308 - - - Q200405250002

Scientific Notebook No. 331: Development of a New Sorption Database for the Geochemist's Workbench (GWB), Release 3.0 (06/01/1999 through 04/06/2000)

222

21
150
R

LAUREN BROWNING

210-522-6642

SWRI/CNWRA

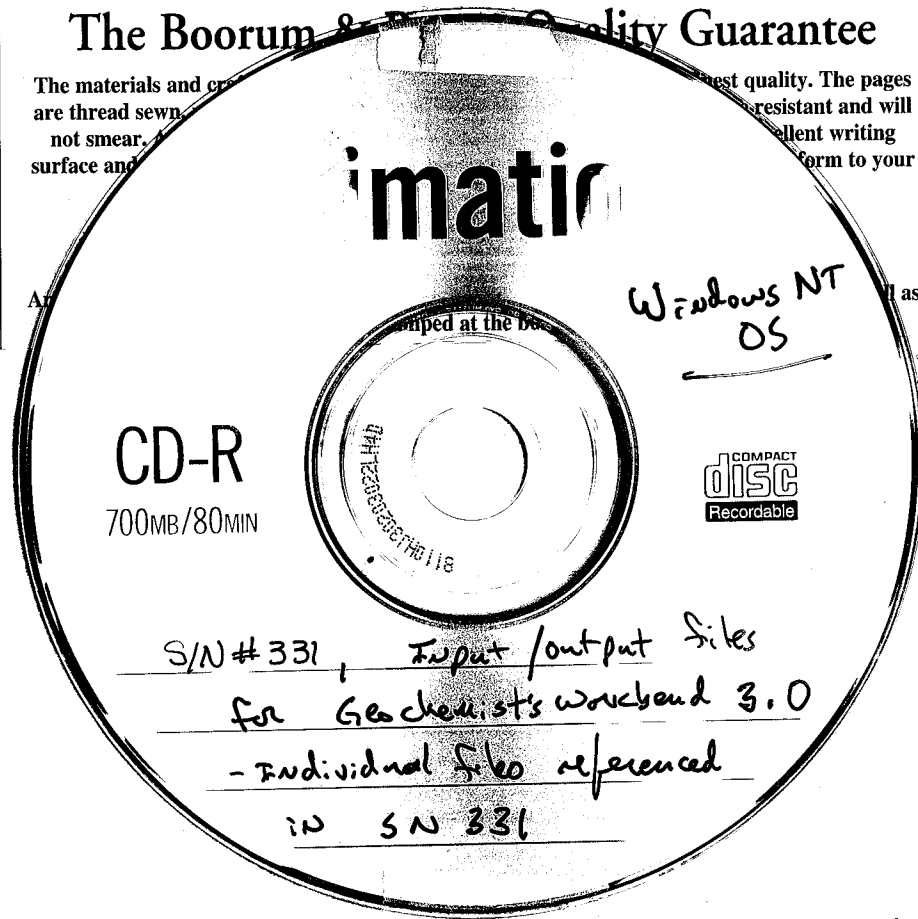
20-1402-871

CNWRA
CONTROLLED
COPY 331

The Boorum & [illegible] Quality Guarantee

The materials and cr[illegible]est quality. The pages
are thread sewn, [illegible]resistant and will
not smear. A[illegible]ellent writing
surface and [illegible]form to your

A[illegible]l as
[illegible]ped at the be[illegible]



Windows NT
OS

S/N #331, Input/output files
for Geochemist's workbench 3.0
- individual files referenced
in SN 331

designed books also available by special order. For more information about our Customized Book Program, contact your office products dealer. See back cover for other books in this series.
Made in Canada

Initial Entry 6-1-99

This notebook describes the development of a new sorption database for the geochemical modeling code called The Geochemist's Workbench (GWB), Release 3.0. The GWB is a commercially available set of software tools for conducting geochemical calculations, and was developed by Craig Bethke at the University of Illinois at Urbana-Champaign. The CNWRA copy of GWB was purchased from Rockware (Golden, Colorado; www.rockware.com) and installed on a Windows NT platform. Control issues for GWB are documented in the CNWRA scientific notebook #278 on Radionuclide Transport, maintained by R. Pabalan.

Formatting of the new sorption database will be modeled after the FeOH.dat database provided in the GWB 3.0 package. Data used in the construction of the new database will be primarily from:

Turner, D.R. 1995. A Uniform Approach to Surface Complexation Modeling of Radionuclide Sorption. CNWRA 95-001. San Antonio, TX: CNWRA.

The addition of ~~new~~ 6-1-99 data from other sources will be documented in this notebook, as appropriate. This notebook describes the new database, and will verify that ~~the~~ 6-1-99 the database is working as expected by comparison with modeling curves presented in Turner (1995). If time permits, an Application will be developed using the new sorption database. This notebook will be maintained by Lauren Browning, who is identified as LauBry or LB.

LB 6-1-99

Database Format

6-1-99

The format of all new GWB sorption databases must be compatible with the GWB coding. To accomplish this, all new databases will be designed after the FeOH.dat database that was included in the GWB 3.0 package. A hardcopy of this database is stapled below for reference. Any deviations ~~or patch~~ 6-1-99 from this design, if necessary, will be discussed in appropriate sections of this notebook.

