```
# Datong Basin Arsenic Analysis'
'-----------------------------------------------------------------------------'
'DEFINITION OF THE GEOCHEMICAL SYSTEM'
'PRIMARY SPECIES'
 alo2-
 ca+2
 cl-
 h+
 h2o
 hco3-
 k+
 mg+2
 na+
 sio2(aq)
 so4-2
 fe+2
 hs-
 mn+2
 fe+3
 nh4+
 h2aso3-
 h2aso4-
 *
 AQUEOUS COMPLEXES
 as(oh)3(aq)
 aso2-
 aso2oh-2
 aso4-3
 cacl+
 cacl2(aq)
 caco3(aq)
 cahco3+
 caoh+
 caso4(aq)
 fe(oh)2(aq)
 fe(oh)2+
 fe(oh)3(aq)
 fe(oh)3-
 fe(oh)4-
 fecl+
 fecl2(aq)
 feco3(aq)
 feco3+
 fehco3+
 feoh+
 feoh+2
```

```
 feso4(aq)
 h2s(aq)
 h2sio4-2
 h2so4(aq)
 h3aso4(aq)
 halo2(aq)
 haso2(aq)
 haso4-2
 hass2(aq)
 hcl(aq)
 hsio3-
 hso4-
 kcl(aq)
 khso4(aq)
 koh(aq)
 kso4-
 mgcl+
 mgco3(aq)
 mghco3+
 mgso4(aq)
 mn(oh)2(aq)
 mn(oh)3-
 mn2(oh)3+
 mn2oh+3
 mncl+
 mncl2(aq)
 mnco3(aq)
 mnhco3+
 mnoh+
 mnso4(aq)
 naalo2(aq)
 nacl(aq)
 naco3-
 nah3sio4(aq)
 nahco3(aq)
 naoh(aq)
 naso4-
 nh3(aq)
 nh4so4-
 al+3
 co3-2
 oh-
 *
'MINERALS'
 calcite                         0           0
     0.000     0.000     0.000
```

```
 mackinawite                    0           0
    0.000     0.000     0.000
 orpiment                       0           0
    0.000     0.000     0.000
 albite                         1           3
 0.251E-15    2     1.000     1.000    69.800     0.000     0.000     0.000
        2
            0.6918E-10   65.0000    1      h+                0.4570
            0.2512E-15   71.0000    1      h+               -0.5720
 0.251E-15    0     1.000     1.000    69.800     0.000     0.000     0.0000.5600E-01  0
    0.000     0.000     0.000
 annite                         1           1
 0.282E-13    2     1.000     1.000    22.000     0.000     0.000     0.000
        2
            0.1413E-11   22.0000    1      h+                0.3700
            0.2818E-14   22.0000    1      h+               -0.2200
 illite                         1           3
 0.166E-12    2     1.000     1.000    35.000     0.000     0.000     0.000
        2
            0.1047E-10   23.6000    1      h+                0.3400
            0.3020E-16   58.8000    1      h+               -0.4000
 0.166E-12    0     1.000     1.000    35.000     0.000     0.000     0.0000.2040E+00  0
    0.000     0.000     0.000
 k-feldspar                     1           3
 0.389E-12    2     1.000     1.000    38.000     0.000     0.000     0.000
        2
            0.8710E-10   51.7000    1      h+                0.5000
            0.6310E-21   94.1000    1      h+               -0.8230
 0.389E-12    0     1.000     1.000    38.000     0.000     0.000     0.0000.9000E-02  0
    0.000     0.000     0.000
 quartz                         1           3
 0.102E-13    0     1.000     1.000    87.700     0.000     0.000     0.000
 0.102E-13    0     1.000     1.000    87.700     0.000     0.000     0.0000.1760E+00  0
    0.000     0.000     0.000
 montmor-na                     1           3
 0.166E-12    2     1.000     1.000    35.000     0.000     0.000     0.000
        2
            0.1047E-10   23.6000    1      h+                0.3400
            0.3020E-16   58.9000    1      h+               -0.4000
 0.166E-12    0     1.000     1.000    35.000     0.000     0.000     0.0000.8900E-01  0
    0.000     0.000     0.000
 chlorite                       1           3
 0.302E-12    2     1.000     1.000    88.000     0.000     0.000     0.000
        1
            0.7762E-11   88.0000    1      h+                0.5000
 0.302E-12    0     1.000     1.000    88.000     0.000     0.000     0.0000.1760E+00  0
```

```
     0.000     0.000     0.000
 *                             0           0

  The following minerals form ideal solid solutions:
   None
'GASES'
 *
'SURFACE COMPLEXES'
 *
'SPECIES W/ Kd and DECAY        decay constant(1/s)'
 *                     0.000000000000000E+000

 GENERAL CHEMICAL SYSTEM
    --> Thermodynamic database: thermodb.txt

'EXCHANGEABLE CATIONS'
'                     master     convention     ex. coef.'
