-03	.2765126D-02	.00D+00	.00D+00
904	0	0	.9233961D-03	.3687215D-02	.00D+00	.00D+00
905	0	0	.9258505D-03	.4610616D-02	.00D+00	.00D+00
906	0	0	.9303653D-03	.5536872D-02	.00D+00	.00D+00
907	0	0	.9378596D-03	.6468322D-02	.00D+00	.00D+00
908	0	0	.9494578D-03	.7408447D-02	.00D+00	.00D+00
909	0	0	.9665068D-03	.8361815D-02	.00D+00	.00D+00
910	0	0	.9906221D-03	.9334418D-02	.00D+00	.00D+00
911	0	0	.1023784D-02	.1033408D-01	.00D+00	.00D+00
912	0	0	.1068413D-02	.1137049D-01	.00D+00	.00D+00
913	0	0	.1127557D-02	.1245605D-01	.00D+00	.00D+00
914	0	0	.1205137D-02	.1360674D-01	.00D+00	.00D+00
915	0	0	.1306221D-02	.1484304D-01	.00D+00	.00D+00
916	0	0	.1437785D-02	.1618950D-01	.00D+00	.00D+00
917	0	0	.1609475D-02	.1767865D-01	.00D+00	.00D+00
918	0	0	.1834874D-02	.1935445D-01	.00D+00	.00D+00
919	0	0	.2134075D-02	.2127397D-01	.00D+00	.00D+00
920	0	0	.2537900D-02	.2351826D-01	.00D+00	.00D+00
921	0	0	.3095320D-02	.2619692D-01	.00D+00	.00D+00
922	0	0	.3888071D-02	.2947317D-01	.00D+00	.00D+00

```
  923     0     0    .5061301D-02    .3359247D-01    .00D+00    .00D+00
  924     0     0    .6891952D-02    .3893836D-01    .00D+00    .00D+00
  925     0     0    .9956792D-02    .4614212D-01    .00D+00    .00D+00
  926     0     0    .1558733D-01    .5628596D-01    .00D+00    .00D+00
  927     0     0    .2723687D-01    .7129737D-01    .00D+00    .00D+00
  928     0     0    .5500913D-01    .9463756D-01    .00D+00    .00D+00
  929     0     0    .1320462D+00    .1320462D+00    .00D+00    .00D+00
  930     0     0    .2464926D+00    .0000000D+00    .00D+00    .00D+00
  931     0     0    .0000000D+00    .0000000D+00    .00D+00    .00D+00
  932     0     0    .0000000D+00    .9217580D-03    .00D+00    .00D+00
  933     0     0    .0000000D+00    .1843550D-02    .00D+00    .00D+00
  934     0     0    .0000000D+00    .2765696D-02    .00D+00    .00D+00
  935     0     0    .0000000D+00    .3688813D-02    .00D+00    .00D+00
  936     0     0    .0000000D+00    .4613813D-02    .00D+00    .00D+00
  937     0     0    .0000000D+00    .5542580D-02    .00D+00    .00D+00
  938     0     0    .0000000D+00    .6477568D-02    .00D+00    .00D+00
  939     0     0    .0000000D+00    .7422374D-02    .00D+00    .00D+00
  940     0     0    .0000000D+00    .8382021D-02    .00D+00    .00D+00
  941     0     0    .0000000D+00    .9362614D-02    .00D+00    .00D+00
  942     0     0    .0000000D+00    .1037232D-01    .00D+00    .00D+00
  943     0     0    .0000000D+00    .1142152D-01    .00D+00    .00D+00
  944     0     0    .0000000D+00    .1252340D-01    .00D+00    .00D+00
  945     0     0    .0000000D+00    .1369463D-01    .00D+00    .00D+00
  946     0     0    .0000000D+00    .1495833D-01    .00D+00    .00D+00
  947     0     0    .0000000D+00    .1633790D-01    .00D+00    .00D+00
  948     0     0    .0000000D+00    .1787386D-01    .00D+00    .00D+00
  949     0     0    .0000000D+00    .1961130D-01    .00D+00    .00D+00
  950     0     0    .0000000D+00    .2161644D-01    .00D+00    .00D+00
  951     0     0    .0000000D+00    .2398402D-01    .00D+00    .00D+00
  952     0     0    .0000000D+00    .2684646D-01    .00D+00    .00D+00
  953     0     0    .0000000D+00    .3041039D-01    .00D+00    .00D+00
  954     0     0    .0000000D+00    .3500342D-01    .00D+00    .00D+00
  955     0     0    .0000000D+00    .4118950D-01    .00D+00    .00D+00
  956     0     0    .0000000D+00    .5001998D-01    .00D+00    .00D+00
  957     0     0    .0000000D+00    .6366838D-01    .00D+00    .00D+00
```