VB
6-1-99

6-1-99
P. 7

FeOH.dat

```
Dataset of surface reactions for gwb programs
Dataset format: jun95
Surface type: HFO
*
* Based on data of Dzombak and Morel (1990)
* Entered by Amy Berger, November 1993.
*

   2 basis species

>(s)FeOH
     charge=  0.0       mole wt.=   72.8543
     3 elements in species
       1.000 Fe              1.000 O              1.000 H

>(w)FeOH
     charge=  0.0       mole wt.=   72.8543
     3 elements in species
       1.000 Fe              1.000 O              1.000 H

-end-

   3 sorbing minerals

Hematite
     surface area=    600.0000 m2/g
     2 sorption sites
     >(s)FeOH                    site density=      0.0100 mol/mol mineral
     >(w)FeOH                    site density=      0.4000 mol/mol mineral

Fe(OH)3(ppd)
     surface area=    600.0000 m2/g
     2 sorption sites
     >(s)FeOH                    site density=      0.0050 mol/mol mineral
     >(w)FeOH                    site density=      0.2000 mol/mol mineral

Goethite
     surface area=    600.0000 m2/g
     2 sorption sites
     >(s)FeOH                    site density=      0.0050 mol/mol mineral
     >(w)FeOH                    site density=      0.2000 mol/mol mineral

-end-

   39 surface species

>(s)FeO-
     charge= -1.0       mole wt.=   71.8464
     2 species in reaction
       1.000 >(s)FeOH       -1.000 H+
     log K=   8.9300    dlogK/dT=   0.0000

>(w)FeO-
     charge= -1.0       mole wt.=   71.8464
     2 species in reaction
       1.000 >(w)FeOH       -1.000 H+
     log K=   8.9300    dlogK/dT=   0.0000

>(s)FeOH2+
     charge=  1.0       mole wt.=   73.8622
     2 species in reaction
       1.000 >(s)FeOH        1.000 H+
     log K=  -7.2900    dlogK/dT=   0.0000
```

```
>(w)FeOH2+
     charge=  1.0       mole wt.=   73.8622
     2 species in reaction
       1.000 >(w)FeOH          1.000 H+
     log K=  -7.2900    dlogK/dT=   0.0000

>(s)FeOAg
     charge=  0.0       mole wt.=  179.7144
     3 species in reaction
       1.000 >(s)FeOH          1.000 Ag+              -1.000 H+
     log K=   1.7200    dlogK/dT=   0.0000

>(s)FeOHBa++
     charge=  2.0       mole wt.=  210.1843
     2 species in reaction
       1.000 >(s)FeOH          1.000 Ba++
     log K=  -5.4600    dlogK/dT=   0.0000

>(s)FeOHCa++
     charge=  2.0       mole wt.=  112.9343
     2 species in reaction
       1.000 >(s)FeOH          1.000 Ca++
     log K=  -4.9700    dlogK/dT=   0.0000

>(w)FeOCa+
     charge=  1.0       mole wt.=  111.9264
     3 species in reaction
       1.000 >(w)FeOH         -1.000 H+               1.000 Ca++
     log K=   5.8500    dlogK/dT=   0.0000

* >(s)FeOCd+
*      charge=  1.0       mole wt.=  184.2564
*      3 species in reaction
*        1.000 >(s)FeOH         -1.000 H+               1.000 Cd++
*      log K=  -0.4700    dlogK/dT=   0.0000

* >(w)FeOCd+
*      charge=  1.0       mole wt.=  184.2564
*      3 species in reaction
*        1.000 >(w)FeOH         -1.000 H+               1.000 Cd++
*      log K=   2.9000    dlogK/dT=   0.0000

>(s)FeOCrOH+
     charge=  1.0       mole wt.=  140.8497
     4 species in reaction
       1.000 >(s)FeOH         -2.000 H+               1.000 Cr+++
       1.000 H2O
     log K=  -2.0600    dlogK/dT=   0.0000

>(s)FeOCo+
     charge=  1.0       mole wt.=  130.7796
     3 species in reaction
       1.000 >(s)FeOH         -1.000 H+               1.000 Co++
     log K=   0.4600    dlogK/dT=   0.0000

>(w)FeOCo+
     charge=  1.0       mole wt.=  130.7796
     3 species in reaction
       1.000 >(w)FeOH         -1.000 H+               1.000 Co++
     log K=   3.0100    dlogK/dT=   0.0000

>(s)FeOCu+
```

```
      charge=  1.0       mole wt.=  135.3924
      3 species in reaction
        1.000 >(s)FeOH       -1.000 H+              1.000 Cu++
      log K=  -2.8900    dlogK/dT=   0.0000

>(s)FeONi+
      charge=  1.0       mole wt.=  130.5564
      3 species in reaction
        1.000 >(s)FeOH       -1.000 H+              1.000 Ni++
      log K=  -0.3700    dlogK/dT=   0.0000

>(s)FeOHg+
      charge=  1.0       mole wt.=  272.4364
      3 species in reaction
        1.000 >(s)FeOH       -1.000 H+              1.000 Hg++
      log K=  -7.7600    dlogK/dT=   0.0000

>(w)FeOHg+
      charge=  1.0       mole wt.=  272.4364
      3 species in reaction
        1.000 >(w)FeOH       -1.000 H+              1.000 Hg++
      log K=  -6.4500    dlogK/dT=   0.0000

>(s)FeOPb+
      charge=  1.0       mole wt.=  279.0464
      3 species in reaction
        1.000 >(s)FeOH       -1.000 H+              1.000 Pb++
      log K=  -4.6500    dlogK/dT=   0.0000

