ANEXO IV

ENSAYO DE EVOLUCIÓN HIDROQUÍMICA ASOCIADA A UN INCREMENTO DE PH: INTRODUCCIÓN DE ALCALINIDAD AL SISTEMA

-Cálculos de la modelización geoquímica mediante PHREEQC a diferentes pHs (4,6, 5,7, 7 y 8)

CÁLCULOS DE ESPECIACIÓN QUÍMICA DE METALES E ÍNDICES DE SATURACIÓN

Aznalcóllar, Noviembre de 2005 pH 4,6

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   Input file: C:\PHEEQC\MODELIZACIÓN\Especiación Aznalcóllar Noviembre 2005.pqi
  Output file: C:\PHEEQC\MODELIZACIÓN\Especiación Aznalcóllar Noviembre 2005.pqo
Database file: C:\Archivos de programa\USGS\Phreeqc Interactive 2.7.1\minteq.dat

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Reading data base.
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       SOLUTION_MASTER_SPECIES
       SOLUTION_SPECIES
       SOLUTION_SPECIES
       PHASES
       SURFACE_MASTER_SPECIES
       SURFACE_SPECIES
       END
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Reading input data for simulation 1.
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       DATABASE C:\Archivos de programa\USGS\Phreeqc Interactive 2.7.1\minteq.dat
       SOLUTION 1 Muestra superficial experimento subida de pH
           temp      21
           pH        4.6
           pe        11
           redox     pe
           units     mg/l
           density   1
           S(6)      7.98 g/l
           Al        86
           Fe(2)     0
           Fe(3)     0.5
           Zn        830
           Cu        36.2
           Mn        190
           K         17.5
           Na        69
           Ca        516
           Cd        1.64
           Ni        2.28
           O(0)      9.6
           As        67 ug/l
           Pb        466 ug/l
           U         36 ug/l
           water    1 # kg
       SOLUTION_MASTER_SPECIES
           Fe(2)         Fe+2            0     Fe
           Fe(3)         Fe+3           -2     Fe
           Mg            Mg+2            0     Mg             24.312
           Na            Na+             0     Na             22.9898
           Ca            Ca+2            0     Ca             40.08
           S             SO4-2           0     SO4            32.064
           S(6)          SO4-2           0     SO4
           K             K+              0     K              39.102
           Al            Al+3            0     Al             26.9815
       SOLUTION_SPECIES
       H2O = OH- + H+
           log_k     -14
           delta_h   13.362 kcal
       Fe+2 = Fe+3 + e-
           log_k     -13.02
           delta_h   9.68 kcal
       Fe+3 + H2O = FeOH+2 + H+
           log_k     -2.19
           delta_h   10.4 kcal
       H+ + SO4-2 = HSO4-
           log_k     1.988
           delta_h   3.85 kcal
       Al+3 + H2O = AlOH+2 + H+
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            log_k     -5
            delta_h   11.49 kcal
        Al+3 + 3H2O = Al(OH)3 + 3H+
            log_k     -16.9
            delta_h   39.89 kcal
        Al+3 + SO4-2 = AlSO4+
            log_k     3.5
            delta_h   2.29 kcal
        PHASES
        Jarosite-K
            KFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + K+ + 2SO4-2
            log_k     -14.8
            delta_h   -31.28 kcal
        Jarosite-Na
            NaFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + Na+ + 2SO4-2
            log_k     -11.2
            delta_h   -36.18 kcal
        Schwertmannite
            Fe8O8(OH)6(SO4) + 22H+ = 8Fe+3 + 14H2O + SO4-2
            log_k     7
        Ferrihydrite
            Fe(OH)3 + 3H+ = Fe+3 + 3H2O
            log_k     5
        Goethite
            FeOOH + 3H+ = Fe+3 + 2H2O
            log_k     0.5
            delta_h   -14.48 kcal
        Jurbanite
            AlOHSO4 + H+ = Al+3 + H2O + SO4-2
            log_k     -3.23
        Basaluminite
            Al4(OH)10SO4 + 10H+ = 4Al+3 + 10H2O + SO4-2
            log_k     22.7
        Alunite
            KAl3(SO4)2(OH)6 + 6H+ = 3Al+3 + 6H2O + K+ + 2SO4-2
            log_k     -1.3
            delta_h   3.918 kcal
        END
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Beginning of initial solution calculations.
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Initial solution 1.   Muestra superficial experimento subida de pH

-----------------------------Solution composition------------------------------

        Elements           Molality       Moles

        Al                3.219e-003  3.219e-003
        As                9.031e-007  9.031e-007
        Ca                1.300e-002  1.300e-002
        Cd                1.473e-005  1.473e-005
        Cu                5.753e-004  5.753e-004
        Fe(3)             9.041e-006  9.041e-006
        K                 4.519e-004  4.519e-004
        Mn                3.492e-003  3.492e-003
        Na                3.031e-003  3.031e-003
        Ni                3.922e-005  3.922e-005
        O(0)              6.059e-004  6.059e-004
        Pb                2.271e-006  2.271e-006
        S(6)              8.389e-002  8.389e-002
        U                 1.527e-007  1.527e-007
        Zn                1.282e-002  1.282e-002

----------------------------Description of solution----------------------------

                                       pH  =   4.600
                                       pe  =  11.000
                          Activity of water  =   0.998
                             Ionic strength  =  1.518e-001
                         Mass of water (kg)  =  1.000e+000
                 Total alkalinity (eq/kg)  = -4.763e-005
                    Total carbon (mol/kg)  =  0.000e+000
                       Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  21.000
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                  Electrical balance (eq)  = -9.468e-002
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -61.16
                                Iterations  =   9
                                   Total H  = 1.110126e+002
                                   Total O  = 5.584243e+001

--------------------------------Redox couples--------------------------------

       Redox couple             pe  Eh (volts)

       O(-2)/O(0)          16.3804      0.9560

----------------------------Distribution of species----------------------------

                                                    Log       Log         Log
       Species            Molality    Activity  Molality  Activity     Gamma

       H+               3.103e-005  2.512e-005    -4.508    -4.600    -0.092
       OH-              3.845e-010  2.925e-010    -9.415    -9.534    -0.119
       H2O              5.551e+001  9.984e-001     1.744    -0.001     0.000
Al              3.219e-003
       AlSO4+           2.045e-003  1.555e-003    -2.689    -2.808    -0.119
       Al(SO4)2-        9.438e-004  7.074e-004    -3.025    -3.150    -0.125
       Al+3             1.981e-004  2.961e-005    -3.703    -4.529    -0.826
       AlOH+2           2.700e-005  9.040e-006    -4.569    -5.044    -0.475
       Al(OH)2+         4.860e-006  3.715e-006    -5.313    -5.430    -0.117
       Al(OH)3          9.047e-009  9.369e-009    -8.044    -8.028     0.015
       Al(OH)4-         3.586e-010  2.688e-010    -9.445    -9.571    -0.125
As(3)           9.633e-021
       H3AsO3           9.633e-021  9.975e-021   -20.016   -20.001     0.015
       H2AsO3-          2.657e-025  2.021e-025   -24.576   -24.694    -0.119
       H4AsO3+          1.632e-025  1.241e-025   -24.787   -24.906    -0.119
       HAsO3-2          1.595e-032  5.338e-033   -31.797   -32.273    -0.475
       AsO3-3           0.000e+000  0.000e+000   -40.078   -41.147    -1.069
As(5)           9.031e-007
       H2AsO4-          8.866e-007  6.744e-007    -6.052    -6.171    -0.119
       HAsO4-2          1.376e-008  4.605e-009    -7.862    -8.337    -0.475
       H3AsO4           2.753e-009  2.851e-009    -8.560    -8.545     0.015
       AsO4-3           4.934e-015  4.206e-016   -14.307   -15.376    -1.069
Ca              1.300e-002
       CaSO4            7.253e-003  7.511e-003    -2.139    -2.124     0.015
       Ca+2             5.748e-003  2.178e-003    -2.240    -2.662    -0.421
       CaOH+            2.024e-011  1.565e-011   -10.694   -10.806    -0.112
Cd              1.473e-005
       CdSO4            6.587e-006  6.822e-006    -5.181    -5.166     0.015
       Cd+2             4.137e-006  1.385e-006    -5.383    -5.859    -0.475
       Cd(SO4)2-2       4.011e-006  1.343e-006    -5.397    -5.872    -0.475
       CdOH+            4.456e-012  3.389e-012   -11.351   -11.470    -0.119
       Cd2OH+3          2.836e-016  2.418e-017   -15.547   -16.617    -1.069
       Cd(OH)2          9.436e-018  9.771e-018   -17.025   -17.010     0.015
       Cd(OH)3-         5.729e-026  4.358e-026   -25.242   -25.361    -0.119
       Cd(OH)4-2        4.611e-035  1.544e-035   -34.336   -34.811    -0.475
Cu(1)           5.604e-013
       Cu+              5.604e-013  3.972e-013   -12.252   -12.401    -0.149
Cu(2)           5.753e-004
       Cu+2             3.113e-004  7.861e-005    -3.507    -4.105    -0.598
       CuSO4            2.639e-004  2.733e-004    -3.579    -3.563     0.015
       CuOH+            4.219e-008  3.124e-008    -7.375    -7.505    -0.130
       Cu(OH)2          2.505e-009  2.595e-009    -8.601    -8.586     0.015
       Cu2(OH)2+2       8.532e-010  2.856e-010    -9.069    -9.544    -0.475
       Cu(OH)3-         8.188e-018  6.228e-018   -17.087   -17.206    -0.119
       Cu(OH)4-2        1.472e-025  4.928e-026   -24.832   -25.307    -0.475
Fe(3)           9.041e-006
       Fe(OH)2+         7.527e-006  5.754e-006    -5.123    -5.240    -0.117
       FeOH+2           1.029e-006  3.444e-007    -5.988    -6.463    -0.475
       FeSO4+           2.992e-007  2.268e-007    -6.524    -6.644    -0.120
       Fe(SO4)2-        1.625e-007  1.236e-007    -6.789    -6.908    -0.119
       Fe+3             1.999e-008  1.704e-009    -7.699    -8.769    -1.069
       Fe(OH)3          2.595e-009  2.687e-009    -8.586    -8.571     0.015
       Fe2(OH)2+4       3.005e-010  3.774e-012    -9.522   -11.423    -1.901
       Fe3(OH)4+5       4.161e-012  4.454e-015   -11.381   -14.351    -2.970
       Fe(OH)4-         1.397e-012  1.068e-012   -11.855   -11.971    -0.117
H(0)            8.982e-035
       H2               4.491e-035  4.651e-035   -34.348   -34.332     0.015
K               4.519e-004
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	K+	4.077e-004	2.952e-004	-3.390	-3.530	-0.140
	KSO4-	4.426e-005	3.383e-005	-4.354	-4.471	-0.117
Mn(2)		3.492e-003				
	MnSO4	1.786e-003	1.850e-003	-2.748	-2.733	0.015
	Mn+2	1.706e-003	6.102e-004	-2.768	-3.214	-0.446
	MnOH+	5.910e-010	4.480e-010	-9.228	-9.349	-0.120
	Mn(OH)3-	8.011e-025	6.073e-025	-24.096	-24.217	-0.120
Mn(3)		2.295e-017				
	Mn+3	2.295e-017	3.430e-018	-16.639	-17.465	-0.826
Mn(6)		0.000e+000				
	MnO4-2	0.000e+000	0.000e+000	-41.871	-42.353	-0.481
Mn(7)		0.000e+000				
	MnO4-	0.000e+000	0.000e+000	-40.859	-41.002	-0.143
Na		3.031e-003				
	Na+	2.793e-003	2.123e-003	-2.554	-2.673	-0.119
	NaSO4-	2.376e-004	1.816e-004	-3.624	-3.741	-0.117
Ni		3.922e-005				
	NiSO4	2.020e-005	2.092e-005	-4.695	-4.679	0.015
	Ni+2	1.895e-005	6.345e-006	-4.722	-5.198	-0.475
	Ni(SO4)2-2	6.085e-008	2.037e-008	-7.216	-7.691	-0.475
	NiOH+	3.442e-011	2.618e-011	-10.463	-10.582	-0.119
	Ni(OH)2	9.679e-016	1.002e-015	-15.014	-14.999	0.015
	Ni(OH)3-	5.238e-022	3.984e-022	-21.281	-21.400	-0.119
O(0)		6.059e-004				
	O2	3.030e-004	3.137e-004	-3.519	-3.503	0.015
Pb		2.271e-006				
	PbSO4	1.421e-006	1.471e-006	-5.847	-5.832	0.015
	Pb+2	4.464e-007	1.494e-007	-6.350	-6.826	-0.475
	Pb(SO4)2-2	4.039e-007	1.352e-007	-6.394	-6.869	-0.475
	PbOH+	1.522e-010	1.158e-010	-9.817	-9.936	-0.119
	Pb2OH+3	4.545e-015	3.874e-016	-14.342	-15.412	-1.069
	Pb(OH)2	1.729e-015	1.791e-015	-14.762	-14.747	0.015
	Pb(OH)3-	1.074e-021	8.172e-022	-20.969	-21.088	-0.119
	Pb3(OH)4+2	1.785e-026	5.975e-027	-25.748	-26.224	-0.475
	Pb(OH)4-2	2.228e-028	7.458e-029	-27.652	-28.127	-0.475
S(6)		8.389e-002				
	SO4-2	5.906e-002	1.751e-002	-1.229	-1.757	-0.528
	CaSO4	7.253e-003	7.511e-003	-2.139	-2.124	0.015
	ZnSO4	5.876e-003	6.085e-003	-2.231	-2.216	0.015
	Zn(SO4)2-2	2.669e-003	8.936e-004	-2.574	-3.049	-0.475
	AlSO4+	2.045e-003	1.555e-003	-2.689	-2.808	-0.119
	MnSO4	1.786e-003	1.850e-003	-2.748	-2.733	0.015
	Al(SO4)2-	9.438e-004	7.074e-004	-3.025	-3.150	-0.125
	CuSO4	2.639e-004	2.733e-004	-3.579	-3.563	0.015
	NaSO4-	2.376e-004	1.816e-004	-3.624	-3.741	-0.117
	HSO4-	5.149e-005	3.917e-005	-4.288	-4.407	-0.119
	KSO4-	4.426e-005	3.383e-005	-4.354	-4.471	-0.117
	NiSO4	2.020e-005	2.092e-005	-4.695	-4.679	0.015
	CdSO4	6.587e-006	6.822e-006	-5.181	-5.166	0.015
	Cd(SO4)2-2	4.011e-006	1.343e-006	-5.397	-5.872	-0.475
	PbSO4	1.421e-006	1.471e-006	-5.847	-5.832	0.015
	Pb(SO4)2-2	4.039e-007	1.352e-007	-6.394	-6.869	-0.475
	FeSO4+	2.992e-007	2.268e-007	-6.524	-6.644	-0.120
	Fe(SO4)2-	1.625e-007	1.236e-007	-6.789	-6.908	-0.119
	UO2(SO4)2-2	8.004e-008	2.680e-008	-7.097	-7.572	-0.475
	Ni(SO4)2-2	6.085e-008	2.037e-008	-7.216	-7.691	-0.475
	UO2SO4	5.076e-008	5.257e-008	-7.294	-7.279	0.015
	U(SO4)2	1.332e-033	1.379e-033	-32.875	-32.860	0.015
	USO4+2	1.326e-035	4.439e-036	-34.877	-35.353	-0.475
U(3)		0.000e+000				
	U+3	0.000e+000	0.000e+000	-57.990	-59.059	-1.069
U(4)		9.718e-030				
	U(OH)5-	5.015e-030	3.815e-030	-29.300	-29.419	-0.119
	U(OH)4	4.141e-030	4.288e-030	-29.383	-29.368	0.015
	U(OH)3+	5.443e-031	4.140e-031	-30.264	-30.383	-0.119
	U(OH)2+2	1.611e-032	5.392e-033	-31.793	-32.268	-0.475
	U(SO4)2	1.332e-033	1.379e-033	-32.875	-32.860	0.015
	UOH+3	7.444e-035	6.345e-036	-34.128	-35.198	-1.069
	USO4+2	1.326e-035	4.439e-036	-34.877	-35.353	-0.475
	U+4	7.602e-038	9.548e-040	-37.119	-39.020	-1.901
	U6(OH)15+9	0.000e+000	0.000e+000	-172.736	-182.360	-9.624
U(5)		5.702e-017				
	UO2+	5.702e-017	4.337e-017	-16.244	-16.363	-0.119
U(6)		1.527e-007				
	UO2(SO4)2-2	8.004e-008	2.680e-008	-7.097	-7.572	-0.475

