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
```