>(s)FeOHSr++
      charge=  2.0       mole wt.=  160.4743
      2 species in reaction
        1.000 >(s)FeOH        1.000 Sr++
      log K=  -5.0100    dlogK/dT=   0.0000

>(w)FeOSr+
      charge=  1.0       mole wt.=  159.4664
      3 species in reaction
        1.000 >(w)FeOH        1.000 Sr++            -1.000 H+
      log K=   6.5800    dlogK/dT=   0.0000

>(w)FeOSrOH
      charge=  0.0       mole wt.=  176.4737
      4 species in reaction
        1.000 >(w)FeOH        1.000 Sr++            -2.000 H+
        1.000 H2O
      log K=  17.6000    dlogK/dT=   0.0000

>(s)FeOZn+
      charge=  1.0       mole wt.=  137.2264
      3 species in reaction
        1.000 >(s)FeOH       -1.000 H+              1.000 Zn++
      log K=  -0.9900    dlogK/dT=   0.0000

>(w)FeOZn+
      charge=  1.0       mole wt.=  137.2264
      3 species in reaction
        1.000 >(w)FeOH       -1.000 H+              1.000 Zn++
      log K=   1.9900    dlogK/dT=   0.0000

>(w)FeH2AsO3
      charge=  0.0       mole wt.=  180.7826
      3 species in reaction
```

```
      1.000 >(w)FeOH          1.000 As(OH)3          -1.000 H2O
     log K=  -5.4100    dlogK/dT=   0.0000

>(w)FeH2AsO4
     charge=  0.0       mole wt.=  196.7820
     4 species in reaction
      1.000 >(w)FeOH          1.000 AsO4---          -1.000 H2O
      3.000 H+
     log K= -29.3100    dlogK/dT=   0.0000

>(w)FeHAsO4-
     charge= -1.0       mole wt.=  195.7741
     4 species in reaction
      1.000 >(w)FeOH          1.000 AsO4---           2.000 H+
     -1.000 H2O
     log K= -23.5100    dlogK/dT=   0.0000

>(w)FeOHAsO4---
     charge= -3.0       mole wt.=  211.7740
     2 species in reaction
      1.000 >(w)FeOH          1.000 AsO4---
     log K= -10.5800    dlogK/dT=   0.0000

>(w)FeH2BO3
     charge=  0.0       mole wt.=  116.6720
     3 species in reaction
      1.000 >(w)FeOH          1.000 B(OH)3           -1.000 H2O
     log K=  -0.6200    dlogK/dT=   0.0000

>(w)FeCrO4-
     charge= -1.0       mole wt.=  171.8406
     4 species in reaction
      1.000 >(w)FeOH          1.000 H+               1.000 CrO4--
     -1.000 H2O
     log K= -10.8500    dlogK/dT=   0.0000

>(w)FeH2PO4
     charge=  0.0       mole wt.=  152.8342
     4 species in reaction
      1.000 >(w)FeOH          1.000 PO4---           3.000 H+
     -1.000 H2O
     log K= -31.2900    dlogK/dT=   0.0000

>(w)FeHPO4-
     charge= -1.0       mole wt.=  151.8263
     4 species in reaction
      1.000 >(w)FeOH          2.000 H+               1.000 PO4---
     -1.000 H2O
     log K= -25.3900    dlogK/dT=   0.0000

>(w)FePO4--
     charge= -2.0       mole wt.=  150.8184
     4 species in reaction
      1.000 >(w)FeOH          1.000 H+               1.000 PO4---
     -1.000 H2O
     log K= -17.7200    dlogK/dT=   0.0000

>(w)FeSO4-
     charge= -1.0       mole wt.=  151.9046
     4 species in reaction
      1.000 >(w)FeOH          1.000 H+               1.000 SO4--
     -1.000 H2O
     log K=  -7.7800    dlogK/dT=   0.0000
```

```
>(w)FeOHSO4--
     charge= -2.0        mole wt.=  168.9119
     2 species in reaction
       1.000 >(w)FeOH          1.000 SO4--
     log K=  -0.7900     dlogK/dT=   0.0000

*>(w)FeOHS2O3--
*     charge= -2.0        mole wt.=  184.9725
*     2 species in reaction
*       1.000 >(w)FeOH          1.000 S2O3--
*     log K=  -0.4900     dlogK/dT=   0.0000
*
>(w)FeSeO4-
     charge= -1.0        mole wt.=  198.8046
     4 species in reaction
       1.000 >(w)FeOH          1.000 SeO4--          -1.000 H2O
       1.000 H+
     log K=  -7.7300     dlogK/dT=   0.0000

>(w)FeOHSeO4--
     charge= -2.0        mole wt.=  215.8119
     2 species in reaction
       1.000 >(w)FeOH          1.000 SeO4--
     log K=  -0.8000     dlogK/dT=   0.0000

>(w)FeSeO3-
     charge= -1.0        mole wt.=  182.8052
     4 species in reaction
       1.000 >(w)FeOH          1.000 SeO3--          -1.000 H2O
       1.000 H+
     log K= -12.6900     dlogK/dT=   0.0000

>(w)FeOHSeO3--
     charge= -2.0        mole wt.=  199.8125
     2 species in reaction
       1.000 >(w)FeOH          1.000 SeO3--
     log K=  -5.1700     dlogK/dT=   0.0000

>(w)FeOHVO4---
     charge= -3.0        mole wt.=  187.7933
     2 species in reaction
       1.000 >(w)FeOH          1.000 VO4---
     log K= -13.5700     dlogK/dT=   0.0000

-end-

Data Template

>__________________
     charge= __._        mole wt.=_____.____
     4 species in reaction
     ___.___ (species)     ___.___ (species)     ___.___ (species)
     ___.___ (species)
     log K=_____.____    dlogK/dT= _____.____
```