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        UO2SO4           5.076e-008  5.257e-008    -7.294    -7.279     0.015
        UO2+2            1.970e-008  6.596e-009    -7.705    -8.181    -0.475
        UO2OH+           2.216e-009  1.686e-009    -8.654    -8.773    -0.119
        (UO2)2(OH)2+2    3.677e-013  1.231e-013   -12.435   -12.910    -0.475
        (UO2)3(OH)5+     5.373e-018  4.087e-018   -17.270   -17.389    -0.119
Zn              1.282e-002
        ZnSO4            5.876e-003  6.085e-003    -2.231    -2.216     0.015
        Zn+2             4.276e-003  1.530e-003    -2.369    -2.815    -0.446
        Zn(SO4)2-2       2.669e-003  8.936e-004    -2.574    -3.049    -0.475
        ZnOH+            6.443e-008  4.901e-008    -7.191    -7.310    -0.119
        Zn(OH)2          2.944e-011  3.049e-011   -10.531   -10.516     0.015
        Zn(OH)3-         5.038e-018  3.832e-018   -17.298   -17.417    -0.119
        Zn(OH)4-2        7.211e-026  2.414e-026   -25.142   -25.617    -0.475

-----------------------------Saturation indices-------------------------------

        Phase               SI log IAP  log KT

        Al(OH)3(a)       -1.38    9.27   10.65  Al(OH)3
        Al2O3            -4.44   18.54   22.98  Al2O3
        Al4(OH)10SO4      3.42   26.12   22.70  Al4(OH)10SO4
        AlAsO4:2H2O      -4.07    0.73    4.80  AlAsO4:2H2O
        AlOHSO4           1.54   -1.69   -3.23  AlOHSO4
        AlumK            -6.34  -11.58   -5.24  KAl(SO4)2:12H2O
        Alunite           8.31    6.97   -1.34  KAl3(SO4)2(OH)6
        Anglesite        -0.77   -8.58   -7.81  PbSO4
        Anhydrite         0.18   -4.42   -4.60  CaSO4
        Antlerite        -3.96    4.33    8.29  Cu3(OH)4SO4
        Arsenolite      -77.06 -158.97  -81.92  As4O6
        As2O5           -23.84  -17.09    6.75  As2O5
        B_UO2(OH)2       -4.66    1.02    5.68  UO2(OH)2
        Basaluminite      3.42   26.12   22.70  Al4(OH)10SO4
        Bianchite        -2.81   -4.58   -1.76  ZnSO4:6H2O
        Birnessite       -6.16   37.18   43.34  MnO2
        Bixbyite         -6.87   43.17   50.04  Mn2O3
        Boehmite          0.41    9.27    8.86  AlOOH
        Brochantite      -5.92    9.42   15.34  Cu4(OH)6SO4
        Bunsenite        -8.69    4.00   12.69  NiO
        Ca3(AsO4)2:6H2O -19.78    2.52   22.30  Ca3(AsO4)2:6H2O
        Cd(Gamma)       -41.63  -27.86   13.77  Cd
        Cd(OH)2(A)      -10.60    3.34   13.94  Cd(OH)2
        Cd(OH)2(C)      -10.31    3.34   13.65  Cd(OH)2
        Cd3(OH)2(SO4)2  -18.60  -11.89    6.71  Cd3(OH)2(SO4)2
        Cd3(OH)4SO4     -23.50   -0.94   22.56  Cd3(OH)4SO4
        Cd4(OH)6SO4     -26.00    2.40   28.40  Cd4(OH)6SO4
        CdMetal         -41.53  -27.86   13.67  Cd
        CdSO4            -7.66   -7.62    0.05  CdSO4
        CdSO4:2.67H2O    -5.79   -7.62   -1.83  CdSO4:2.67H2O
        CdSO4:H2O        -6.03   -7.62   -1.58  CdSO4:H2O
        Chalcanthite     -3.21   -5.86   -2.65  CuSO4:5H2O
        Claudetite      -76.80 -158.97  -82.17  As4O6
        Cu(OH)2          -3.70    5.09    8.79  Cu(OH)2
        Cu2SO4          -24.65  -31.97   -7.31  Cu2SO4
        Cu3(AsO4)2:6H2O  -7.91   -1.81    6.10  Cu3(AsO4)2:6H2O
        CuMetal         -14.47  -26.10  -11.63  Cu
        CuOCuSO4        -12.65   -0.77   11.88  CuO:CuSO4
        CupricFerrite     8.89   15.16    6.27  CuFe2O4
        Cuprite         -13.99  -21.01   -7.02  Cu2O
        CuprousFerrite    6.11   -5.47  -11.59  CuFeO2
        CuSO4             -9.05   -5.86    3.19  CuSO4
        Diaspore           2.15    9.27    7.12  AlOOH
        Fe2(SO4)3        -26.98  -22.81    4.17  Fe2(SO4)3
        FeAsO4:2H2O       -3.91   -3.51    0.40  FeAsO4:2H2O
        Ferrihydrite       0.03    5.03    5.00  Fe(OH)3
        Gibbsite(C)        0.27    9.27    9.00  Al(OH)3
        Goethite           4.39    5.03    0.64  FeOOH
        Goslarite         -2.58   -4.58   -1.99  ZnSO4:7H2O
        Gummite           -9.61    1.02   10.63  UO3
        Gypsum             0.43   -4.42   -4.85  CaSO4:2H2O
        Hausmannite      -13.19   49.15   62.34  Mn3O4
        Hematite          13.76   10.06   -3.70  Fe2O3
        Jarosite-H         4.73   -6.82  -11.55  (H3O)Fe3(SO4)2(OH)6
        Jarosite-K         8.73   -5.75  -14.49  KFe3(SO4)2(OH)6
        Jarosite-Na        5.94   -4.90  -10.84  NaFe3(SO4)2(OH)6
        Jurbanite          1.54   -1.69   -3.23  AlOHSO4
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        Langite          -7.76    9.42   17.18  Cu4(OH)6SO4:H2O
        Larnakite        -5.99   -6.21   -0.22  PbO:PbSO4
        Lepidocrocite     3.66    5.03    1.37  FeOOH
        Lime            -26.72    6.54   33.26  CaO
        Litharge        -10.51    2.37   12.88  PbO
        Maghemite         3.67   10.06    6.39  Fe2O3
        Manganite        -3.43   21.58   25.01  MnOOH
        Massicot        -10.70    2.37   13.08  PbO
        Minium          -36.39   38.32   74.71  Pb3O4
        Mirabilite       -5.81   -7.11   -1.30  Na2SO4:10H2O
        Mn2(SO4)3       -34.88   10.30   45.18  Mn2(SO4)3
        Mn3(AsO4)2:8H2O -11.64    0.86   12.50  Mn3(AsO4)2:8H2O
        MnSO4            -7.79   -4.97    2.82  MnSO4
        Monteponite     -12.03    3.34   15.37  CdO
        Morenosite       -4.57   -6.96   -2.39  NiSO4:7H2O
        Ni(OH)2          -6.50    4.00   10.50  Ni(OH)2
        Ni3(AsO4)2:8H2O -20.79   -5.09   15.70  Ni3(AsO4)2:8H2O
        Ni4(OH)6SO4     -26.95    5.05   32.00  Ni4(OH)6SO4
        Nsutite          -5.57   37.18   42.75  MnO2
        O2(g)           -22.06   62.40   84.45  O2
        Pb(OH)2(C)       -5.92    2.37    8.29  Pb(OH)2
        Pb2O(OH)2       -21.45    4.75   26.20  Pb2O(OH)2
        Pb2O3           -25.09   35.95   61.04  Pb2O3
        Pb3(AsO4)2      -15.77   -9.97    5.80  Pb3(AsO4)2
        Pb3O2SO4        -14.44   -3.83   10.61  Pb3O2SO4
        Pb4(OH)6SO4     -22.56   -1.46   21.10  Pb4(OH)6SO4
        Pb4O3SO4        -23.91   -1.46   22.45  Pb4O3SO4
        PbMetal         -33.09  -28.83    4.27  Pb
        PbO:0.3H2O      -10.61    2.37   12.98  PbO:0.33H2O
        Plattnerite     -16.43   33.57   50.01  PbO2
        Portlandite     -16.44    6.54   22.98  Ca(OH)2
        Pyrocroite       -9.33    5.98   15.31  Mn(OH)2
        Pyrolusite       -4.22   37.18   41.40  MnO2
        Retgersite       -4.91   -6.96   -2.05  NiSO4:6H2O
        Schoepite        -4.51    1.02    5.52  UO2(OH)2:H2O
        Schwertmannite   22.28   29.28    7.00  Fe8O8(OH)6(SO4)
        Tenorite         -2.68    5.09    7.77  CuO
        Thenardite       -6.93   -7.10   -0.17  Na2SO4
        U3O8(C)         -21.73  -28.14   -6.41  U3O8
        U4O9(C)         -48.91  -89.52  -40.61  U4O9
        UO2(am)         -21.82  -30.18   -8.36  UO2
        UO3(C)           -6.89    1.02    7.91  UO3
        Uraninite       -16.11  -30.18  -14.07  UO2
        Zincite          -4.97    6.38   11.36  ZnO
        Zincosite        -7.77   -4.57    3.20  ZnSO4
        Zn(OH)2(A)       -6.07    6.38   12.45  Zn(OH)2
        Zn(OH)2(B)       -5.37    6.38   11.75  Zn(OH)2
        Zn(OH)2(C)       -5.82    6.38   12.20  Zn(OH)2
        Zn(OH)2(E)       -5.12    6.38   11.50  Zn(OH)2
        Zn(OH)2(G)       -5.33    6.38   11.71  Zn(OH)2
        Zn2(OH)2SO4      -5.69    1.81    7.50  Zn2(OH)2SO4
        Zn3(AsO4)2:2.5H2O -11.59    2.06   13.65  Zn3(AsO4)2:2.5H2O
        Zn3O(SO4)2      -22.40   -2.76   19.64  Zn3O(SO4)2
        Zn4(OH)6SO4     -13.82   14.58   28.40  Zn4(OH)6SO4
        ZnMetal         -50.94  -24.82   26.12  Zn
        ZnO(Active)      -4.93    6.38   11.31  ZnO
        ZnSO4:H2O        -4.11   -4.57   -0.46  ZnSO4:H2O