 ca+2                 0            3            0.40
 h+                   0            3            0.00
 k+                   0            3            0.20
 mg+2                 0            3            0.50
 na+                  1            3            1.00
 *                    0            0            0.00
   Components     a0    charge
  alo2-          1.810   -1.0
  ca+2           2.870    2.0
  cl-            1.810   -1.0
  h+             3.080    1.0
  h2o            0.000    0.0
  hco3-          2.100   -1.0
  k+             2.270    1.0
  mg+2           2.540    2.0
  na+            1.910    1.0
  sio2(aq)       0.000    0.0
  so4-2          3.150   -2.0
  fe+2           2.620    2.0
  hs-            1.810   -1.0
  mn+2           2.680    2.0
  fe+3           3.600    3.0
  nh4+           2.410    1.0
  h2aso3-        0.000    0.0
  h2aso4-        0.000    0.0


 Log K interpolation coefficients (a,b,c,d,e)
 valid temperature range (deg.C.):   0.0 to 300.0
```

	a*ln(TK)	b	c*TK	d*(TK)**-1	e*(TK)**-2
as(oh)3(aq)	0.0000E+00	-9.2048E+00	0.0000E+00	0.0000E+00	0.0000E+00
aso2-	0.0000E+00	-1.1140E-02	0.0000E+00	0.0000E+00	0.0000E+00
aso2oh-2	0.0000E+00	1.1017E+01	0.0000E+00	0.0000E+00	0.0000E+00
aso4-3	0.0000E+00	1.8360E+01	0.0000E+00	0.0000E+00	0.0000E+00
cacl+	1.3103E+02	-8.3024E+02	-1.3376E-01	4.6829E+04	-2.9136E+06
cacl2(aq)	2.6397E+02	-1.6725E+03	-2.6682E-01	9.3589E+04	-5.7991E+06
caco3(aq)	1.4428E+02	-9.0987E+02	-1.4188E-01	4.9758E+04	-2.6449E+06
cahco3+	1.4238E+02	-9.0678E+02	-1.4307E-01	5.1998E+04	-3.3081E+06
caoh+	4.8490E+01	-3.0192E+02	-5.1744E-02	1.8938E+04	-8.5279E+05
caso4(aq)	2.6777E+02	-1.7008E+03	-2.6432E-01	9.3540E+04	-5.5017E+06
fe(oh)2(aq)	-4.9796E+00	2.9729E+01	6.8993E-03	5.0397E+03	2.4624E+04
fe(oh)2+	0.0000E+00	5.6700E+00	0.0000E+00	0.0000E+00	0.0000E+00
fe(oh)3(aq)	0.0000E+00	1.3600E+01	0.0000E+00	0.0000E+00	0.0000E+00
fe(oh)3-	0.0000E+00	3.2962E+01	0.0000E+00	0.0000E+00	0.0000E+00
fe(oh)4-	0.0000E+00	2.1000E+01	0.0000E+00	0.0000E+00	0.0000E+00
fecl+	1.3604E+02	-8.6383E+02	-1.3730E-01	4.8907E+04	-3.0401E+06
fecl2(aq)	2.7002E+02	-1.7116E+03	-2.7172E-01	9.6352E+04	-5.9118E+06
feco3(aq)	-4.9426E+02	3.1460E+03	4.8872E-01	-1.7444E+05	1.0224E+07
feco3+	0.0000E+00	6.0880E-01	0.0000E+00	0.0000E+00	0.0000E+00
fehco3+	1.5321E+02	-9.6630E+02	-1.5586E-01	5.1442E+04	-3.0882E+06
feoh+	2.8176E+01	-1.7774E+02	-2.5611E-02	1.2397E+04	-5.2002E+05
feoh+2	0.0000E+00	2.1900E+00	0.0000E+00	0.0000E+00	0.0000E+00
feso4(aq)	2.5058E+02	-1.5940E+03	-2.4250E-01	8.7676E+04	-5.1239E+06
h2s(aq)	0.0000E+00	-6.9877E+00	0.0000E+00	0.0000E+00	0.0000E+00
h2sio4-2	9.9570E+01	-6.5687E+02	-5.1514E-02	4.7876E+04	-2.9104E+06
h2so4(aq)	0.0000E+00	1.0200E+00	0.0000E+00	0.0000E+00	0.0000E+00
h3aso4(aq)	0.0000E+00	-2.2490E+00	0.0000E+00	0.0000E+00	0.0000E+00
halo2(aq)	8.5813E+01	-5.4438E+02	-8.8781E-02	2.9201E+04	-1.9974E+06
haso2(aq)	0.0000E+00	-9.2792E+00	0.0000E+00	0.0000E+00	0.0000E+00
haso4-2	0.0000E+00	6.7583E+00	0.0000E+00	0.0000E+00	0.0000E+00
hass2(aq)	0.0000E+00	-3.0480E+01	0.0000E+00	0.0000E+00	0.0000E+00
hcl(aq)	3.1813E+02	-2.0125E+03	-3.1404E-01	1.0851E+05	-6.1992E+06
hsio3-	-5.6009E+00	1.2880E+01	3.5279E-02	8.2277E+03	-8.1249E+05
hso4-	1.5437E+02	-9.9063E+02	-1.5057E-01	5.8117E+04	-3.6369E+06
kcl(aq)	1.1449E+02	-7.2588E+02	-1.1354E-01	4.0160E+04	-2.2906E+06
khso4(aq)	2.4309E+02	-1.5539E+03	-2.3929E-01	9.0003E+04	-5.5513E+06
koh(aq)	0.0000E+00	1.4460E+01	0.0000E+00	0.0000E+00	0.0000E+00
kso4-	1.5172E+02	-9.6700E+02	-1.4844E-01	5.4823E+04	-3.3736E+06
mgcl+	1.4464E+02	-9.2065E+02	-1.4462E-01	5.3131E+04	-3.4131E+06