FeOHNpAll3.dat 6-30-99

The new sorption database FeOHNpAll3.dat is stapled below. This database describes Np species sorption onto 3 different minerals: Fe(OH)3(ppd), Goethite, & Magnetite. To prepare this database:

1) Surface species were selected from Turner (1995) based on how well the surface species modeling curves matched the data.

2) One ~~form~~ Np-based surface species was selected for each sorbing mineral.

3) surface complexation model binding constants were taken from Appendix B (Turner, 1995)

4) Diffuse Layer model data from Turner (1995) was used.

5) Because protonation/deprotonation log k values differ for each mineral, dummy basis species were constructed.
ex >FeOH is the basis species for Fe(OH)3(ppd)
>g-FeOH " " " Goethite
>m-FeOH " " " Magnetite

6) Note that the surface species reactions have log k values that differ in sign from Turner (1995), because the reactions must be written in reverse order for GWB.

7) Site densities were calculated from sites/NM^2 to mol sites/mol mineral.

ex (Goethite-Np):

LB 6-30-99

FeOHNpAll3.dat (continued) 6-30-99

ex. (Goethite-Np) - continued

$$\text{site density} = 2.31 \frac{\text{sites}}{NM^2} \cdot \frac{(1E9\,NM)^2}{m^2} \cdot \frac{15.7\,m^2}{g} \cdot \frac{88.854\,g}{mol} \cdot \frac{\text{mol sites}}{6.022E23\ \text{site}}$$
$$= 0.0535$$

8) Sorption reactions were written

NOTE: For simplicity, the general approach taken here is to develop databases for individual classes of surface species, such as Np in this case, and then make efforts to link the individual databases together.

LB 6-30-99

FeOHNpAl13.dat (continued) 6-30-99

```
                                                    FEOHNpAl13.dat
Dataset of surface reactions for gwb programs
Dataset format: jun95
Surface type:
*
* Based on calculations of David Turner: a DT Uniform Approach, CNWRA 95-001
* Entered by Lauren Browning, May 1999.
*

   3 basis species

>FeOH
     charge=  0.0       mole wt.=   72.8543
     3 elements in species
       1.000 Fe              1.000 O              1.000 H

>g-FeOH
     charge=  0.0       mole wt.=   72.8543
     3 elements in species
       1.000 Fe              1.000 O              1.000 H

>m-FeOH
     charge=  0.0       mole wt.=   72.8543
     3 elements in species
       1.000 Fe              1.000 O              1.000 H

-end-

   3 sorbing mineral

Fe(OH)3(ppd)
     surface area=    600.0000 m2/g
     1 sorption sites
     >FeOH                    site density=      0.2050 mol/mol mineral

Goethite
     surface area=     15.7000 m2/g
     1 sorption sites
     >g-FeOH                  site density=     0.00535 mol/mol mineral

Magnetite
     surface area=      5.5000 m2/g
     1 sorption sites
     >m-FeOH                  site density=     0.00489 mol/mol mineral

-end-

   9 surface species


>FeO-
     charge= -1.0       mole wt.=   71.8464
     2 species in reaction
       1.000 >FeOH        -1.000 H+
     log K=   8.9300    dlogK/dT=   0.0000


>FeOH2+
     charge=  1.0       mole wt.=   73.8622
     2 species in reaction
       1.000 >FeOH         1.000 H+
     log K=  -7.2900    dlogK/dT=   0.0000
```

FeOHNpAll3.dat (continued) 6-30-99


```
>FeO-NpO2
     charge=  0.0        mole wt.=   340.9007
     3 species in reaction
       1.000 >FeOH          1.000 NpO2+         -1.000 H+
     log K=  3.02     dlogK/dT=   0.0000

>g-FeO-
     charge= -1.0        mole wt.=   71.8464
     2 species in reaction
       1.000 >g-FeOH       -1.000 H+
     log K=   9.1700     dlogK/dT=   0.0000


>g-FeOH2+
     charge=  1.0        mole wt.=   73.8622
     2 species in reaction
       1.000 >g-FeOH        1.000 H+
     log K=  -7.3500     dlogK/dT=   0.0000


>FeOH2-NpO2OH+
     charge=  1.0        mole wt.=   359.9164
     3 species in reaction
       1.000 >g-FeOH     1.000 NpO2+          1.000 H2O
     log K=  -5.21       dlogK/dT=   0.0000

>m-FeO-
     charge= -1.0        mole wt.=   71.8464
     2 species in reaction
       1.000 >m-FeOH       -1.000 H+
     log K=   6.3700     dlogK/dT=   0.0000


>m-FeOH2+
     charge=  1.0        mole wt.=   73.8622
     2 species in reaction
       1.000 >m-FeOH        1.000 H+
     log K=  -6.7200     dlogK/dT=   0.0000


>FeOH2-NpO2OH+
     charge=  1.0        mole wt.=   359.9164
     3 species in reaction
       1.000 >m-FeOH     1.000 NpO2+          1.000 H2O
     log K=  -3.55       dlogK/dT=   0.0000

-end-

Data Template

>____________________
     charge= __._        mole wt.=_____.____
     4 species in reaction
     ___.___ (species)      ___.___ (species)      ___.___ (species)
     ___.___ (species)
     log K=_____.____     dlogK/dT= _____.____
```

Np(V)-goethite sorption 10-28-99

Binding constants for Np(V)-goethite sorption were taken from Turner (1995), and are stapled below. Input/Output files relevant to Np(V)-Goethite sorption are located at:
D:\Reds.Transport\FeO-Np-Ferr-Goet-Mt\FeO-Np-Goet

LB 10-28-99

Table B-5. Neptunium (V)-goethite sorption binding constants: monodentate, mononuclear compounds

Solid: Natural Goethite A_{SP}: 15.7 m^2/g Data Source: Nakayama and Sakamoto (1991) Concentration: [Np(V)] = 6E-6 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0E-9	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_S = 2.31 sites/nm^2 M/V = 1 g/L

No CO_2	DLM			CCM			TLM		
	$Log K_+$ = 7.35 $Log K_-$ = −9.17			$Log K_+$ = 6.47 $Log K_-$ = −9.03			$Log K_+$ = 6.00 $Log K_-$ = −10.00 $Log K_{Cat}$ = −7.64 $Log K_{An}$ = 8.78		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
XO-NpO_2^o	−2.54	16.7	.0253	−2.60	14.6	.0242	−5.43	93.4	.0401
XOH-NpO_2^+	5.21	8.4	.0195	4.75	6.3	.0189	2.34	95.1	.0472
XO-NpO_2OH^-	−10.39	23.4	.0312	−9.92	21.5	.0305	−9.98	6.3	.0283
XOH-NpO_2OH^o	−2.54	16.7	.0253	−2.60	14.6	.0242	−2.44	14.1	.0239
XOH_2-NpO_2OH^+	5.21	8.4	.0195	4.75	6.3	.0189	5.86	6.9	.0257
OTHER SPECIES									
$(XO)_2$-NpO_2^-	−5.96	23.0	.0334	−5.54	20.7	.0320	−8.61	88.8	.0335

LB

Np(V) Goethite Sorption (cont.) 10-28-99

The react script NpGoet (stapled below) is an example of how the database was benchmarked. This same file was run multiple times, with only the pH changed. Because the extent of sorption varies strongly with pH, this approach allows the benchmarking against modeling & experimental curves in Turner (1995).