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End of simulation.
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Reading input data for simulation 2.
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End of run.
```

Aznalcóllar, Noviembre de 2005 a pH 5,7

```
Input file: C:\PHEEQC\MODELIZACIÓN\Especiación Aznalcóllar Noviembre 2005.pqi
Output file: C:\PHEEQC\MODELIZACIÓN\Noviembre 2005pH5.7.pqo
Database file: C:\Archivos de programa\USGS\Phreeqc Interactive 2.7.1\minteq.dat

------------------
Reading data base.
------------------

       SOLUTION_MASTER_SPECIES
       SOLUTION_SPECIES
       SOLUTION_SPECIES
       PHASES
       SURFACE_MASTER_SPECIES
       SURFACE_SPECIES
       END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

       DATABASE C:\Archivos de programa\USGS\Phreeqc Interactive 2.7.1\minteq.dat
       SOLUTION 1 Muestra superficial experimento subida de pH
           temp      21
           pH        5.7
           pe        11
           redox     pe
           units     mg/l
           density   1
           S(6)      7.98 g/l
           Al        86
           Fe(2)     0
           Fe(3)     0.5
           Zn        830
           Cu        36.2
           Mn        190
           K         17.5
           Na        69
           Ca        516
           Cd        1.64
           Ni        2.28
           O(0)      9.6
           As        67 ug/l
           Pb        466 ug/l
           U         36 ug/l
           water    1 # kg
       SOLUTION_MASTER_SPECIES
           Fe(2)         Fe+2            0     Fe
           Fe(3)         Fe+3           -2     Fe
           Mg            Mg+2            0     Mg              24.312
           Na            Na+             0     Na              22.9898
           Ca            Ca+2            0     Ca              40.08
           S             SO4-2           0     SO4             32.064
           S(6)          SO4-2           0     SO4
           K             K+              0     K               39.102
           Al            Al+3            0     Al              26.9815
       SOLUTION_SPECIES
       H2O = OH- + H+
           log_k     -14
           delta_h   13.362 kcal
       Fe+2 = Fe+3 + e-
           log_k     -13.02
           delta_h   9.68 kcal
       Fe+3 + H2O = FeOH+2 + H+
           log_k     -2.19
           delta_h   10.4 kcal
       H+ + SO4-2 = HSO4-
           log_k     1.988
           delta_h   3.85 kcal
       Al+3 + H2O = AlOH+2 + H+
           log_k     -5
           delta_h   11.49 kcal
       Al+3 + 3H2O = Al(OH)3 + 3H+
           log_k     -16.9
```

```
            delta_h   39.89 kcal
        Al+3 + SO4-2 = AlSO4+
            log_k     3.5
            delta_h   2.29 kcal
        PHASES
        Jarosite-K
            KFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + K+ + 2SO4-2
            log_k     -14.8
            delta_h   -31.28 kcal
        Jarosite-Na
            NaFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + Na+ + 2SO4-2
            log_k     -11.2
            delta_h   -36.18 kcal
        Schwertmannite
            Fe8O8(OH)6(SO4) + 22H+ = 8Fe+3 + 14H2O + SO4-2
            log_k     7
        Ferrihydrite
            Fe(OH)3 + 3H+ = Fe+3 + 3H2O
            log_k     5
        Goethite
            FeOOH + 3H+ = Fe+3 + 2H2O
            log_k     0.5
            delta_h   -14.48 kcal
        Jurbanite
            AlOHSO4 + H+ = Al+3 + H2O + SO4-2
            log_k     -3.23
        Basaluminite
            Al4(OH)10SO4 + 10H+ = 4Al+3 + 10H2O + SO4-2
            log_k     22.7
        Alunite
            KAl3(SO4)2(OH)6 + 6H+ = 3Al+3 + 6H2O + K+ + 2SO4-2
            log_k     -1.3
            delta_h   3.918 kcal
        END
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.   Muestra superficial experimento subida de pH

-----------------------------Solution composition------------------------------

        Elements           Molality       Moles

        Al               3.219e-003  3.219e-003
        As               9.031e-007  9.031e-007
        Ca               1.300e-002  1.300e-002
        Cd               1.473e-005  1.473e-005
        Cu               5.753e-004  5.753e-004
        Fe(3)            9.041e-006  9.041e-006
        K                4.519e-004  4.519e-004
        Mn               3.492e-003  3.492e-003
        Na               3.031e-003  3.031e-003
        Ni               3.922e-005  3.922e-005
        O(0)             6.059e-004  6.059e-004
        Pb               2.271e-006  2.271e-006
        S(6)             8.389e-002  8.389e-002
        U                1.527e-007  1.527e-007
        Zn               1.282e-002  1.282e-002