mgco3(aq)	1.5467E+02	-9.7579E+02	-1.4997E-01	5.3376E+04	-2.8826E+06
mghco3+	1.4465E+02	-9.2374E+02	-1.4285E-01	5.3640E+04	-3.4446E+06
mgso4(aq)	5.4072E+02	-3.4368E+03	-5.2632E-01	1.8893E+05	-1.0945E+07
mn(oh)2(aq)	0.0000E+00	2.2200E+01	0.0000E+00	0.0000E+00	0.0000E+00
mn(oh)3-	0.0000E+00	3.4228E+01	0.0000E+00	0.0000E+00	0.0000E+00
mn2(oh)3+	0.0000E+00	2.3900E+01	0.0000E+00	0.0000E+00	0.0000E+00

mn2oh+3	0.0000E+00	1.0560E+01	0.0000E+00	0.0000E+00	0.0000E+00
mncl+	1.4367E+02	-9.1505E+02	-1.4582E-01	5.2441E+04	-3.2219E+06
mncl2(aq)	0.0000E+00	-2.5000E-01	0.0000E+00	0.0000E+00	0.0000E+00
mnco3(aq)	0.0000E+00	5.8090E+00	0.0000E+00	0.0000E+00	0.0000E+00
mnhco3+	0.0000E+00	-8.8200E-01	0.0000E+00	0.0000E+00	0.0000E+00
mnoh+	0.0000E+00	1.0590E+01	0.0000E+00	0.0000E+00	0.0000E+00
mnso4(aq)	2.7771E+02	-1.7657E+03	-2.7277E-01	9.7419E+04	-5.7214E+06
naalo2(aq)	1.5177E+02	-9.6704E+02	-1.4725E-01	5.4975E+04	-3.3276E+06
nacl(aq)	1.2748E+02	-8.0980E+02	-1.2503E-01	4.5318E+04	-2.7066E+06
naco3-	5.5748E+01	-3.5618E+02	-2.4308E-02	1.9021E+04	-7.2732E+05
nah3sio4(aq)	-5.2360E+02	3.3235E+03	5.1452E-01	-1.7955E+05	1.0420E+07
nahco3(aq)	-1.9296E+02	1.2242E+03	1.9025E-01	-6.6962E+04	3.8160E+06
naoh(aq)	-3.9778E+02	2.5265E+03	3.8913E-01	-1.3467E+05	7.9779E+06
naso4-	2.2849E+02	-1.4587E+03	-2.1256E-01	8.1356E+04	-4.7528E+06
nh3(aq)	0.0000E+00	9.2400E+00	0.0000E+00	0.0000E+00	0.0000E+00
nh4so4-	0.0000E+00	-1.0300E+00	0.0000E+00	0.0000E+00	0.0000E+00
al+3	3.6067E+01	-2.2324E+02	-3.3211E-02	4.4829E+03	-9.1283E+05
co3-2	-1.2715E+02	8.1537E+02	1.2850E-01	-4.5171E+04	2.8995E+06
oh-	-1.1609E+02	7.4186E+02	1.1647E-01	-3.8963E+04	2.6264E+06
calcite	1.4263E+02	-9.0477E+02	-1.4455E-01	5.0724E+04	-2.9370E+06
mackinawite	0.0000E+00	-3.6000E+00	0.0000E+00	0.0000E+00	0.0000E+00
orpiment	0.0000E+00	-7.9416E+01	0.0000E+00	0.0000E+00	0.0000E+00
albite	4.3838E+02	-2.8635E+03	-3.5565E-01	1.7711E+05	-1.2655E+07
annite	5.8724E+02	-3.8145E+03	-5.0201E-01	2.3819E+05	-1.5466E+07
illite	9.7662E+02	-6.3134E+03	-8.3515E-01	3.6292E+05	-2.3691E+07
k-feldspar	2.2819E+01	-1.2055E+02	-4.7299E-02	-7.0465E+03	4.7707E+05
quartz	-2.3561E+01	1.5445E+02	1.7816E-02	-1.0900E+04	6.4851E+05
montmor-na	6.3477E+02	-4.1348E+03	-5.2688E-01	2.5007E+05	-1.7845E+07
chlorite	7.3086E+02	-4.6982E+03	-6.7072E-01	2.7387E+05	-1.6018E+07

Derived Species Reactions

species	a0	charge	logK(25. C)	alo2-	ca+2	cl-	h+	h2o	hco3-	k+	mg+2	na+
sio2(aqso4-2	fe+2	hs-	mn+2	fe+3	nh4+	h2aso3-	h2aso4-					
as(oh)3(aq)	0.000	0.0	-9.205	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00				
aso2-	2.810	-1.0	-0.011	0.00	0.00	0.00	-1.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00				
aso2oh-2	2.810	-2.0	11.017	0.00	0.00	0.00	-1.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00				
aso4-3	2.810	-3.0	18.360	0.00	0.00	0.00	-2.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00				
cacl+	2.310	1.0	0.701	0.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00				
cacl2(aq)	0.000	0.0	0.654	0.00	1.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00				
caco3(aq)	0.000	0.0	7.009	0.00	1.00	0.00	-1.00	0.00	1.00	0.00	0.00	0.00

```
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 cahco3+        2.310   1.0       -1.043   0.00   1.00   0.00   0.00   0.00   1.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 caoh+          2.310   1.0       12.852   0.00   1.00   0.00  -1.00   1.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 caso4(aq)      0.000   0.0       -2.100   0.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 0.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 fe(oh)2(aq)    0.000   0.0       20.595   0.00   0.00   0.00  -2.00   2.00   0.00   0.00   0.00   0.00