10-28-99

NpGoet

```
# React script, saved Tue Apr 04 2000 by lbrowning
data = thermo.dat verify
surface_data = D:\Radio.Transport\FeO-NpO2-Ferrihydrite\FEOHNpAll.dat
work_dir  =  D:\
temperature = 25
decouple Fe+++
swap Goethite for Fe+++
swap O2(g) for O2(aq)
swap NpO2+ for Np++++
1 kg free H2O
free gram Goethite = 1
fugacity O2(g) = .2
total molality NpO2+ = 6e-6
pH = 8
balance on NO3-
total molality NO3- = .1
total molality Na+ = .1

suppress  Fe(OH)2+ Fe(OH)3 FeOH++
suppress ALL
unsuppress  Fe(OH)3(ppd) Goethite
```

Note that a few aqueous species (see ✱) were suppressed. This was necessary to improve the benchmarking, & will be checked again when the compiled database is complete to see if it is still necessary.

LB 10-28-99

Np(V) Goethite Sorption (cont.)

10-28-99

Attached below is an example of NpGoet output, with pH set to 6. The predicted fraction of Np sorbed is circled on pg 2.

OutputNpGoetpH=6.txt

Step # 0
Temperature = 25.0 C
pH = 6.000
Eh = 0.8637 volts
Xi = 0.0000
Pressure = 1.013 bars
log fO2 = -0.699
pe = 14.6010

Ionic strength	=	0.100017
Activity of water	=	1.000000
Solvent mass	=	1.000000 kg
Solution mass	=	1.008511 kg
Solution density	=	1.013 g/cm3
Chlorinity	=	0.000000 molal
Dissolved solids	=	8439 mg/kg sol'n
sorbing surface:		
Surface charge	=	11.9 uC/cm2
Surface potential	=	96.8 mV
Surface area	=	1.57e+005 cm2

Nernst redox couples	Eh (volts)	pe
e- + .25*O2(aq) + H+ = .5*H2O	0.8637	14.6010

Minerals in system	moles	log moles	grams	volume (cm3)
Goethite	0.01125	-1.949	1.000	0.2343
(total)			1.000	0.2343

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.1000	6150.	0.7609	-1.1186
Na+	0.1000	2280.	0.7768	-1.1097
O2(aq)	0.0002460	7.804	1.0260	-3.5980
NpO2+	5.995e-006	1.599	0.7768	-5.3319
H+	1.200e-006	0.001199	0.8334	-6.0000
OH-	1.340e-008	0.0002260	0.7691	-7.9868

(only species > 1e-8 molal listed)

Surface species	molality	moles	Boltzman fct.	log molality
>g-FeOH	3.852e-005	3.852e-005	1.0000	-4.4143
>g-FeOH2+	1.989e-005	1.989e-005	43.352	-4.7013
>g-FeO-	1.129e-006	1.129e-006	0.023067	-5.9473
>FeOH2-NpO2OH+	6.711e-007	6.711e-007	43.352	-6.1732

(Boltzman factor = exp(zF PSI/RT), where PSI is surface potential)

Mineral saturation states	log Q/K		log Q/K
Hematite	0.9565s/sat	NpO2	-1.2191
Goethite	0.0000 sat		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
N2(g)	1.597e-010	-9.797
H2(g)	6.282e-042	-41.202

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg
>FeOH	0.0000				

>Fe-OH	6.021e-005				
Fe+++	0.01125	9.439e-016	5.227e-011		
H+	-0.03376	-1.682e-005	-0.01681	1.675e-005	0.01674
H2O	55.53	55.51	9.916e+005	1.678e-006	0.02997
NO3-	0.1000	0.1000	6150.		
Na+	0.1000	0.1000	2280.		
Np++++	6.671e-006	6.000e-006	1.410	6.711e-007	0.1577
O2(aq)	0.0002476	0.0002475	7.852	1.678e-007	0.005323