----------------------------Description of solution----------------------------

                                    pH  =   5.700
                                    pe  =  11.000
                       Activity of water  =   0.998
                          Ionic strength  =  1.537e-001
                      Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  1.449e-003
                   Total carbon (mol/kg)  =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  21.000
                  Electrical balance (eq)  = -9.618e-002
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -61.39
                               Iterations  =  13
                                  Total H  = 1.110139e+002
```

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                                  Total O  = 5.584385e+001

---------------------------------Redox couples---------------------------------

       Redox couple             pe  Eh (volts)

       O(-2)/O(0)          15.2804      0.8918

----------------------------Distribution of species----------------------------

                                                    Log       Log         Log
       Species            Molality    Activity  Molality  Activity     Gamma

       H+               2.466e-006  1.995e-006    -5.608    -5.700    -0.092
       OH-              4.845e-009  3.682e-009    -8.315    -8.434    -0.119
       H2O              5.551e+001  9.984e-001     1.744    -0.001     0.000
Al              3.219e-003
       AlSO4+           1.523e-003  1.157e-003    -2.817    -2.937    -0.119
       Al(SO4)2-        7.105e-004  5.320e-004    -3.148    -3.274    -0.126
       Al(OH)2+         5.677e-004  4.335e-004    -3.246    -3.363    -0.117
       AlOH+2           2.511e-004  8.379e-005    -3.600    -4.077    -0.477
       Al+3             1.467e-004  2.180e-005    -3.834    -4.662    -0.828
       Al(OH)3          1.328e-005  1.376e-005    -4.877    -4.861     0.015
       Al(OH)4-         6.639e-006  4.970e-006    -5.178    -5.304    -0.126
As(3)           4.108e-024
       H3AsO3           4.107e-024  4.255e-024   -23.387   -23.371     0.015
       H2AsO3-          1.428e-027  1.085e-027   -26.845   -26.965    -0.119
       H4AsO3+          5.534e-030  4.206e-030   -29.257   -29.376    -0.119
       HAsO3-2          1.081e-033  3.608e-034   -32.966   -33.443    -0.477
       AsO3-3           0.000e+000  0.000e+000   -40.145   -41.217    -1.072
As(5)           9.031e-007
       H2AsO4-          7.550e-007  5.739e-007    -6.122    -6.241    -0.119
       HAsO4-2          1.478e-007  4.933e-008    -6.830    -7.307    -0.477
       H3AsO4           1.860e-010  1.927e-010    -9.730    -9.715     0.015
       AsO4-3           6.703e-013  5.672e-014   -12.174   -13.246    -1.072
Ca              1.300e-002
       CaSO4            7.276e-003  7.538e-003    -2.138    -2.123     0.015
       Ca+2             5.725e-003  2.163e-003    -2.242    -2.665    -0.423
       CaOH+            2.532e-010  1.956e-010    -9.597    -9.709    -0.112
Cd              1.473e-005
       CdSO4            6.574e-006  6.811e-006    -5.182    -5.167     0.015
       Cd+2             4.100e-006  1.368e-006    -5.387    -5.864    -0.477
       Cd(SO4)2-2       4.060e-006  1.355e-006    -5.391    -5.868    -0.477
       CdOH+            5.546e-011  4.215e-011   -10.256   -10.375    -0.119
       Cd2OH+3          3.510e-015  2.971e-016   -14.455   -15.527    -1.072
       Cd(OH)2          1.477e-015  1.530e-015   -14.831   -14.815     0.015
       Cd(OH)3-         1.130e-022  8.589e-023   -21.947   -22.066    -0.119
       Cd(OH)4-2        1.148e-030  3.830e-031   -29.940   -30.417    -0.477
Cu(1)           5.556e-013
       Cu+              5.556e-013  3.932e-013   -12.255   -12.405    -0.150
Cu(2)           5.753e-004
       Cu+2             3.102e-004  7.781e-005    -3.508    -4.109    -0.601
       CuSO4            2.639e-004  2.734e-004    -3.579    -3.563     0.015
       CuOH+            5.265e-007  3.893e-007    -6.279    -6.410    -0.131
       Cu(OH)2          3.929e-007  4.070e-007    -6.406    -6.390     0.015
       Cu2(OH)2+2       1.329e-007  4.435e-008    -6.876    -7.353    -0.477
       Cu(OH)3-         1.618e-014  1.230e-014   -13.791   -13.910    -0.119
       Cu(OH)4-2        3.672e-021  1.225e-021   -20.435   -20.912    -0.477
Fe(3)           9.041e-006
       Fe(OH)2+         8.902e-006  6.798e-006    -5.051    -5.168    -0.117
       FeOH+2           9.684e-008  3.232e-008    -7.014    -7.491    -0.477
       Fe(OH)3          3.857e-008  3.996e-008    -7.414    -7.398     0.015
       FeSO4+           2.257e-009  1.709e-009    -8.647    -8.767    -0.121
       Fe(SO4)2-        1.238e-009  9.413e-010    -8.907    -9.026    -0.119
       Fe(OH)4-         2.618e-010  2.000e-010    -9.582    -9.699    -0.117
       Fe+3             1.501e-010  1.270e-011    -9.824   -10.896    -1.072
       Fe2(OH)2+4       2.681e-012  3.323e-014   -11.572   -13.478    -1.907
       Fe3(OH)4+5       4.417e-014  4.634e-017   -13.355   -16.334    -2.979
H(0)            5.665e-037
       H2               2.832e-037  2.934e-037   -36.548   -36.532     0.015
K               4.519e-004
       K+               4.073e-004  2.945e-004    -3.390    -3.531    -0.141
       KSO4-            4.467e-005  3.411e-005    -4.350    -4.467    -0.117
Mn(2)           3.492e-003
       MnSO4            1.792e-003  1.857e-003    -2.747    -2.731     0.015
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        Mn+2            1.700e-003  6.060e-004    -2.769    -3.218    -0.448
        MnOH+           7.396e-009  5.601e-009    -8.131    -8.252    -0.121
        Mn(OH)3-        1.589e-021  1.203e-021   -20.799   -20.920    -0.121
Mn(3)           2.292e-017
        Mn+3            2.292e-017  3.406e-018   -16.640   -17.468    -0.828
Mn(6)           8.461e-034
        MnO4-2          8.461e-034  2.782e-034   -33.073   -33.556    -0.483
Mn(7)           8.676e-033
        MnO4-           8.676e-033  6.239e-033   -32.062   -32.205    -0.143
Na              3.031e-003
        Na+             2.791e-003  2.120e-003    -2.554    -2.674    -0.120
        NaSO4-          2.399e-004  1.832e-004    -3.620    -3.737    -0.117
Ni              3.922e-005
        NiSO4           2.027e-005  2.100e-005    -4.693    -4.678     0.015
        Ni+2            1.889e-005  6.302e-006    -4.724    -5.201    -0.477
        Ni(SO4)2-2      6.193e-008  2.067e-008    -7.208    -7.685    -0.477
        NiOH+           4.306e-010  3.273e-010    -9.366    -9.485    -0.119
        Ni(OH)2         1.523e-013  1.578e-013   -12.817   -12.802     0.015
        Ni(OH)3-        1.039e-018  7.894e-019   -17.984   -18.103    -0.119
O(0)            6.059e-004
        O2              3.030e-004  3.139e-004    -3.519    -3.503     0.015
Pb              2.271e-006
        PbSO4           1.418e-006  1.469e-006    -5.848    -5.833     0.015
        Pb+2            4.424e-007  1.476e-007    -6.354    -6.831    -0.477
        Pb(SO4)2-2      4.089e-007  1.364e-007    -6.388    -6.865    -0.477
        PbOH+           1.895e-009  1.440e-009    -8.722    -8.842    -0.119
        Pb(OH)2         2.706e-013  2.804e-013   -12.568   -12.552     0.015
        Pb2OH+3         5.625e-014  4.760e-015   -13.250   -14.322    -1.072
        Pb(OH)3-        2.119e-018  1.611e-018   -17.674   -17.793    -0.119
        Pb3(OH)4+2      4.337e-022  1.447e-022   -21.363   -21.839    -0.477
        Pb(OH)4-2       5.546e-024  1.851e-024   -23.256   -23.733    -0.477
S(6)            8.389e-002
        SO4-2           6.000e-002  1.770e-002    -1.222    -1.752    -0.530
        CaSO4           7.276e-003  7.538e-003    -2.138    -2.123     0.015
        ZnSO4           5.871e-003  6.083e-003    -2.231    -2.216     0.015
        Zn(SO4)2-2      2.705e-003  9.027e-004    -2.568    -3.044    -0.477
        MnSO4           1.792e-003  1.857e-003    -2.747    -2.731     0.015
        AlSO4+          1.523e-003  1.157e-003    -2.817    -2.937    -0.119
        Al(SO4)2-       7.105e-004  5.320e-004    -3.148    -3.274    -0.126
        CuSO4           2.639e-004  2.734e-004    -3.579    -3.563     0.015
        NaSO4-          2.399e-004  1.832e-004    -3.620    -3.737    -0.117
        KSO4-           4.467e-005  3.411e-005    -4.350    -4.467    -0.117
        NiSO4           2.027e-005  2.100e-005    -4.693    -4.678     0.015
        CdSO4           6.574e-006  6.811e-006    -5.182    -5.167     0.015
        HSO4-           4.137e-006  3.144e-006    -5.383    -5.502    -0.119
        Cd(SO4)2-2      4.060e-006  1.355e-006    -5.391    -5.868    -0.477
        PbSO4           1.418e-006  1.469e-006    -5.848    -5.833     0.015
        Pb(SO4)2-2      4.089e-007  1.364e-007    -6.388    -6.865    -0.477
        UO2(SO4)2-2     6.917e-008  2.308e-008    -7.160    -7.637    -0.477
        Ni(SO4)2-2      6.193e-008  2.067e-008    -7.208    -7.685    -0.477
        UO2SO4          4.325e-008  4.481e-008    -7.364    -7.349     0.015
        FeSO4+          2.257e-009  1.709e-009    -8.647    -8.767    -0.121
        Fe(SO4)2-       1.238e-009  9.413e-010    -8.907    -9.026    -0.119
        U(SO4)2         4.566e-038  4.731e-038   -37.340   -37.325     0.015
        USO4+2          4.514e-040  1.506e-040   -39.345   -39.822    -0.477
U(3)            0.000e+000
        U+3             0.000e+000  0.000e+000   -62.461   -63.533    -1.072
U(4)            5.682e-029
        U(OH)5-         5.329e-029  4.050e-029   -28.273   -28.393    -0.119
        U(OH)4          3.491e-030  3.616e-030   -29.457   -29.442     0.015
        U(OH)3+         3.649e-032  2.774e-032   -31.438   -31.557    -0.119
        U(OH)2+2        8.599e-035  2.869e-035   -34.066   -34.542    -0.477
        U(SO4)2         4.566e-038  4.731e-038   -37.340   -37.325     0.015
        UOH+3           3.169e-038  2.682e-039   -37.499   -38.572    -1.072
        USO4+2          4.514e-040  1.506e-040   -39.345   -39.822    -0.477
        U+4             0.000e+000  0.000e+000   -41.587   -43.494    -1.907
        U6(OH)15+9      0.000e+000  0.000e+000  -183.052  -192.704    -9.652
U(5)            4.812e-017
        UO2+            4.812e-017  3.658e-017   -16.318   -16.437    -0.119
U(6)            1.527e-007
        UO2(SO4)2-2     6.917e-008  2.308e-008    -7.160    -7.637    -0.477
        UO2SO4          4.325e-008  4.481e-008    -7.364    -7.349     0.015
        UO2OH+          2.355e-008  1.790e-008    -7.628    -7.747    -0.119
        UO2+2           1.667e-008  5.563e-009    -7.778    -8.255    -0.477
        (UO2)2(OH)2+2   4.158e-011  1.387e-011   -10.381   -10.858    -0.477
```

```
        (UO2)3(OH)5+     1.020e-012  7.752e-013   -11.991   -12.111    -0.119
Zn              1.282e-002
        ZnSO4            5.871e-003  6.083e-003    -2.231    -2.216     0.015
        Zn+2             4.245e-003  1.513e-003    -2.372    -2.820    -0.448
        Zn(SO4)2-2       2.705e-003  9.027e-004    -2.568    -3.044    -0.477
        ZnOH+            8.029e-007  6.102e-007    -6.095    -6.215    -0.119
        Zn(OH)2          4.613e-009  4.779e-009    -8.336    -8.321     0.015
        Zn(OH)3-         9.949e-015  7.562e-015   -14.002   -14.121    -0.119
        Zn(OH)4-2        1.797e-021  5.997e-022   -20.745   -21.222    -0.477

------------------------------Saturation indices-------------------------------

        Phase               SI log IAP  log KT

        Al(OH)3(a)        1.79   12.44   10.65  Al(OH)3
        Al2O3             1.89   24.87   22.98  Al2O3
        Al4(OH)10SO4     13.89   36.59   22.70  Al4(OH)10SO4
        AlAsO4:2H2O      -2.08    2.72    4.80  AlAsO4:2H2O
        AlOHSO4           2.52   -0.71   -3.23  AlOHSO4
        AlumK            -6.46  -11.71   -5.24  KAl(SO4)2:12H2O
        Alunite          14.51   13.18   -1.34  KAl3(SO4)2(OH)6
        Anglesite        -0.77   -8.58   -7.81  PbSO4
        Anhydrite         0.18   -4.42   -4.60  CaSO4
        Antlerite         0.43    8.72    8.29  Cu3(OH)4SO4
        Arsenolite      -90.54 -172.45  -81.92  As4O6
        As2O5           -26.18  -19.43    6.75  As2O5
        B_UO2(OH)2       -2.54    3.14    5.68  UO2(OH)2
        Basaluminite     13.89   36.59   22.70  Al4(OH)10SO4
        Bianchite        -2.81   -4.58   -1.76  ZnSO4:6H2O
        Birnessite       -1.76   41.58   43.34  MnO2
        Bixbyite         -0.28   49.76   50.04  Mn2O3
        Boehmite          3.58   12.44    8.86  AlOOH
        Brochantite       0.67   16.01   15.34  Cu4(OH)6SO4
        Bunsenite        -6.49    6.20   12.69  NiO
        Ca3(AsO4)2:6H2O -15.53    6.77   22.30  Ca3(AsO4)2:6H2O
        Cd(Gamma)       -41.63  -27.86   13.77  Cd
        Cd(OH)2(A)       -8.40    5.53   13.94  Cd(OH)2
        Cd(OH)2(C)       -8.12    5.53   13.65  Cd(OH)2
        Cd3(OH)2(SO4)2  -16.41   -9.70    6.71  Cd3(OH)2(SO4)2
        Cd3(OH)4SO4     -19.11    3.45   22.56  Cd3(OH)4SO4
        Cd4(OH)6SO4     -19.41    8.99   28.40  Cd4(OH)6SO4
        CdMetal         -41.53  -27.86   13.67  Cd
        CdSO4            -7.66   -7.62    0.05  CdSO4
        CdSO4:2.67H2O    -5.79   -7.62   -1.83  CdSO4:2.67H2O
        CdSO4:H2O        -6.03   -7.62   -1.58  CdSO4:H2O
        Chalcanthite     -3.21   -5.86   -2.65  CuSO4:5H2O
        Claudetite      -90.28 -172.45  -82.17  As4O6
        Cu(OH)2          -1.50    7.29    8.79  Cu(OH)2
        Cu2SO4          -24.66  -31.97   -7.31  Cu2SO4
        Cu3(AsO4)2:6H2O  -3.66    2.44    6.10  Cu3(AsO4)2:6H2O
        CuMetal         -14.47  -26.11  -11.63  Cu
        CuOCuSO4        -10.46    1.43   11.88  CuO:CuSO4
        CupricFerrite    13.43   19.70    6.27  CuFe2O4
        Cuprite         -11.80  -18.82   -7.02  Cu2O
        CuprousFerrite    8.38   -3.21  -11.59  CuFeO2
        CuSO4             -9.05   -5.86    3.19  CuSO4
        Diaspore           5.32   12.44    7.12  AlOOH
        Fe2(SO4)3       -31.22  -27.05    4.17  Fe2(SO4)3
        FeAsO4:2H2O      -3.91   -3.51    0.40  FeAsO4:2H2O
        Ferrihydrite      1.20    6.20    5.00  Fe(OH)3
        Gibbsite(C)       3.44   12.44    9.00  Al(OH)3
        Goethite          5.56    6.20    0.64  FeOOH
        Goslarite        -2.58   -4.58   -1.99  ZnSO4:7H2O
        Gummite          -7.49    3.14   10.63  UO3
        Gypsum            0.43   -4.42   -4.85  CaSO4:2H2O
        Hausmannite      -4.39   57.94   62.34  Mn3O4
        Hematite         16.11   12.41   -3.70  Fe2O3
        Jarosite-H        3.85   -7.70  -11.55  (H3O)Fe3(SO4)2(OH)6
        Jarosite-K        8.96   -5.53  -14.49  KFe3(SO4)2(OH)6
        Jarosite-Na       6.17   -4.67  -10.84  NaFe3(SO4)2(OH)6
        Jurbanite         2.52   -0.71   -3.23  AlOHSO4
        Langite          -1.18   16.01   17.18  Cu4(OH)6SO4:H2O
        Larnakite        -3.80   -4.01   -0.22  PbO:PbSO4
        Lepidocrocite     4.83    6.20    1.37  FeOOH
        Lime            -24.52    8.73   33.26  CaO
```

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       Litharge          -8.31    4.57   12.88  PbO
       Maghemite          6.02   12.41    6.39  Fe2O3
       Manganite         -0.13   24.88   25.01  MnOOH
       Massicot          -8.51    4.57   13.08  PbO
       Minium           -27.61   47.10   74.71  Pb3O4
       Mirabilite        -5.80   -7.11   -1.30  Na2SO4:10H2O
       Mn2(SO4)3        -34.87   10.31   45.18  Mn2(SO4)3
       Mn3(AsO4)2:8H2O   -7.39    5.11   12.50  Mn3(AsO4)2:8H2O
       MnSO4             -7.79   -4.97    2.82  MnSO4
       Monteponite       -9.83    5.54   15.37  CdO
       Morenosite        -4.57   -6.96   -2.39  NiSO4:7H2O
       Ni(OH)2           -4.30    6.20   10.50  Ni(OH)2
       Ni3(AsO4)2:8H2O  -16.54   -0.84   15.70  Ni3(AsO4)2:8H2O
       Ni4(OH)6SO4      -20.36   11.64   32.00  Ni4(OH)6SO4
       Nsutite           -1.17   41.58   42.75  MnO2
       O2(g)            -17.66   66.80   84.45  O2
       Pb(OH)2(C)        -3.72    4.57    8.29  Pb(OH)2
       Pb2O(OH)2        -17.06    9.14   26.20  Pb2O(OH)2
       Pb2O3            -18.50   42.54   61.04  Pb2O3
       Pb3(AsO4)2       -11.52   -5.72    5.80  Pb3(AsO4)2
       Pb3O2SO4         -10.05    0.55   10.61  Pb3O2SO4
       Pb4(OH)6SO4      -15.98    5.12   21.10  Pb4(OH)6SO4
       Pb4O3SO4         -17.33    5.12   22.45  Pb4O3SO4
       PbMetal          -33.10  -28.83    4.27  Pb
       PbO:0.3H2O        -8.41    4.57   12.98  PbO:0.33H2O
       Plattnerite      -12.04   37.97   50.01  PbO2
       Portlandite      -14.25    8.73   22.98  Ca(OH)2
       Pyrocroite        -7.13    8.18   15.31  Mn(OH)2
       Pyrolusite         0.18   41.58   41.40  MnO2
       Retgersite        -4.91   -6.96   -2.05  NiSO4:6H2O
       Schoepite         -2.38    3.14    5.52  UO2(OH)2:H2O
       Schwertmannite    29.47   36.47    7.00  Fe8O8(OH)6(SO4)
       Tenorite          -0.48    7.29    7.77  CuO
       Thenardite        -6.93   -7.10   -0.17  Na2SO4
       U3O8(C)          -17.55  -23.97   -6.41  U3O8
       U4O9(C)          -47.01  -87.62  -40.61  U4O9
       UO2(am)          -21.89  -30.25   -8.36  UO2
       UO3(C)            -4.77    3.14    7.91  UO3
       Uraninite        -16.18  -30.25  -14.07  UO2
       Zincite           -2.78    8.58   11.36  ZnO
       Zincosite         -7.77   -4.57    3.20  ZnSO4
       Zn(OH)2(A)        -3.87    8.58   12.45  Zn(OH)2
       Zn(OH)2(B)        -3.17    8.58   11.75  Zn(OH)2
       Zn(OH)2(C)        -3.62    8.58   12.20  Zn(OH)2
       Zn(OH)2(E)        -2.92    8.58   11.50  Zn(OH)2
       Zn(OH)2(G)        -3.13    8.58   11.71  Zn(OH)2
       Zn2(OH)2SO4       -3.49    4.01    7.50  Zn2(OH)2SO4
       Zn3(AsO4)2:2.5H2O  -7.34    6.31   13.65  Zn3(AsO4)2:2.5H2O
       Zn3O(SO4)2       -20.20   -0.57   19.64  Zn3O(SO4)2
       Zn4(OH)6SO4       -7.24   21.16   28.40  Zn4(OH)6SO4
       ZnMetal          -50.94  -24.82   26.12  Zn
       ZnO(Active)       -2.73    8.58   11.31  ZnO
       ZnSO4:H2O         -4.11   -4.57   -0.46  ZnSO4:H2O