 0.00   0.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00
 fe(oh)2+       2.310   1.0        5.670   0.00   0.00   0.00  -2.00   2.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   0.00   1.00   0.00   0.00   0.00
 fe(oh)3(aq)    0.000   0.0       13.600   0.00   0.00   0.00  -3.00   3.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   0.00   1.00   0.00   0.00   0.00
 fe(oh)3-       1.810  -1.0       32.962   0.00   0.00   0.00  -3.00   3.00   0.00   0.00   0.00   0.00
 0.00   0.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00
 fe(oh)4-       1.810  -1.0       21.000   0.00   0.00   0.00  -4.00   4.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   0.00   1.00   0.00   0.00   0.00
 fecl+          2.310   1.0        0.165   0.00   0.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00
 0.00   0.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00
 fecl2(aq)      0.000   0.0        2.464   0.00   0.00   2.00   0.00   0.00   0.00   0.00   0.00   0.00
 0.00   0.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00
 feco3(aq)      0.000   0.0        5.568   0.00   0.00   0.00  -1.00   0.00   1.00   0.00   0.00   0.00
 0.00   0.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00
 feco3+         0.000   1.0        0.609   0.00   0.00   0.00  -1.00   0.00   1.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   0.00   1.00   0.00   0.00   0.00
 fehco3+        2.310   1.0       -2.044   0.00   0.00   0.00   0.00   0.00   1.00   0.00   0.00   0.00
 0.00   0.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00
 feoh+          2.310   1.0       10.895   0.00   0.00   0.00  -1.00   1.00   0.00   0.00   0.00   0.00
 0.00   0.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00
 feoh+2         2.800   2.0        2.190   0.00   0.00   0.00  -1.00   1.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   0.00   1.00   0.00   0.00   0.00
 feso4(aq)      0.000   0.0       -2.189   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 0.00   1.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00
 h2s(aq)        0.000   0.0       -6.988   0.00   0.00   0.00   1.00   0.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   1.00   0.00   0.00   0.00   0.00   0.00
 h2sio4-2       3.000  -2.0       22.910   0.00   0.00   0.00  -2.00   2.00   0.00   0.00   0.00   0.00
 1.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 h2so4(aq)      0.000   0.0        1.020   0.00   0.00   0.00   2.00   0.00   0.00   0.00   0.00   0.00
 0.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 h3aso4(aq)     3.000   0.0       -2.249   0.00   0.00   0.00   1.00   0.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   1.00
 halo2(aq)      0.000   0.0       -6.448   1.00   0.00   0.00   1.00   0.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 haso2(aq)      3.000   0.0       -9.279   0.00   0.00   0.00   1.00  -1.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   1.00   0.00
 haso4-2        3.000  -2.0        6.758   0.00   0.00   0.00  -1.00   0.00   0.00   0.00   0.00   0.00
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 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   1.00
 hass2(aq)      0.000   0.0      -30.480   0.00   0.00   0.00   3.00  -3.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   2.00   0.00   0.00   0.00   1.00   0.00
 hcl(aq)        0.000   0.0        0.700   0.00   0.00   1.00   1.00   0.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 hsio3-         1.810  -1.0        9.942   0.00   0.00   0.00  -1.00   1.00   0.00   0.00   0.00   0.00