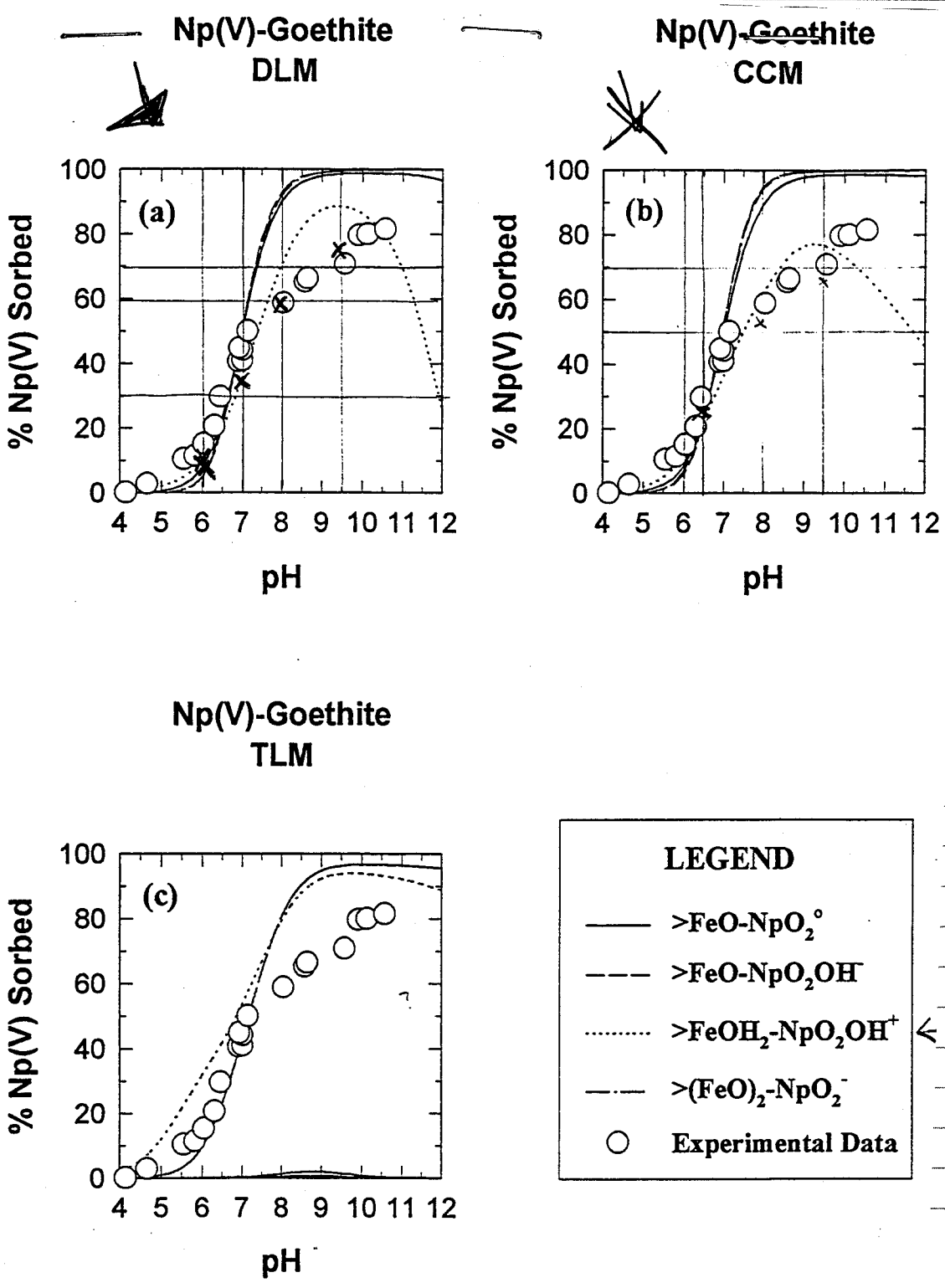
Sorbed	fraction	log fraction
Np++++	0.1006	-0.997

Elemental composition	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg
Hydrogen	111.0	111.0	1.110e+005	2.011e-005	0.02009
Iron	0.01125	9.439e-016	5.227e-011		
Neptunium	6.671e-006	6.000e-006	1.410	6.711e-007	0.1577
Nitrogen	0.1000	0.1000	1389.		
Oxygen	55.83	55.81	8.854e+005	2.013e-006	0.03194
Sodium	0.1000	0.1000	2280.		

10

Np (V) Sorption of Goethite (continued) 10-28-99

Qualitative comparisons were made between Turner's (1995) calculated & experimental curves for the diffuse layer model (DLM). Points calculated in this study are indicated by X's.



10-28-99

Figure 4-5. Np(V) sorption on goethite. SCM results are calculated using parameters derive the experimental data shown in the figure, and assuming a single adsorbed species (see (a) DLM; (b) CCM; and (c) TLM results. $Np(V)_T = 6 \times 10^{-6}$ M, 0.1 M $NaNO_3$, M/V = 1 g/L. parameters from Tables 3-1 and B-5. Data from Nakayama and Sakamoto (1991).