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End of simulation.
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-----------------------------------
Reading input data for simulation 2.
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End of run.
-----------
```

Aznalcóllar, Noviembre de 2005 pH 7

```
  Input file: C:\PHEEQC\MODELIZACIÓN\Especiación Aznalcóllar Noviembre 2005.pqi
 Output file: C:\PHEEQC\MODELIZACIÓN\Noviembre 2005pH7.0.pqo
Database file: C:\Archivos de programa\USGS\Phreeqc Interactive 2.7.1\minteq.dat

------------------
Reading data base.
------------------

       SOLUTION_MASTER_SPECIES
       SOLUTION_SPECIES
       SOLUTION_SPECIES
       PHASES
       SURFACE_MASTER_SPECIES
       SURFACE_SPECIES
       END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

       DATABASE C:\Archivos de programa\USGS\Phreeqc Interactive 2.7.1\minteq.dat
       SOLUTION 1 Muestra superficial experimento subida de pH
           temp      21
           pH        7
           pe        11
           redox     pe
           units     mg/l
           density   1
           S(6)      7.98 g/l
           Al        86
           Fe(2)     0
           Fe(3)     0.5
           Zn        830
           Cu        36.2
           Mn        190
           K         17.5
           Na        69
           Ca        516
           Cd        1.64
           Ni        2.28
           O(0)      9.6
           As        67 ug/l
           Pb        466 ug/l
           U         36 ug/l
           water    1 # kg
       SOLUTION_MASTER_SPECIES
           Fe(2)         Fe+2            0     Fe
           Fe(3)         Fe+3           -2     Fe
           Mg            Mg+2            0     Mg             24.312
           Na            Na+             0     Na             22.9898
           Ca            Ca+2            0     Ca             40.08
           S             SO4-2           0     SO4            32.064
           S(6)          SO4-2           0     SO4
           K             K+              0     K              39.102
           Al            Al+3            0     Al             26.9815
       SOLUTION_SPECIES
       H2O = OH- + H+
           log_k     -14
           delta_h   13.362 kcal
       Fe+2 = Fe+3 + e-
           log_k     -13.02
           delta_h   9.68 kcal
       Fe+3 + H2O = FeOH+2 + H+
           log_k     -2.19
           delta_h   10.4 kcal
       H+ + SO4-2 = HSO4-
           log_k     1.988
           delta_h   3.85 kcal
       Al+3 + H2O = AlOH+2 + H+
           log_k     -5
           delta_h   11.49 kcal
       Al+3 + 3H2O = Al(OH)3 + 3H+
           log_k     -16.9
           delta_h   39.89 kcal
```

```
        Al+3 + SO4-2 = AlSO4+
            log_k     3.5
            delta_h   2.29 kcal
        PHASES
        Jarosite-K
            KFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + K+ + 2SO4-2
            log_k     -14.8
            delta_h   -31.28 kcal
        Jarosite-Na
            NaFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + Na+ + 2SO4-2
            log_k     -11.2
            delta_h   -36.18 kcal
        Schwertmannite
            Fe8O8(OH)6(SO4) + 22H+ = 8Fe+3 + 14H2O + SO4-2
            log_k     7
        Ferrihydrite
            Fe(OH)3 + 3H+ = Fe+3 + 3H2O
            log_k     5
        Goethite
            FeOOH + 3H+ = Fe+3 + 2H2O
            log_k     0.5
            delta_h   -14.48 kcal
        Jurbanite
            AlOHSO4 + H+ = Al+3 + H2O + SO4-2
            log_k     -3.23
        Basaluminite
            Al4(OH)10SO4 + 10H+ = 4Al+3 + 10H2O + SO4-2
            log_k     22.7
        Alunite
            KAl3(SO4)2(OH)6 + 6H+ = 3Al+3 + 6H2O + K+ + 2SO4-2
            log_k     -1.3
            delta_h   3.918 kcal
        END
------------------------------------------
Beginning of initial solution calculations.
------------------------------------------

Initial solution 1.   Muestra superficial experimento subida de pH

-----------------------------Solution composition------------------------------

        Elements           Molality       Moles

        Al                3.219e-003  3.219e-003
        As                9.031e-007  9.031e-007
        Ca                1.300e-002  1.300e-002
        Cd                1.473e-005  1.473e-005
        Cu                5.753e-004  5.753e-004
        Fe(3)             9.041e-006  9.041e-006
        K                 4.519e-004  4.519e-004
        Mn                3.492e-003  3.492e-003
        Na                3.031e-003  3.031e-003
        Ni                3.922e-005  3.922e-005
        O(0)              6.059e-004  6.059e-004
        Pb                2.271e-006  2.271e-006
        S(6)              8.389e-002  8.389e-002
        U                 1.527e-007  1.527e-007
        Zn                1.282e-002  1.282e-002

----------------------------Description of solution----------------------------

                                       pH  =   7.000
                                       pe  =  11.000
                          Activity of water  =   0.998
                             Ionic strength  =  1.577e-001
                         Mass of water (kg)  =  1.000e+000
                 Total alkalinity (eq/kg)  =  1.182e-002
                    Total carbon (mol/kg)  =  0.000e+000
                       Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  21.000
                  Electrical balance (eq)  = -1.066e-001
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -66.20
                                Iterations  =  15
                                   Total H  = 1.110243e+002
                                   Total O  = 5.585422e+001
```

```
--------------------------------Redox couples--------------------------------

       Redox couple             pe  Eh (volts)

       O(-2)/O(0)          13.9805      0.8159

----------------------------Distribution of species----------------------------

                                                  Log       Log         Log
       Species            Molality    Activity  Molality  Activity     Gamma

       H+               1.237e-007  1.000e-007    -6.907    -7.000    -0.093
       OH-              9.682e-008  7.346e-008    -7.014    -7.134    -0.120
       H2O              5.551e+001  9.983e-001     1.744    -0.001     0.000
Al              3.219e-003
       Al(OH)4-         2.435e-003  1.819e-003    -2.613    -2.740    -0.127
       Al(OH)2+         5.229e-004  3.985e-004    -3.282    -3.400    -0.118
       Al(OH)3          2.434e-004  2.524e-004    -3.614    -3.598     0.016
       AlOH+2           1.164e-005  3.860e-006    -4.934    -5.413    -0.479
       AlSO4+           3.642e-006  2.763e-006    -5.439    -5.559    -0.120
       Al(SO4)2-        1.758e-006  1.313e-006    -5.755    -5.882    -0.127
       Al+3             3.426e-007  5.034e-008    -6.465    -7.298    -0.833
As(3)           1.261e-028
       H3AsO3           1.252e-028  1.298e-028   -27.902   -27.887     0.016
       H2AsO3-          8.707e-031  6.607e-031   -30.060   -30.180    -0.120
       HAsO3-2          1.322e-035  4.384e-036   -34.879   -35.358    -0.479
       H4AsO3+          8.477e-036  6.433e-036   -35.072   -35.192    -0.120
       AsO3-3           0.000e+000  0.000e+000   -40.754   -41.832    -1.079
As(5)           9.031e-007
       HAsO4-2          7.197e-007  2.386e-007    -6.143    -6.622    -0.479
       H2AsO4-          1.833e-007  1.391e-007    -6.737    -6.857    -0.120
       AsO4-3           6.564e-011  5.474e-012   -10.183   -11.262    -1.079
       H3AsO4           2.258e-012  2.341e-012   -11.646   -11.631     0.016
Ca              1.300e-002
       CaSO4            7.361e-003  7.633e-003    -2.133    -2.117     0.016
       Ca+2             5.640e-003  2.118e-003    -2.249    -2.674    -0.425
       CaOH+            4.957e-009  3.823e-009    -8.305    -8.418    -0.113
Cd              1.473e-005
       CdSO4            6.545e-006  6.787e-006    -5.184    -5.168     0.016
       Cd(SO4)2-2       4.211e-006  1.396e-006    -5.376    -5.855    -0.479
       Cd+2             3.977e-006  1.319e-006    -5.400    -5.880    -0.479
       CdOH+            1.068e-009  8.106e-010    -8.971    -9.091    -0.120
       Cd(OH)2          5.660e-013  5.870e-013   -12.247   -12.231     0.016
       Cd2OH+3          6.602e-014  5.506e-015   -13.180   -14.259    -1.079
       Cd(OH)3-         8.665e-019  6.575e-019   -18.062   -18.182    -0.120
       Cd(OH)4-2        1.765e-025  5.850e-026   -24.753   -25.233    -0.479
Cu(1)           3.874e-013
       Cu+              3.874e-013  2.733e-013   -12.412   -12.563    -0.152
Cu(2)           5.753e-004
       Cu+2             2.185e-004  5.408e-005    -3.661    -4.267    -0.606
       CuSO4            1.894e-004  1.964e-004    -3.723    -3.707     0.016
       Cu(OH)2          1.086e-004  1.126e-004    -3.964    -3.948     0.016
       Cu2(OH)2+2       2.572e-005  8.527e-006    -4.590    -5.069    -0.479
       CuOH+            7.318e-006  5.399e-006    -5.136    -5.268    -0.132
       Cu(OH)3-         8.947e-011  6.789e-011   -10.048   -10.168    -0.120
       Cu(OH)4-2        4.070e-016  1.349e-016   -15.390   -15.870    -0.479
Fe(3)           9.041e-006
       Fe(OH)2+         8.231e-006  6.272e-006    -5.085    -5.203    -0.118
       Fe(OH)3          7.095e-007  7.357e-007    -6.149    -6.133     0.016
       Fe(OH)4-         9.638e-008  7.345e-008    -7.016    -7.134    -0.118
       FeOH+2           4.508e-009  1.495e-009    -8.346    -8.825    -0.479
       FeSO4+           5.421e-012  4.096e-012   -11.266   -11.388    -0.122
       Fe(SO4)2-        3.074e-012  2.332e-012   -11.512   -11.632    -0.120
       Fe+3             3.530e-013  2.944e-014   -12.452   -13.531    -1.079
       Fe2(OH)2+4       5.885e-015  7.109e-017   -14.230   -16.148    -1.918
       Fe3(OH)4+5       9.080e-017  9.146e-020   -16.042   -19.039    -2.997
H(0)            1.422e-039
       H2               7.108e-040  7.371e-040   -39.148   -39.132     0.016
K               4.519e-004
       K+               4.060e-004  2.926e-004    -3.392    -3.534    -0.142
       KSO4-            4.600e-005  3.505e-005    -4.337    -4.455    -0.118
Mn(2)           3.492e-003
       MnSO4            1.814e-003  1.881e-003    -2.741    -2.726     0.016
       Mn+2             1.679e-003  5.938e-004    -2.775    -3.226    -0.451
```