 1.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 hso4-          2.370  -1.0       -1.974   0.00   0.00   0.00   1.00   0.00   0.00   0.00   0.00   0.00
 0.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00
 kcl(aq)        0.000   0.0        1.500   0.00   0.00   1.00   0.00   0.00   0.00   1.00   0.00   0.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 khso4(aq)      0.000   0.0       -0.806   0.00   0.00   0.00   1.00   0.00   0.00   1.00   0.00   0.00
 0.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 koh(aq)        0.000   0.0       14.460   0.00   0.00   0.00  -1.00   1.00   0.00   1.00   0.00   0.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 kso4-          1.810  -1.0       -0.875   0.00   0.00   0.00   0.00   0.00   0.00   1.00   0.00   0.00
 0.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 mgcl+          2.310   1.0        0.139   0.00   0.00   1.00   0.00   0.00   0.00   0.00   1.00   0.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 mgco3(aq)      0.000   0.0        7.356   0.00   0.00   0.00  -1.00   0.00   1.00   0.00   1.00   0.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 mghco3+        2.310   1.0       -1.033   0.00   0.00   0.00   0.00   0.00   1.00   0.00   1.00   0.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 mgso4(aq)      0.000   0.0       -2.382   0.00   0.00   0.00   0.00   0.00   0.00   0.00   1.00   0.00
 0.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 mn(oh)2(aq)    0.000   0.0       22.200   0.00   0.00   0.00  -2.00   2.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   1.00   0.00   0.00   0.00   0.00
 mn(oh)3-       1.810  -1.0       34.228   0.00   0.00   0.00  -3.00   3.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   1.00   0.00   0.00   0.00   0.00
 mn2(oh)3+      2.310   1.0       23.900   0.00   0.00   0.00  -3.00   3.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   2.00   0.00   0.00   0.00   0.00
 mn2oh+3        3.600   3.0       10.560   0.00   0.00   0.00  -1.00   1.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   2.00   0.00   0.00   0.00   0.00
 mncl+          2.310   1.0       -0.297   0.00   0.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   1.00   0.00   0.00   0.00   0.00
 mncl2(aq)      0.000   0.0       -0.250   0.00   0.00   2.00   0.00   0.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   1.00   0.00   0.00   0.00   0.00
 mnco3(aq)      0.000   0.0        5.809   0.00   0.00   0.00  -1.00   0.00   1.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   1.00   0.00   0.00   0.00   0.00
 mnhco3+        2.310   1.0       -0.882   0.00   0.00   0.00   0.00   0.00   1.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   1.00   0.00   0.00   0.00   0.00
 mnoh+          2.310   1.0       10.590   0.00   0.00   0.00  -1.00   1.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   1.00   0.00   0.00   0.00   0.00
 mnso4(aq)      0.000   0.0       -2.342   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 0.00   1.00   0.00   0.00   1.00   0.00   0.00   0.00   0.00
 naalo2(aq)     0.000   0.0        0.748   1.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   1.00
```

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 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 nacl(aq)       0.000   0.0        0.782   0.00   0.00   1.00   0.00   0.00   0.00   0.00   0.00   1.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 naco3-         1.810  -1.0        9.816   0.00   0.00   0.00  -1.00   0.00   1.00   0.00   0.00   1.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 nah3sio4(aq)   0.000   0.0        8.622   0.00   0.00   0.00  -1.00   2.00   0.00   0.00   0.00   1.00