Table 6.15 Input Data Sets for Problem 8 (continued)

```
  958     0     0    .0000000D+00    .8721404D-01    .00D+00    .00D+00
  959     0     0    .0000000D+00    .1342666D+00    .00D+00    .00D+00
  960     0     0    .0000000D+00    .2464926D+00    .00D+00    .00D+00
  961     0     0    .5396279D+00    .5396279D+00    .00D+00    .00D+00
    0     0     0      0.0    0.0     0.0    0.0       END OF VELOCITY (dm/hr)
    1   899     1      0.05   0.0
    0     0     0      0.0    0.0     0.0               END OF TH
    1   960     1      1.000  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
6 1 13 4 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 20: Adsorption Information
 1 0
0 0
0 0 0
c ******* DATA SET 22: Basic real and integer parameters
1.0 1 1000 1.0d-6 1.0d0 1.0d0 1 omegac npcyl niterc epsc cnstrx,y ipiv
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
 >SOH
  2 0
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
>SOH
  0  0 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
```

Table 6.15 Input Data Sets for Problem 8 (continued)

```
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
C ******** DATA SET 26:  ADSORBED SPECIES
>SOH2+
0    1  0  0  0  0  0  1       1  0  0  0  0  0  1
```

```
>SO-
0   -1  0  0  0  0  0  1       -1  0  0  0  0  0  1
>SOH2-CoNTA(ads)
0    1  0  0  0  1  1  1        1  0  0  0  1  1  1
>SO-Co(ads)
0   -2  0  0  0  0  1  2       -2  0  0  0  0  1  2
C ******** DATA SET 28:  MICROBIAL SPECIES
C5H7O2N(aq cells)
  0  -2.681936665037 0
C5H7O2N(ads cells)
  0  -2.681936665037 0
C ******** DATA SET 29:  reaction data
20
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
```

Table 6.15 Input Data Sets for Problem 8 (continued)

```
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
1 1 0    NRTS NPDS KRTYP           REACTION 13 - OH
-14.0      LOGKEQ
 -1  1
 1   20
2 1 0    NRTS NPDS KRTYP           REACTION 14 - >SOH2+
 5.6       LOGKEQ
 1   1  1
 7   1  21
2 1 0    NRTS NPDS KRTYP           REACTION 15 - >SO-
-11.6      LOGKEQ
 1  -1  1
 7   1  22
2 1 1           NRTS NPDS KRTYP    REACTION 16 - CoNTA (ads) * rates revised
-2.279039227   -0.09690     LOGKB  LOGKF
 1  1  1
 11 21  23
2 1 1           NRTS NPDS KRTYP    REACTION 16 - Co(ads)
-1.279039227   -0.574031267728     LOGKB  LOGKF
 1  2  1
 6  22 24
3 3 2           NRTS NPDS KRTYP    REACTION 17 - MB rxn - aq species
```

Table 6.15 Input Data Sets for Problem 8 (concluded)

```
0.0916519  7.64D-7 6.25D-6 0.0 1 2 0 0.0 0.0 grmax ks ka kn locsan taul taue
1  1.620  2.424    17.370666  3.120  0.424
10 4      1        25         2      3
0 0 0 0 0             inhib hscinh hscinh p q
3 3 2           NRTS NPDS KRTYP    REACTION 18 - MB rxn - ads species
0.0916519  7.64D-7 6.25D-6 0.0 1 2 0 0.0 0.0 grmax ks ka kn locsan taul taue
1  1.620  2.424    17.370666  3.120  0.424
10 4      1        26         2      3
0 0 0 0 0             inhib hscinh hscinh p q
1 1 3           NRTS NPDS KRTYP    REACTION 19 - MB phase transfer rxn
-1.279039227   -0.574031267728  LOGKB  LOGKF
 1    1
 25   26
                                END OF JOB
```