```
        MnOH+           1.449e-007  1.095e-007    -6.839    -6.961    -0.122
        Mn(OH)3-        1.239e-017  9.363e-018   -16.907   -17.029    -0.122
Mn(3)           2.271e-017
        Mn+3            2.271e-017  3.337e-018   -16.644   -17.477    -0.833
Mn(6)           2.100e-023
        MnO4-2          2.100e-023  6.845e-024   -22.678   -23.165    -0.487
Mn(7)           2.142e-022
        MnO4-           2.142e-022  1.535e-022   -21.669   -21.814    -0.145
Na              3.031e-003
        Na+             2.783e-003  2.110e-003    -2.555    -2.676    -0.120
        NaSO4-          2.474e-004  1.886e-004    -3.607    -3.725    -0.118
Ni              3.922e-005
        NiSO4           2.052e-005  2.128e-005    -4.688    -4.672     0.016
        Ni+2            1.863e-005  6.175e-006    -4.730    -5.209    -0.479
        Ni(SO4)2-2      6.530e-008  2.165e-008    -7.185    -7.665    -0.479
        NiOH+           8.433e-009  6.399e-009    -8.074    -8.194    -0.120
        Ni(OH)2         5.935e-011  6.154e-011   -10.227   -10.211     0.016
        Ni(OH)3-        8.097e-015  6.144e-015   -14.092   -14.212    -0.120
O(0)            6.059e-004
        O2              3.030e-004  3.142e-004    -3.519    -3.503     0.016
Pb              2.271e-006
        PbSO4           1.393e-006  1.445e-006    -5.856    -5.840     0.016
        Pb+2            4.235e-007  1.404e-007    -6.373    -6.853    -0.479
        Pb(SO4)2-2      4.185e-007  1.387e-007    -6.378    -6.858    -0.479
        PbOH+           3.602e-008  2.733e-008    -7.443    -7.563    -0.120
        Pb(OH)2         1.024e-010  1.062e-010    -9.990    -9.974     0.016
        Pb2OH+3         1.030e-012  8.591e-014   -11.987   -13.066    -1.079
        Pb(OH)3-        1.603e-014  1.217e-014   -13.795   -13.915    -0.120
        Pb3(OH)4+2      5.951e-017  1.973e-017   -16.225   -16.705    -0.479
        Pb(OH)4-2       8.413e-019  2.789e-019   -18.075   -18.555    -0.479
S(6)            8.389e-002
        SO4-2           6.270e-002  1.830e-002    -1.203    -1.738    -0.535
        CaSO4           7.361e-003  7.633e-003    -2.133    -2.117     0.016
        ZnSO4           5.860e-003  6.077e-003    -2.232    -2.216     0.016
        Zn(SO4)2-2      2.813e-003  9.324e-004    -2.551    -3.030    -0.479
        MnSO4           1.814e-003  1.881e-003    -2.741    -2.726     0.016
        NaSO4-          2.474e-004  1.886e-004    -3.607    -3.725    -0.118
        CuSO4           1.894e-004  1.964e-004    -3.723    -3.707     0.016
        KSO4-           4.600e-005  3.505e-005    -4.337    -4.455    -0.118
        NiSO4           2.052e-005  2.128e-005    -4.688    -4.672     0.016
        CdSO4           6.545e-006  6.787e-006    -5.184    -5.168     0.016
        Cd(SO4)2-2      4.211e-006  1.396e-006    -5.376    -5.855    -0.479
        AlSO4+          3.642e-006  2.763e-006    -5.439    -5.559    -0.120
        Al(SO4)2-       1.758e-006  1.313e-006    -5.755    -5.882    -0.127
        PbSO4           1.393e-006  1.445e-006    -5.856    -5.840     0.016
        Pb(SO4)2-2      4.185e-007  1.387e-007    -6.378    -6.858    -0.479
        HSO4-           2.147e-007  1.629e-007    -6.668    -6.788    -0.120
        Ni(SO4)2-2      6.530e-008  2.165e-008    -7.185    -7.665    -0.479
        UO2(SO4)2-2     1.271e-008  4.213e-009    -7.896    -8.375    -0.479
        UO2SO4          7.628e-009  7.910e-009    -8.118    -8.102     0.016
        FeSO4+          5.421e-012  4.096e-012   -11.266   -11.388    -0.122
        Fe(SO4)2-       3.074e-012  2.332e-012   -11.512   -11.632    -0.120
        U(SO4)2         0.000e+000  0.000e+000   -43.279   -43.264     0.016
        USO4+2          0.000e+000  0.000e+000   -45.296   -45.775    -0.479
U(3)            0.000e+000
        U+3             0.000e+000  0.000e+000   -68.422   -69.501    -1.079
U(4)            1.824e-028
        U(OH)5-         1.818e-028  1.380e-028   -27.740   -27.860    -0.120
        U(OH)4          5.953e-031  6.173e-031   -30.225   -30.209     0.016
        U(OH)3+         3.128e-034  2.373e-034   -33.505   -33.625    -0.120
        U(OH)2+2        3.712e-038  1.230e-038   -37.430   -37.910    -0.479
        UOH+3           0.000e+000  0.000e+000   -42.160   -43.239    -1.079
        U(SO4)2         0.000e+000  0.000e+000   -43.279   -43.264     0.016
        USO4+2          0.000e+000  0.000e+000   -45.296   -45.775    -0.479
        U+4             0.000e+000  0.000e+000   -47.544   -49.462    -1.918
        U6(OH)15+9      0.000e+000  0.000e+000  -199.301  -209.010    -9.710
U(5)            8.230e-018
        UO2+            8.230e-018  6.245e-018   -17.085   -17.204    -0.120
U(6)            1.527e-007
        UO2OH+          8.034e-008  6.096e-008    -7.095    -7.215    -0.120
        (UO2)3(OH)5+    1.607e-008  1.220e-008    -7.794    -7.914    -0.120
        UO2(SO4)2-2     1.271e-008  4.213e-009    -7.896    -8.375    -0.479
        UO2SO4          7.628e-009  7.910e-009    -8.118    -8.102     0.016
        UO2+2           2.865e-009  9.498e-010    -8.543    -9.022    -0.479
        (UO2)2(OH)2+2   4.856e-010  1.610e-010    -9.314    -9.793    -0.479
```

```
Zn              1.282e-002
       ZnSO4            5.860e-003  6.077e-003    -2.232    -2.216     0.016
       Zn+2             4.132e-003  1.462e-003    -2.384    -2.835    -0.451
       Zn(SO4)2-2       2.813e-003  9.324e-004    -2.551    -3.030    -0.479
       ZnOH+            1.550e-005  1.176e-005    -4.810    -4.929    -0.120
       Zn(OH)2          1.773e-006  1.838e-006    -5.751    -5.736     0.016
       Zn(OH)3-         7.647e-011  5.803e-011   -10.116   -10.236    -0.120
       Zn(OH)4-2        2.769e-016  9.181e-017   -15.558   -16.037    -0.479

------------------------------Saturation indices-------------------------------

       Phase               SI log IAP  log KT

       Al(OH)3(a)        3.05   13.70   10.65  Al(OH)3
       Al2O3             4.42   27.40   22.98  Al2O3
       Al4(OH)10SO4     16.36   39.06   22.70  Al4(OH)10SO4
       AlAsO4:2H2O      -2.73    2.07    4.80  AlAsO4:2H2O
       AlOHSO4           1.19   -2.04   -3.23  AlOHSO4
       AlumK            -9.07  -14.32   -5.24  KAl(SO4)2:12H2O
       Alunite          14.43   13.09   -1.34  KAl3(SO4)2(OH)6
       Anglesite        -0.78   -8.59   -7.81  PbSO4
       Anhydrite         0.19   -4.41   -4.60  CaSO4
       Antlerite         5.17   13.46    8.29  Cu3(OH)4SO4
       Arsenolite     -108.60 -190.51  -81.92  As4O6
       As2O5           -30.01  -23.26    6.75  As2O5
       B_UO2(OH)2       -0.70    4.98    5.68  UO2(OH)2
       Basaluminite     16.36   39.06   22.70  Al4(OH)10SO4
       Bianchite        -2.81   -4.58   -1.76  ZnSO4:6H2O
       Birnessite        3.43   46.77   43.34  MnO2
       Bixbyite          7.50   57.55   50.04  Mn2O3
       Boehmite          4.84   13.70    8.86  AlOOH
       Brochantite       7.85   23.19   15.34  Cu4(OH)6SO4
       Bunsenite        -3.90    8.79   12.69  NiO
       Ca3(AsO4)2:6H2O -11.59   10.71   22.30  Ca3(AsO4)2:6H2O
       Cd(Gamma)       -41.65  -27.88   13.77  Cd
       Cd(OH)2(A)       -5.82    8.12   13.94  Cd(OH)2
       Cd(OH)2(C)       -5.53    8.12   13.65  Cd(OH)2
       Cd3(OH)2(SO4)2  -13.83   -7.12    6.71  Cd3(OH)2(SO4)2
       Cd3(OH)4SO4     -13.94    8.62   22.56  Cd3(OH)4SO4
       Cd4(OH)6SO4     -11.66   16.74   28.40  Cd4(OH)6SO4
       CdMetal         -41.55  -27.88   13.67  Cd
       CdSO4            -7.66   -7.62    0.05  CdSO4
       CdSO4:2.67H2O    -5.79   -7.62   -1.83  CdSO4:2.67H2O
       CdSO4:H2O        -6.04   -7.62   -1.58  CdSO4:H2O
       Chalcanthite     -3.35   -6.01   -2.65  CuSO4:5H2O
       Claudetite     -108.34 -190.51  -82.17  As4O6
       Cu(OH)2           0.94    9.73    8.79  Cu(OH)2
       Cu2SO4          -24.96  -32.27   -7.31  Cu2SO4
       Cu3(AsO4)2:6H2O  -0.17    5.93    6.10  Cu3(AsO4)2:6H2O
       CuMetal         -14.63  -26.27  -11.63  Cu
       CuOCuSO4         -8.16    3.73   11.88  CuO:CuSO4
       CupricFerrite    18.40   24.67    6.27  CuFe2O4
       Cuprite          -9.52  -16.53   -7.02  Cu2O
       CuprousFerrite   10.79   -0.80  -11.59  CuFeO2
       CuSO4            -9.20   -6.00    3.19  CuSO4
       Diaspore          6.58   13.70    7.12  AlOOH
       Fe2(SO4)3       -36.44  -32.28    4.17  Fe2(SO4)3
       FeAsO4:2H2O      -4.56   -4.16    0.40  FeAsO4:2H2O
       Ferrihydrite      2.47    7.47    5.00  Fe(OH)3
       Gibbsite(C)       4.70   13.70    9.00  Al(OH)3
       Goethite          6.82    7.47    0.64  FeOOH
       Goslarite        -2.59   -4.58   -1.99  ZnSO4:7H2O
       Gummite          -5.66    4.98   10.63  UO3
       Gypsum            0.44   -4.41   -4.85  CaSO4:2H2O
       Hausmannite       5.98   68.32   62.34  Mn3O4
       Hematite         18.64   14.94   -3.70  Fe2O3
       Jarosite-H        2.48   -9.07  -11.55  (H3O)Fe3(SO4)2(OH)6
       Jarosite-K        8.88   -5.61  -14.49  KFe3(SO4)2(OH)6
       Jarosite-Na       6.09   -4.75  -10.84  NaFe3(SO4)2(OH)6
       Jurbanite         1.19   -2.04   -3.23  AlOHSO4
       Langite           6.00   23.19   17.18  Cu4(OH)6SO4:H2O
       Larnakite        -1.23   -1.44   -0.22  PbO:PbSO4
       Lepidocrocite     6.10    7.47    1.37  FeOOH
       Lime            -21.93   11.33   33.26  CaO
       Litharge         -5.74    7.15   12.88  PbO
```

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       Maghemite          8.55   14.94    6.39  Fe2O3
       Manganite          3.76   28.77   25.01  MnOOH
       Massicot          -5.93    7.15   13.08  PbO
       Minium           -17.28   57.44   74.71  Pb3O4
       Mirabilite        -5.79   -7.10   -1.30  Na2SO4:10H2O
       Mn2(SO4)3        -34.84   10.33   45.18  Mn2(SO4)3
       Mn3(AsO4)2:8H2O   -3.45    9.05   12.50  Mn3(AsO4)2:8H2O
       MnSO4             -7.79   -4.96    2.82  MnSO4
       Monteponite       -7.25    8.12   15.37  CdO
       Morenosite        -4.56   -6.95   -2.39  NiSO4:7H2O
       Ni(OH)2           -1.71    8.79   10.50  Ni(OH)2
       Ni3(AsO4)2:8H2O  -12.60    3.10   15.70  Ni3(AsO4)2:8H2O
       Ni4(OH)6SO4      -12.58   19.42   32.00  Ni4(OH)6SO4
       Nsutite            4.02   46.77   42.75  MnO2
       O2(g)            -12.46   72.00   84.45  O2
       Pb(OH)2(C)        -1.14    7.15    8.29  Pb(OH)2
       Pb2O(OH)2        -11.91   14.29   26.20  Pb2O(OH)2
       Pb2O3            -10.75   50.29   61.04  Pb2O3
       Pb3(AsO4)2        -7.62   -1.82    5.80  Pb3(AsO4)2
       Pb3O2SO4          -4.90    5.70   10.61  Pb3O2SO4
       Pb4(OH)6SO4       -8.25   12.85   21.10  Pb4(OH)6SO4
       Pb4O3SO4          -9.60   12.85   22.45  Pb4O3SO4
       PbMetal          -33.12  -28.85    4.27  Pb
       PbO:0.3H2O        -5.83    7.15   12.98  PbO:0.33H2O
       Plattnerite       -6.86   43.15   50.01  PbO2
       Portlandite      -11.66   11.32   22.98  Ca(OH)2
       Pyrocroite        -4.54   10.77   15.31  Mn(OH)2
       Pyrolusite         5.37   46.77   41.40  MnO2
       Retgersite        -4.90   -6.95   -2.05  NiSO4:6H2O
       Schoepite         -0.55    4.98    5.52  UO2(OH)2:H2O
       Schwertmannite    37.00   44.00    7.00  Fe8O8(OH)6(SO4)
       Tenorite           1.96    9.73    7.77  CuO
       Thenardite        -6.92   -7.09   -0.17  Na2SO4
       U3O8(C)          -14.65  -21.07   -6.41  U3O8
       U4O9(C)          -47.48  -88.09  -40.61  U4O9
       UO2(am)          -22.66  -31.02   -8.36  UO2
       UO3(C)            -2.93    4.98    7.91  UO3
       Uraninite        -16.95  -31.02  -14.07  UO2
       Zincite           -0.19   11.16   11.36  ZnO
       Zincosite         -7.77   -4.57    3.20  ZnSO4
       Zn(OH)2(A)        -1.29   11.16   12.45  Zn(OH)2
       Zn(OH)2(B)        -0.59   11.16   11.75  Zn(OH)2
       Zn(OH)2(C)        -1.04   11.16   12.20  Zn(OH)2
       Zn(OH)2(E)        -0.34   11.16   11.50  Zn(OH)2
       Zn(OH)2(G)        -0.55   11.16   11.71  Zn(OH)2
       Zn2(OH)2SO4       -0.91    6.59    7.50  Zn2(OH)2SO4
       Zn3(AsO4)2:2.5H2O  -3.42   10.23   13.65  Zn3(AsO4)2:2.5H2O
       Zn3O(SO4)2       -17.62    2.02   19.64  Zn3O(SO4)2
       Zn4(OH)6SO4        0.52   28.92   28.40  Zn4(OH)6SO4
       ZnMetal          -50.96  -24.84   26.12  Zn
       ZnO(Active)       -0.15   11.16   11.31  ZnO
       ZnSO4:H2O         -4.11   -4.57   -0.46  ZnSO4:H2O

------------------
End of simulation.
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Reading input data for simulation 2.
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End of run.
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```

Aznalcóllar, Noviembre de 2005 pH 8