 1.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 nahco3(aq)     0.000   0.0       -0.170   0.00   0.00   0.00   0.00   0.00   1.00   0.00   0.00   1.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 naoh(aq)       0.000   0.0       14.154   0.00   0.00   0.00  -1.00   1.00   0.00   0.00   0.00   1.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 naso4-         1.810  -1.0       -0.811   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   1.00
 0.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 nh3(aq)        0.000   0.0        9.240   0.00   0.00   0.00  -1.00   0.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   0.00   0.00   1.00   0.00   0.00
 nh4so4-        5.000  -1.0       -1.030   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 0.00   1.00   0.00   0.00   0.00   0.00   1.00   0.00   0.00
 al+3           3.330   3.0      -22.879   1.00   0.00   0.00   4.00  -2.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 co3-2          2.810  -2.0       10.325   0.00   0.00   0.00  -1.00   0.00   1.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 oh-            1.400  -1.0       13.991   0.00   0.00   0.00  -1.00   1.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00

 Mineral Reactions
  minerals    m.vol(L/mol)  logK(25. C)  alo2-  ca+2   cl-    h+     h2o    hco3-  k+     mg+2   na+
  sio2(aqso4-2  fe+2   hs-    mn+2   fe+3   nh4+   h2aso3-h2aso4-
 calcite           0.0369       1.854    0.00   1.00   0.00  -1.00   0.00   1.00   0.00   0.00   0.00   0.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 mackinawite       0.5000      -3.600    0.00   0.00   0.00  -1.00   0.00   0.00   0.00   0.00   0.00   0.00
 0.00   1.00   1.00   0.00   0.00   0.00   0.00   0.00
 orpiment          0.0705     -79.416    0.00   0.00   0.00   5.00  -6.00   0.00   0.00   0.00   0.00   0.00
 0.00   0.00   3.00   0.00   0.00   0.00   2.00   0.00
 albite            0.1003     -20.133    1.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   1.00   3.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 annite            0.1543       6.574    1.00   0.00   0.00  -6.00   4.00   0.00   1.00   0.00   0.00   3.00
 0.00   3.00   0.00   0.00   0.00   0.00   0.00   0.00
 illite            0.1389     -47.328    2.30   0.00   0.00   1.20   0.40   0.00   0.60   0.25   0.00   3.50
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 k-feldspar        0.1089     -22.910    1.00   0.00   0.00   0.00   0.00   0.00   1.00   0.00   0.00   3.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 quartz            0.0227      -3.745    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   1.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 montmor-na        0.1343     -37.175    1.67   0.00   0.00   0.68   0.66   0.00   0.00   0.33   0.33   4.00
 0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
 chlorite          0.2103       4.298    2.00   0.00   0.00  -8.00   8.00   0.00   0.00   2.50   0.00   3.00
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 0.00   2.50   0.00   0.00   0.00   0.00   0.00   0.00
'--------------------------------------------------------------------------------'
'INITIAL AND BOUNDARY WATER TYPES'
 number of initial-water types=   4
 number of boundary (+ injecting) water types=   1

 Initial Water Type =   1
 water temperature (C)=    8.75
'                     icon   guess       ctot   nameq   qksat'
 alo2-    1        0.7083E-07        0.7083E-07
 ca+2     1        0.3121E-03        0.3121E-03