Np(V)-Ferrihydrite Sorption 10-28-99

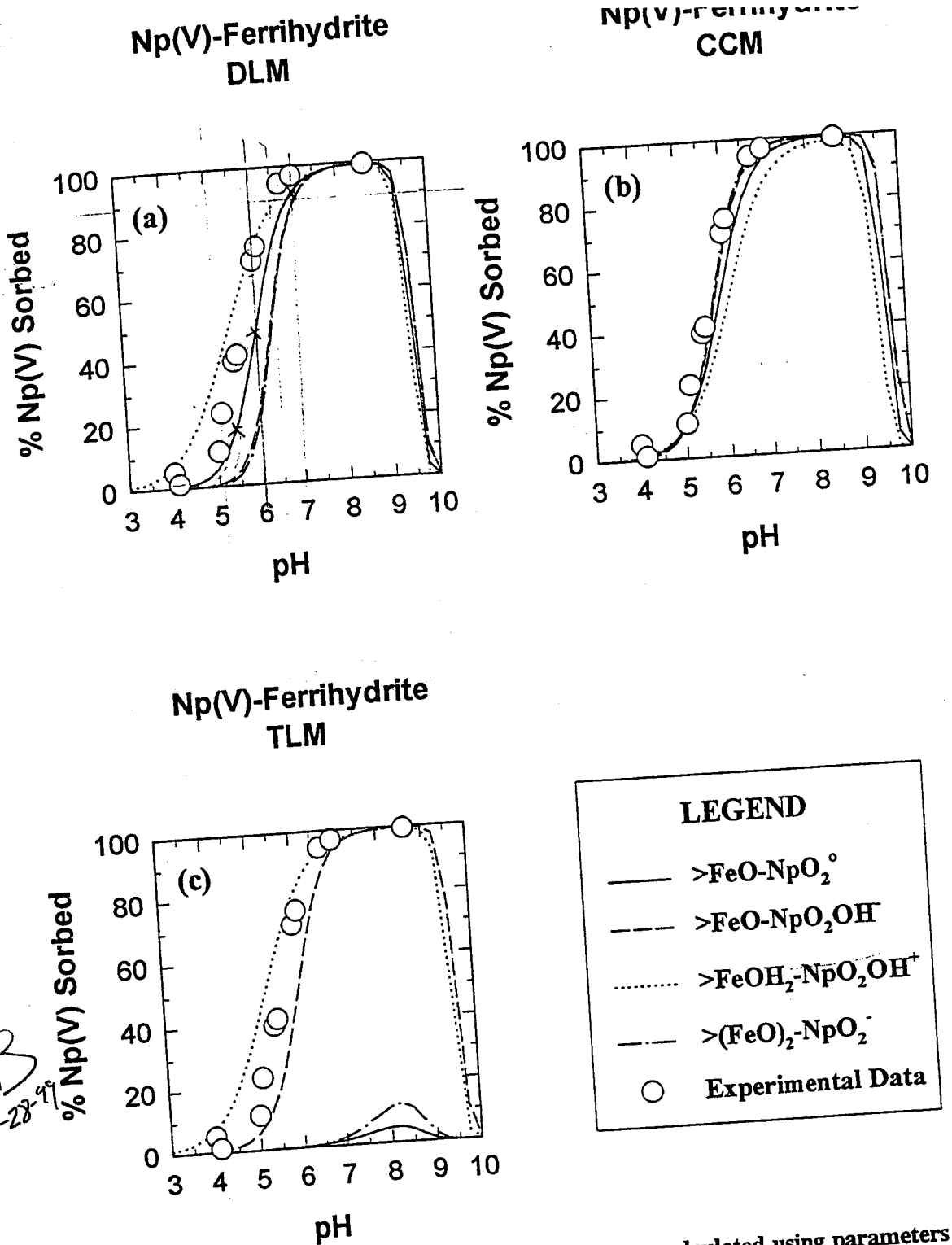


Figure 4-10. Np(V) sorption on ferrihydrite. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $Np(V)_T = 4.7 \times 10^{-12}$ M, 0.1 M $NaNO_3$, M/V=0.89 g/L. Model parameters from Tables 3-1 and B-10. Data from Girvin et al. (1991).

Np(V)-Ferrihydrite Sorption

10-28-99

Input/Output files relevant to Np(V)-Ferrihydrite sorption are located at:
D:\Radio.Transport\FeO-Np-Ferri-Goet-Mt\FeO-NpO_2-Ferrihydrite

GWB input file & benchmarking results are attached below.

GWB file: Dave2.

```
React> show
    Temperature is 25 C
    Thermo dataset:  thermo.dat
    Surface reactions:  FeOH.dat ()
    Working directory:  d:\
    Options: Debye-Huckel

    Basis is:
    H2O                  1 kg solvent
    Fe(OH)3(ppd)  (swapped for Fe+++)  free gram = 1
    O2(g)  (swapped for O2(aq))    fugacity = .2
    NpO2+  (swapped for Np++++)    total molality = 4.70002318e-12
    H+                   pH = 7
    NO3-                 total molality = .1 (charge balance)
    Na+                  total molality = .1

    No reactants specified.

    Other "show" options: type "show show"
```

Np(V) - Magnetite Sorption

10-28-99

Input/Output files relevant to Np(V)-Magnetite Sorption are located at:

~~D:\Radio Transport\FeO Np Ferri-Goet-Mt\FeO Np Mt~~

GWB input file & Benchmarking results are attached below

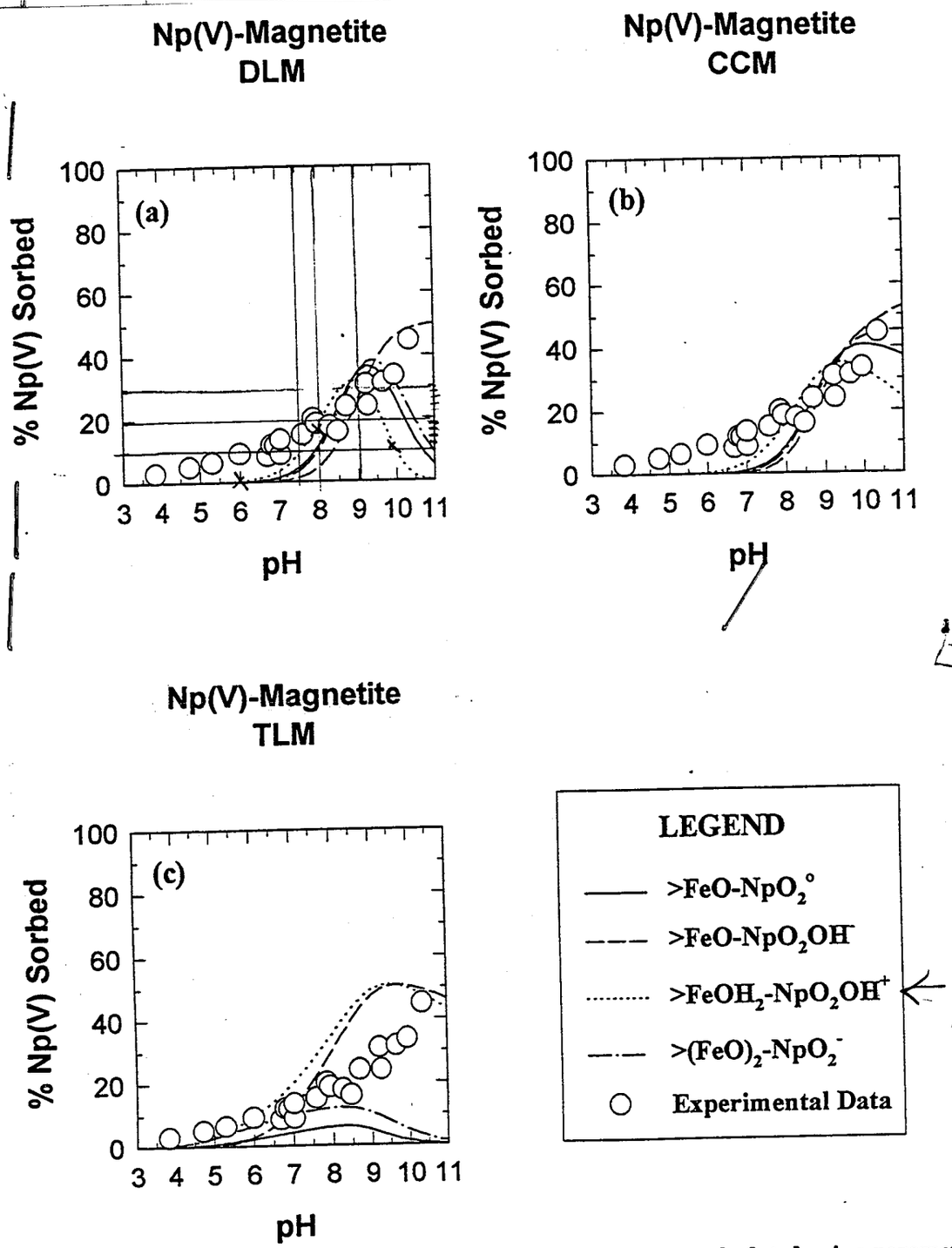
NpMt

```
# React script, saved Wed Apr 05 2000 by lbrowning
data = thermo.dat verify
work_dir  =  D:\
temperature = 25
swap O2(g) for O2(aq)
swap NpO2+ for Np++++
swap Magnetite for Fe++
1 kg free H2O
fugacity O2(g) = .199986187
total molality NpO2+ = 6e-6
pH = 9
balance on NO3-
total molality NO3- = .1
total molality Na+ = .1
free gram Magnetite = 1


suppress ALL
unsuppress  Magnetite
```