```
  Input file: C:\PHEEQC\MODELIZACIÓN\Especiación Aznalcóllar Noviembre 2005.pqi
  Output file: C:\PHEEQC\MODELIZACIÓN\Noviembre 2005pH8.pqo
Database file: C:\Archivos de programa\USGS\Phreeqc Interactive 2.7.1\minteq.dat

------------------
Reading data base.
------------------

       SOLUTION_MASTER_SPECIES
       SOLUTION_SPECIES
       SOLUTION_SPECIES
       PHASES
       SURFACE_MASTER_SPECIES
       SURFACE_SPECIES
       END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

       DATABASE C:\Archivos de programa\USGS\Phreeqc Interactive 2.7.1\minteq.dat
       SOLUTION 1 Muestra superficial experimento subida de pH
           temp      21
           pH        8
           pe        11
           redox     pe
           units     mg/l
           density   1
           S(6)      7.98 g/l
           Al        86
           Fe(2)     0
           Fe(3)     0.5
           Zn        830
           Cu        36.2
           Mn        190
           K         17.5
           Na        69
           Ca        516
           Cd        1.64
           Ni        2.28
           O(0)      9.6
           As        67 ug/l
           Pb        466 ug/l
           U         36 ug/l
           water    1 # kg
       SOLUTION_MASTER_SPECIES
           Fe(2)         Fe+2            0     Fe
           Fe(3)         Fe+3           -2     Fe
           Mg            Mg+2            0     Mg             24.312
           Na            Na+             0     Na             22.9898
           Ca            Ca+2            0     Ca             40.08
           S             SO4-2           0     SO4            32.064
           S(6)          SO4-2           0     SO4
           K             K+              0     K              39.102
           Al            Al+3            0     Al             26.9815
       SOLUTION_SPECIES
       H2O = OH- + H+
           log_k     -14
           delta_h   13.362 kcal
       Fe+2 = Fe+3 + e-
           log_k     -13.02
           delta_h   9.68 kcal
       Fe+3 + H2O = FeOH+2 + H+
           log_k     -2.19
           delta_h   10.4 kcal
       H+ + SO4-2 = HSO4-
           log_k     1.988
           delta_h   3.85 kcal
       Al+3 + H2O = AlOH+2 + H+
           log_k     -5
           delta_h   11.49 kcal
       Al+3 + 3H2O = Al(OH)3 + 3H+
           log_k     -16.9
           delta_h   39.89 kcal
```

```
        Al+3 + SO4-2 = AlSO4+
            log_k     3.5
            delta_h   2.29 kcal
        PHASES
        Jarosite-K
            KFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + K+ + 2SO4-2
            log_k     -14.8
            delta_h   -31.28 kcal
        Jarosite-Na
            NaFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + Na+ + 2SO4-2
            log_k     -11.2
            delta_h   -36.18 kcal
        Schwertmannite
            Fe8O8(OH)6(SO4) + 22H+ = 8Fe+3 + 14H2O + SO4-2
            log_k     7
        Ferrihydrite
            Fe(OH)3 + 3H+ = Fe+3 + 3H2O
            log_k     5
        Goethite
            FeOOH + 3H+ = Fe+3 + 2H2O
            log_k     0.5
            delta_h   -14.48 kcal
        Jurbanite
            AlOHSO4 + H+ = Al+3 + H2O + SO4-2
            log_k     -3.23
        Basaluminite
            Al4(OH)10SO4 + 10H+ = 4Al+3 + 10H2O + SO4-2
            log_k     22.7
        Alunite
            KAl3(SO4)2(OH)6 + 6H+ = 3Al+3 + 6H2O + K+ + 2SO4-2
            log_k     -1.3
            delta_h   3.918 kcal
        END
------------------------------------------
Beginning of initial solution calculations.
------------------------------------------

Initial solution 1.   Muestra superficial experimento subida de pH

-----------------------------Solution composition------------------------------

        Elements           Molality       Moles

        Al               3.219e-003  3.219e-003
        As               9.031e-007  9.031e-007
        Ca               1.300e-002  1.300e-002
        Cd               1.473e-005  1.473e-005
        Cu               5.753e-004  5.753e-004
        Fe(3)            9.041e-006  9.041e-006
        K                4.519e-004  4.519e-004
        Mn               3.492e-003  3.492e-003
        Na               3.031e-003  3.031e-003
        Ni               3.922e-005  3.922e-005
        O(0)             6.059e-004  6.059e-004
        Pb               2.271e-006  2.271e-006
        S(6)             8.389e-002  8.389e-002
        U                1.527e-007  1.527e-007
        Zn               1.282e-002  1.282e-002

----------------------------Description of solution----------------------------

                                       pH  =   8.000
                                       pe  =  11.000
                          Activity of water  =   0.998
                             Ionic strength  =  1.578e-001
                         Mass of water (kg)  =  1.000e+000
                 Total alkalinity (eq/kg)  =  1.443e-002
                    Total carbon (mol/kg)  =  0.000e+000
                       Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  21.000
                  Electrical balance (eq)  = -1.092e-001
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -67.70
                                Iterations  =  11
                                   Total H  = 1.110269e+002
                                   Total O  = 5.585682e+001
```

```
--------------------------------Redox couples--------------------------------

       Redox couple             pe  Eh (volts)

       O(-2)/O(0)          12.9805      0.7576

----------------------------Distribution of species----------------------------

                                                    Log       Log         Log
       Species            Molality    Activity  Molality  Activity     Gamma

       OH-              9.682e-007  7.346e-007    -6.014    -6.134    -0.120
       H+               1.238e-008  1.000e-008    -7.907    -8.000    -0.093
       H2O              5.551e+001  9.983e-001     1.744    -0.001     0.000
Al             3.219e-003
       Al(OH)4-         3.180e-003  2.375e-003    -2.498    -2.624    -0.127
       Al(OH)3          3.178e-005  3.296e-005    -4.498    -4.482     0.016
       Al(OH)2+         6.829e-006  5.204e-006    -5.166    -5.284    -0.118
       AlOH+2           1.521e-008  5.041e-009    -7.818    -8.297    -0.480
       AlSO4+           4.785e-010  3.631e-010    -9.320    -9.440    -0.120
       Al(SO4)2-        2.324e-010  1.736e-010    -9.634    -9.760    -0.127
       Al+3             4.475e-011  6.574e-012   -10.349   -11.182    -0.833
As(3)          1.637e-032
       H3AsO3           1.530e-032  1.587e-032   -31.815   -31.799     0.016
       H2AsO3-          1.064e-033  8.076e-034   -32.973   -33.093    -0.120
       HAsO3-2          1.617e-037  5.359e-038   -36.791   -37.271    -0.480
       H4AsO3+          1.036e-040  0.000e+000   -39.985   -40.104    -0.120
       AsO3-3           0.000e+000  0.000e+000   -41.666   -42.745    -1.079
As(5)          9.031e-007
       HAsO4-2          8.799e-007  2.916e-007    -6.056    -6.535    -0.480
       H2AsO4-          2.241e-008  1.700e-008    -7.650    -7.769    -0.120
       AsO4-3           8.026e-010  6.691e-011    -9.095   -10.175    -1.079
       H3AsO4           2.760e-014  2.862e-014   -13.559   -13.543     0.016
Ca             1.300e-002
       CaSO4            7.380e-003  7.653e-003    -2.132    -2.116     0.016
       Ca+2             5.621e-003  2.111e-003    -2.250    -2.676    -0.425
       CaOH+            4.940e-008  3.809e-008    -7.306    -7.419    -0.113
Cd             1.473e-005
       CdSO4            6.540e-006  6.782e-006    -5.184    -5.169     0.016
       Cd(SO4)2-2       4.233e-006  1.403e-006    -5.373    -5.853    -0.480
       Cd+2             3.951e-006  1.310e-006    -5.403    -5.883    -0.480
       CdOH+            1.061e-008  8.050e-009    -7.974    -8.094    -0.120
       Cd(OH)2          5.621e-011  5.829e-011   -10.250   -10.234     0.016
       Cd2OH+3          6.514e-013  5.431e-014   -12.186   -13.265    -1.079
       Cd(OH)3-         8.606e-016  6.530e-016   -15.065   -15.185    -0.120
       Cd(OH)4-2        1.753e-021  5.810e-022   -20.756   -21.236    -0.480
Cu(1)          1.922e-014
       Cu+              1.922e-014  1.356e-014   -13.716   -13.868    -0.152
Cu(2)          5.753e-004
       Cu(OH)2          5.387e-004  5.586e-004    -3.269    -3.253     0.016
       Cu+2             1.084e-005  2.683e-006    -4.965    -5.571    -0.607
       CuSO4            9.455e-006  9.805e-006    -5.024    -5.009     0.016
       Cu2(OH)2+2       6.331e-006  2.099e-006    -5.199    -5.678    -0.480
       CuOH+            3.631e-006  2.678e-006    -5.440    -5.572    -0.132
       Cu(OH)3-         4.439e-009  3.368e-009    -8.353    -8.473    -0.120
       Cu(OH)4-2        2.019e-013  6.693e-014   -12.695   -13.174    -0.480
Fe(3)          9.041e-006
       Fe(OH)4-         3.491e-006  2.660e-006    -5.457    -5.575    -0.118
       Fe(OH)2+         2.981e-006  2.272e-006    -5.526    -5.644    -0.118
       Fe(OH)3          2.569e-006  2.664e-006    -5.590    -5.574     0.016
       FeOH+2           1.633e-010  5.413e-011    -9.787   -10.267    -0.480
       FeSO4+           1.975e-014  1.492e-014   -13.704   -13.826    -0.122
       Fe(SO4)2-        1.127e-014  8.550e-015   -13.948   -14.068    -0.120
       Fe+3             1.279e-015  1.066e-016   -14.893   -15.972    -1.079
       Fe2(OH)2+4       7.725e-018  9.324e-020   -17.112   -19.030    -1.918
       Fe3(OH)4+5       4.318e-020  4.345e-023   -19.365   -22.362    -2.997
H(0)           0.000e+000
       H2               0.000e+000  0.000e+000   -41.148   -41.132     0.016
K              4.519e-004
       K+               4.057e-004  2.924e-004    -3.392    -3.534    -0.142
       KSO4-            4.625e-005  3.524e-005    -4.335    -4.453    -0.118
Mn(2)          3.492e-003
       MnSO4            1.818e-003  1.885e-003    -2.740    -2.725     0.016
       Mn+2             1.673e-003  5.916e-004    -2.777    -3.228    -0.451
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        MnOH+           1.444e-006  1.091e-006    -5.840    -5.962    -0.122
        Mn(OH)3-        1.235e-014  9.329e-015   -13.908   -14.030    -0.122
Mn(3)           2.264e-017
        Mn+3            2.264e-017  3.325e-018   -16.645   -17.478    -0.833
Mn(6)           2.093e-015
        MnO4-2          2.093e-015  6.820e-016   -14.679   -15.166    -0.487
Mn(7)           2.134e-014
        MnO4-           2.134e-014  1.530e-014   -13.671   -13.815    -0.145
Na              3.031e-003
        Na+             2.782e-003  2.109e-003    -2.556    -2.676    -0.120
        NaSO4-          2.488e-004  1.896e-004    -3.604    -3.722    -0.118
Ni              3.922e-005
        NiSO4           2.053e-005  2.129e-005    -4.688    -4.672     0.016
        Ni+2            1.853e-005  6.142e-006    -4.732    -5.212    -0.480
        NiOH+           8.389e-008  6.365e-008    -7.076    -7.196    -0.120
        Ni(SO4)2-2      6.575e-008  2.179e-008    -7.182    -7.662    -0.480
        Ni(OH)2         5.903e-009  6.121e-009    -8.229    -8.213     0.016
        Ni(OH)3-        8.054e-012  6.111e-012   -11.094   -11.214    -0.120
O(0)            6.059e-004
        O2              3.030e-004  3.142e-004    -3.519    -3.503     0.016
Pb              2.271e-006
        PbSO4           1.215e-006  1.260e-006    -5.915    -5.900     0.016
        Pb+2            3.673e-007  1.218e-007    -6.435    -6.915    -0.480
        Pb(SO4)2-2      3.673e-007  1.218e-007    -6.435    -6.915    -0.480
        PbOH+           3.123e-007  2.370e-007    -6.505    -6.625    -0.120
        Pb(OH)2         8.876e-009  9.205e-009    -8.052    -8.036     0.016
        Pb(OH)3-        1.390e-011  1.055e-011   -10.857   -10.977    -0.120
        Pb2OH+3         7.749e-012  6.460e-013   -11.111   -12.190    -1.079
        Pb3(OH)4+2      3.881e-013  1.286e-013   -12.411   -12.891    -0.480
        Pb(OH)4-2       7.296e-015  2.418e-015   -14.137   -14.616    -0.480
S(6)            8.389e-002
        SO4-2           6.310e-002  1.841e-002    -1.200    -1.735    -0.535
        CaSO4           7.380e-003  7.653e-003    -2.132    -2.116     0.016
        ZnSO4           5.723e-003  5.935e-003    -2.242    -2.227     0.016
        Zn(SO4)2-2      2.764e-003  9.162e-004    -2.558    -3.038    -0.480
        MnSO4           1.818e-003  1.885e-003    -2.740    -2.725     0.016
        NaSO4-          2.488e-004  1.896e-004    -3.604    -3.722    -0.118
        KSO4-           4.625e-005  3.524e-005    -4.335    -4.453    -0.118
        NiSO4           2.053e-005  2.129e-005    -4.688    -4.672     0.016
        CuSO4           9.455e-006  9.805e-006    -5.024    -5.009     0.016
        CdSO4           6.540e-006  6.782e-006    -5.184    -5.169     0.016
        Cd(SO4)2-2      4.233e-006  1.403e-006    -5.373    -5.853    -0.480
        PbSO4           1.215e-006  1.260e-006    -5.915    -5.900     0.016
        Pb(SO4)2-2      3.673e-007  1.218e-007    -6.435    -6.915    -0.480
        Ni(SO4)2-2      6.575e-008  2.179e-008    -7.182    -7.662    -0.480
        HSO4-           2.160e-008  1.639e-008    -7.665    -7.785    -0.120
        AlSO4+          4.785e-010  3.631e-010    -9.320    -9.440    -0.120
        UO2(SO4)2-2     3.837e-010  1.272e-010    -9.416    -9.896    -0.480
        Al(SO4)2-       2.324e-010  1.736e-010    -9.634    -9.760    -0.127
        UO2SO4          2.289e-010  2.374e-010    -9.640    -9.625     0.016
        FeSO4+          1.975e-014  1.492e-014   -13.704   -13.826    -0.122
        Fe(SO4)2-       1.127e-014  8.550e-015   -13.948   -14.068    -0.120
        U(SO4)2         0.000e+000  0.000e+000   -48.800   -48.784     0.016
        USO4+2          0.000e+000  0.000e+000   -50.818   -51.298    -0.480
U(3)            0.000e+000
        U+3             0.000e+000  0.000e+000   -73.947   -75.026    -1.079
U(4)            5.425e-029
        U(OH)5-         5.423e-029  4.115e-029   -28.266   -28.386    -0.120
        U(OH)4          1.776e-032  1.841e-032   -31.751   -31.735     0.016
        U(OH)3+         9.330e-037  7.079e-037   -36.030   -36.150    -0.120
        U(OH)2+2        0.000e+000  0.000e+000   -40.956   -41.435    -0.480
        UOH+3           0.000e+000  0.000e+000   -46.686   -47.765    -1.079
        U(SO4)2         0.000e+000  0.000e+000   -48.800   -48.784     0.016
        USO4+2          0.000e+000  0.000e+000   -50.818   -51.298    -0.480
        U+4             0.000e+000  0.000e+000   -53.069   -54.987    -1.918
        U6(OH)15+9      0.000e+000  0.000e+000  -217.451  -227.163    -9.711
U(5)            2.455e-019
        UO2+            2.455e-019  1.863e-019   -18.610   -18.730    -0.120
U(6)            1.527e-007
        (UO2)3(OH)5+    4.266e-008  3.237e-008    -7.370    -7.490    -0.120
        UO2OH+          2.397e-008  1.818e-008    -7.620    -7.740    -0.120
        UO2(SO4)2-2     3.837e-010  1.272e-010    -9.416    -9.896    -0.480
        UO2SO4          2.289e-010  2.374e-010    -9.640    -9.625     0.016
        UO2+2           8.547e-011  2.833e-011   -10.068   -10.548    -0.480
        (UO2)2(OH)2+2   4.321e-011  1.432e-011   -10.364   -10.844    -0.480
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Zn              1.282e-002
       ZnSO4            5.723e-003  5.935e-003    -2.242    -2.227     0.016
       Zn+2             4.012e-003  1.419e-003    -2.397    -2.848    -0.451
       Zn(SO4)2-2       2.764e-003  9.162e-004    -2.558    -3.038    -0.480
       Zn(OH)2          1.721e-004  1.784e-004    -3.764    -3.749     0.016
       ZnOH+            1.505e-004  1.142e-004    -3.822    -3.942    -0.120
       Zn(OH)3-         7.424e-008  5.633e-008    -7.129    -7.249    -0.120
       Zn(OH)4-2        2.689e-012  8.913e-013   -11.570   -12.050    -0.480