 cl-      1        0.6240E-03        0.6240E-03
 h+       3        0.7405E-08        0.7405E-08
 h2o      1        0.1000E+01        0.1000E+01
 hco3-    1        0.6256E-02        0.6256E-02
 k+       1        0.1126E-04        0.1126E-04
 mg+2     1        0.7809E-03        0.7809E-03
 na+      1        0.4753E-02        0.4753E-02
 sio2(aq)1        0.8739E-04        0.8739E-04
 so4-2    1        0.5768E-04        0.5768E-04
 fe+2     1        0.1433E-05        0.1433E-05
 hs-      1        0.4680E-06        0.4680E-06
 mn+2     1        0.2344E-05        0.2344E-05
 fe+3     1        0.1335E-05        0.1335E-05
 nh4+     1        0.1429E-04        0.1429E-04
 h2aso3-  1        0.1855E-04        0.1855E-04
 h2aso4-  1        0.2792E-05        0.2792E-05
 *        0        0.0000E+00        0.0000E+00

 Initial Water Type =   2
 water temperature (C)=    8.90
'                     icon   guess       ctot   nameq   qksat'
 alo2-    1        0.2170E-06        0.2170E-06
 ca+2     1        0.3848E-03        0.3848E-03
 cl-      1        0.7466E-03        0.7466E-03
 h+       3        0.1273E-07        0.1273E-07
 h2o      1        0.1000E+01        0.1000E+01
 hco3-    1        0.8063E-02        0.8063E-02
 k+       1        0.1357E-04        0.1357E-04
 mg+2     1        0.7761E-03        0.7761E-03
 na+      1        0.6895E-02        0.6895E-02
 sio2(aq)1        0.9474E-04        0.9474E-04
 so4-2    1        0.3759E-03        0.3759E-03
 fe+2     1        0.4301E-05        0.4301E-05
 hs-      1        0.9363E-06        0.9363E-06
 mn+2     1        0.3348E-05        0.3348E-05
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 fe+3    1        0.5680E-06        0.5680E-06
 nh4+    1        0.1093E-03        0.1093E-03
 h2aso3- 1        0.2518E-04        0.2518E-04
 h2aso4- 1        0.9908E-05        0.9908E-05
 *       0        0.0000E+00        0.0000E+00

 Initial Water Type =   3
 water temperature (C)=    8.51
'                      icon   guess       ctot   nameq   qksat'
 alo2-   1        0.2066E-06        0.2066E-06
 ca+2    1        0.6154E-03        0.6154E-03
 cl-     1        0.6257E-02        0.6257E-02
 h+      3        0.2313E-07        0.2313E-07
 h2o     1        0.1000E+01        0.1000E+01
 hco3-   1        0.7584E-02        0.7584E-02
 k+      1        0.2842E-04        0.2842E-04
 mg+2    1        0.1344E-02        0.1344E-02
 na+     1        0.1043E-01        0.1043E-01
 sio2(aq)1        0.8277E-04        0.8277E-04
 so4-2   1        0.5211E-04        0.5211E-04
 fe+2    1        0.3585E-06        0.3585E-06
 hs-     1        0.9147E-05        0.9147E-05
 mn+2    1        0.2915E-05        0.2915E-05
 fe+3    1        0.1524E-05        0.1524E-05
 nh4+    1        0.6503E-04        0.6503E-04
 h2aso3- 1        0.9486E-07        0.9486E-07
 h2aso4- 1        0.2044E-06        0.2044E-06
 *       0        0.0000E+00        0.0000E+00

 Initial Water Type =   4
 water temperature (C)=    8.40
'                      icon   guess       ctot   nameq   qksat'
 alo2-   1        0.2236E-06        0.2236E-06
 ca+2    1        0.4790E-03        0.4790E-03
 cl-     1        0.7874E-03        0.7874E-03
 h+      3        0.1550E-07        0.1550E-07
 h2o     1        0.1000E+01        0.1000E+01
 hco3-   1        0.6332E-02        0.6332E-02
 k+      1        0.1331E-04        0.1331E-04
 mg+2    1        0.9341E-03        0.9341E-03
 na+     1        0.4090E-02        0.4090E-02
 sio2(aq)1        0.1276E-03        0.1276E-03
 so4-2   1        0.8313E-04        0.8313E-04
 fe+2    1        0.7166E-06        0.7166E-06
 hs-     1        0.3744E-06        0.3744E-06
 mn+2    1        0.2725E-05        0.2725E-05
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 fe+3    1        0.7919E-06        0.7919E-06
 nh4+    1        0.2286E-04        0.2286E-04
 h2aso3- 1        0.3628E-05        0.3628E-05
 h2aso4- 1        0.2814E-05        0.2814E-05
 *       0        0.0000E+00        0.0000E+00

 Boundary (+ injection) Water Type =   1
 water temperature (C)=    8.40
'                     icon   guess       ctot         constrain'
 alo2-   1        0.2236E-06        0.2236E-06
 ca+2    1        0.4790E-03        0.4790E-03
 cl-     1        0.7874E-03        0.7874E-03
 h+      3        0.1550E-07        0.1550E-07
 h2o     1        0.1000E+01        0.1000E+01
 hco3-   1        0.6332E-02        0.6332E-02
 k+      1        0.1331E-04        0.1331E-04
 mg+2    1        0.9341E-03        0.9341E-03
 na+     1        0.4090E-02        0.4090E-02
 sio2(aq)1        0.1276E-03        0.1276E-03
 so4-2   1        0.8313E-04        0.8313E-04
 fe+2    1        0.7166E-06        0.7166E-06
 hs-     1        0.3744E-06        0.3744E-06
 mn+2    1        0.2725E-05        0.2725E-05
 fe+3    1        0.7919E-06        0.7919E-06
 nh4+    1        0.2286E-04        0.2286E-04
 h2aso3- 1        0.3628E-05        0.3628E-05
 h2aso4- 1        0.2814E-05        0.2814E-05
 *       0        0.0000E+00        0.0000E+00

'-------------------------------------------------------------------------------'
'INITIAL MINERAL ZONES'
 total number of mineral zones=   1
 MINERAL ZONE=   1
'mineral          vol.frac.     msw33'
 calcite        0.9700E-01 equilibrium
 mackinawite    0.0000E+00 equilibrium
 orpiment       0.0000E+00 equilibrium
 albite         0.5600E-01 kinetic
  0.1000E-02  0.9800E+01    0
 annite         0.2030E+00 kinetic
  0.1000E-02  0.9800E+01    0
 illite         0.2040E+00 kinetic
  0.1000E-02  0.1516E+03    0
 k-feldspar     0.9000E-02 kinetic
  0.1000E-02  0.9800E+01    0
 quartz         0.1760E+00 kinetic
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  0.1000E-02  0.9800E+01    0
 montmor-na     0.8900E-01 kinetic
  0.1000E-02  0.1516E+03    0
 chlorite       0.1760E+00 kinetic
  0.1000E-02  0.9800E+01    0
 Sum of mineral volume fractions in zone: 0.1010E+01

'-------------------------------------------------------------------------------'
INITIAL GAS ZONES
 total number of gas zones=   1
 gas ZONE=   1
'gas      partial pressure'
'-------------------------------------------------------------------------------'
PERMEABILITY-POROSITY
 total number of permeability zones=   1
   1
'perm law     a-par     b-par'
   3           .00E+00               .00E+00
'-------------------------------------------------------------------------------'
INITIAL SURFACE ADSORPTION ZONES
 total number of adsorption zones=   0
'zone       ad.surf.(m2/kg)  total ad.sites (mol/l)'

'-------------------------------------------------------------------------------'
'INITIAL LINEAR EQUILIBRIUM Kd ZONES'
 total number of Kd zones=   1
 Kd ZONE=   1
'species   solid-density(Sden,kg/dm**3)  Kd(l/kg=mass/kg solid / mass/l'
 *              0.0000E+000.0000E+00
'-------------------------------------------------------------------------------'
'INITIAL ZONES OF CATION EXCHANGE'
 total number of cation-exchange zones=   1
'zone          ex. capacity'
   1           14.40
'-------------------------------------------------------------------------------'
 '------------------------------------------------------------------------------
 '
    --> read input data complete
```