------------------------------Saturation indices-------------------------------

       Phase               SI log IAP  log KT

       Al(OH)3(a)        2.17   12.82   10.65  Al(OH)3
       Al2O3             2.65   25.63   22.98  Al2O3
       Al4(OH)10SO4     10.83   33.53   22.70  Al4(OH)10SO4
       AlAsO4:2H2O      -5.53   -0.73    4.80  AlAsO4:2H2O
       AlOHSO4          -1.69   -4.92   -3.23  AlOHSO4
       AlumK           -12.95  -18.20   -5.24  KAl(SO4)2:12H2O
       Alunite           8.78    7.45   -1.34  KAl3(SO4)2(OH)6
       Anglesite        -0.84   -8.65   -7.81  PbSO4
       Anhydrite         0.19   -4.41   -4.60  CaSO4
       Antlerite         5.26   13.55    8.29  Cu3(OH)4SO4
       Arsenolite     -124.25 -206.17  -81.92  As4O6
       As2O5           -33.84  -27.08    6.75  As2O5
       B_UO2(OH)2       -0.23    5.45    5.68  UO2(OH)2
       Basaluminite     10.83   33.53   22.70  Al4(OH)10SO4
       Bianchite        -2.82   -4.59   -1.76  ZnSO4:6H2O
       Birnessite        7.43   50.77   43.34  MnO2
       Bixbyite         13.50   63.54   50.04  Mn2O3
       Boehmite          3.96   12.82    8.86  AlOOH
       Brochantite       8.63   23.97   15.34  Cu4(OH)6SO4
       Bunsenite        -1.90   10.79   12.69  NiO
       Ca3(AsO4)2:6H2O  -9.42   12.88   22.30  Ca3(AsO4)2:6H2O
       Cd(Gamma)       -41.65  -27.88   13.77  Cd
       Cd(OH)2(A)       -3.82   10.12   13.94  Cd(OH)2
       Cd(OH)2(C)       -3.53   10.12   13.65  Cd(OH)2
       Cd3(OH)2(SO4)2  -11.83   -5.12    6.71  Cd3(OH)2(SO4)2
       Cd3(OH)4SO4      -9.95   12.61   22.56  Cd3(OH)4SO4
       Cd4(OH)6SO4      -5.67   22.73   28.40  Cd4(OH)6SO4
       CdMetal         -41.55  -27.88   13.67  Cd
       CdSO4            -7.66   -7.62    0.05  CdSO4
       CdSO4:2.67H2O    -5.79   -7.62   -1.83  CdSO4:2.67H2O
       CdSO4:H2O        -6.04   -7.62   -1.58  CdSO4:H2O
       Chalcanthite     -4.66   -7.31   -2.65  CuSO4:5H2O
       Claudetite     -124.00 -206.17  -82.17  As4O6
       Cu(OH)2           1.64   10.43    8.79  Cu(OH)2
       Cu2SO4          -27.57  -34.88   -7.31  Cu2SO4
       Cu3(AsO4)2:6H2O  -1.91    4.19    6.10  Cu3(AsO4)2:6H2O
       CuMetal         -15.94  -27.57  -11.63  Cu
       CuOCuSO4         -8.76    3.12   11.88  CuO:CuSO4
       CupricFerrite    20.22   26.48    6.27  CuFe2O4
       Cuprite         -10.12  -17.14   -7.02  Cu2O
       CuprousFerrite   11.04   -0.55  -11.59  CuFeO2
       CuSO4           -10.50   -7.31    3.19  CuSO4
       Diaspore          5.70   12.82    7.12  AlOOH
       Fe2(SO4)3       -41.32  -37.15    4.17  Fe2(SO4)3
       FeAsO4:2H2O      -5.92   -5.52    0.40  FeAsO4:2H2O
       Ferrihydrite      3.03    8.03    5.00  Fe(OH)3
       Gibbsite(C)       3.82   12.82    9.00  Al(OH)3
       Goethite          7.38    8.03    0.64  FeOOH
       Goslarite        -2.60   -4.59   -1.99  ZnSO4:7H2O
       Gummite          -5.18    5.45   10.63  UO3
       Gypsum            0.44   -4.41   -4.85  CaSO4:2H2O
       Hausmannite      13.97   76.31   62.34  Mn3O4
       Hematite         19.75   16.05   -3.70  Fe2O3
       Jarosite-H        0.16  -11.39  -11.55  (H3O)Fe3(SO4)2(OH)6
       Jarosite-K        7.56   -6.92  -14.49  KFe3(SO4)2(OH)6
       Jarosite-Na       4.77   -6.07  -10.84  NaFe3(SO4)2(OH)6
       Jurbanite        -1.69   -4.92   -3.23  AlOHSO4
       Langite           6.79   23.97   17.18  Cu4(OH)6SO4:H2O
       Larnakite         0.65    0.44   -0.22  PbO:PbSO4
       Lepidocrocite     6.66    8.03    1.37  FeOOH
       Lime            -19.93   13.32   33.26  CaO
       Litharge         -3.80    9.08   12.88  PbO
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       Maghemite          9.67   16.05    6.39  Fe2O3
       Manganite          6.76   31.77   25.01  MnOOH
       Massicot          -3.99    9.08   13.08  PbO
       Minium            -9.46   65.25   74.71  Pb3O4
       Mirabilite        -5.79   -7.09   -1.30  Na2SO4:10H2O
       Mn2(SO4)3        -34.84   10.34   45.18  Mn2(SO4)3
       Mn3(AsO4)2:8H2O   -1.28   11.22   12.50  Mn3(AsO4)2:8H2O
       MnSO4             -7.79   -4.96    2.82  MnSO4
       Monteponite       -5.25   10.12   15.37  CdO
       Morenosite        -4.56   -6.95   -2.39  NiSO4:7H2O
       Ni(OH)2            0.29   10.79   10.50  Ni(OH)2
       Ni3(AsO4)2:8H2O  -10.43    5.27   15.70  Ni3(AsO4)2:8H2O
       Ni4(OH)6SO4       -6.59   25.41   32.00  Ni4(OH)6SO4
       Nsutite            8.02   50.77   42.75  MnO2
       O2(g)             -8.46   76.00   84.45  O2
       Pb(OH)2(C)         0.79    9.08    8.29  Pb(OH)2
       Pb2O(OH)2         -8.03   18.17   26.20  Pb2O(OH)2
       Pb2O3             -4.87   56.17   61.04  Pb2O3
       Pb3(AsO4)2        -5.63    0.17    5.80  Pb3(AsO4)2
       Pb3O2SO4          -1.09    9.52   10.61  Pb3O2SO4
       Pb4(OH)6SO4       -2.50   18.60   21.10  Pb4(OH)6SO4
       Pb4O3SO4          -3.84   18.60   22.45  Pb4O3SO4
       PbMetal          -33.18  -28.91    4.27  Pb
       PbO:0.3H2O        -3.90    9.08   12.98  PbO:0.33H2O
       Plattnerite       -2.92   47.08   50.01  PbO2
       Portlandite       -9.66   13.32   22.98  Ca(OH)2
       Pyrocroite        -2.54   12.77   15.31  Mn(OH)2
       Pyrolusite         9.37   50.77   41.40  MnO2
       Retgersite        -4.90   -6.95   -2.05  NiSO4:6H2O
       Schoepite         -0.07    5.45    5.52  UO2(OH)2:H2O
       Schwertmannite    39.48   46.48    7.00  Fe8O8(OH)6(SO4)
       Tenorite           2.66   10.43    7.77  CuO
       Thenardite        -6.91   -7.09   -0.17  Na2SO4
       U3O8(C)          -15.23  -21.64   -6.41  U3O8
       U4O9(C)          -51.58  -92.19  -40.61  U4O9
       UO2(am)          -24.18  -32.55   -8.36  UO2
       UO3(C)            -2.46    5.45    7.91  UO3
       Uraninite        -18.47  -32.55  -14.07  UO2
       Zincite            1.79   13.15   11.36  ZnO
       Zincosite         -7.78   -4.58    3.20  ZnSO4
       Zn(OH)2(A)         0.70   13.15   12.45  Zn(OH)2
       Zn(OH)2(B)         1.40   13.15   11.75  Zn(OH)2
       Zn(OH)2(C)         0.95   13.15   12.20  Zn(OH)2
       Zn(OH)2(E)         1.65   13.15   11.50  Zn(OH)2
       Zn(OH)2(G)         1.44   13.15   11.71  Zn(OH)2
       Zn2(OH)2SO4        1.07    8.57    7.50  Zn2(OH)2SO4
       Zn3(AsO4)2:2.5H2O  -1.28   12.37   13.65  Zn3(AsO4)2:2.5H2O
       Zn3O(SO4)2       -15.65    3.99   19.64  Zn3O(SO4)2
       Zn4(OH)6SO4        6.47   34.87   28.40  Zn4(OH)6SO4
       ZnMetal          -50.97  -24.85   26.12  Zn
       ZnO(Active)        1.84   13.15   11.31  ZnO
       ZnSO4:H2O         -4.12   -4.58   -0.46  ZnSO4:H2O

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End of simulation.
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Reading input data for simulation 2.
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End of run.
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