GWB file: NpMt

LB



LB

Figure 4-6. Np(V) sorption on synthetic magnetite. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $Np(V)_T = 6 \times 10^{-6}$ M, 0.1 M $NaNO_3$, M/V=1 g/L. Model parameters from Tables 3-1 and B-6. Data from Nakayama and Sakamoto (1991).

U(VI) sorption on Goethite, Magnetite, & Ferrihydrite

Input/Output files relevant to U(VI) sorption on Goethite, Magnetite, & Ferrihydrite are located at:

D:|Radio.Transport|FeO-UO_2-Ferri-Goet-Mt|

Folder names for the following are:

for Goethite : U-Goethite

for Magnetite : U-Mt

for Ferrihydrite: U-Ferrihydrite

DatabASE : not in subfolder

LB 4-6-00

14

U(VI) Sorption (continued) 4-6-99

Information needed to model U(VI) sorption on Magnetite, Goethite, & Ferrihydrite is presented in the database Attached below:

VB

FEOHU3.dat

```
Dataset of surface reactions for gwb programs
Dataset format: jun95
Surface type:
*
* Based on calculations of David Turner: a DT Uniform Approach, CNWRA 95-001
* Entered by Lauren Browning, June 1999.
*

   3 basis species

>FeOH
     charge=  0.0       mole wt.=   72.8543
     3 elements in species
       1.000 Fe              1.000 O              1.000 H

>g-FeOH
     charge=  0.0       mole wt.=   72.8543
     3 elements in species
       1.000 Fe              1.000 O              1.000 H

>m-FeOH
     charge=  0.0       mole wt.=   72.8543
     3 elements in species
       1.000 Fe              1.000 O              1.000 H

-end-

   3 sorbing minerals

Fe(OH)3(ppd)
     surface area=    600.0000 m2/g
     1 sorption sites
     >FeOH                 site density=      0.2050 mol/mol mineral

Goethite
     surface area=     50.0000 m2/g
     1 sorption sites
     >g-FeOH               site density=      0.0170 mol/mol mineral

Magnetite
     surface area=      5.0000 m2/g
     1 sorption sites
     >m-FeOH               site density=      0.00444 mol/mol mineral

-end-

   9 surface species


>FeO-
     charge= -1.0       mole wt.=   71.8464
     2 species in reaction
       1.000 >FeOH        -1.000 H+
     log K=   8.9300    dlogK/dT=   0.0000


>FeOH2+
     charge=  1.0       mole wt.=   73.8622
     2 species in reaction
       1.000 >FeOH         1.000 H+
     log K=  -7.2900    dlogK/dT=   0.0000
```

U(VI) Sorption (continued) 4-6-99

Information needed to model U(VI) sorption on Magnetite, Goethite, & Ferrihydrite is presented in the database attached below:

FEOHU3.dat

```
>FeO-UO2OH
     charge=  0.0       mole wt.=   358.8815
     4 species in reaction
       1.000 >FeOH        1.000 UO2++       -2.000 H+
       1.000 H2O
     log K=  3.65    dlogK/dT=   0.0000


>g-FeO-
     charge= -1.0       mole wt.=   71.8464
     2 species in reaction
       1.000 >g-FeOH       -1.000 H+
     log K=   9.1700    dlogK/dT=   0.0000


>g-FeOH2+
     charge=  1.0       mole wt.=   73.8622
     2 species in reaction
       1.000 >g-FeOH        1.000 H+
     log K=  -7.3500    dlogK/dT=   0.0000


>FeO-UO2OH
     charge=  0.0       mole wt.=   358.8815
     4 species in reaction
       1.000 >g-FeOH        1.000 UO2++       -2.000 H+
       1.000 H2O
     log K=  3.54    dlogK/dT=   0.0000

>m-FeO-
     charge= -1.0       mole wt.=   71.8464
     2 species in reaction
       1.000 >m-FeOH       -1.000 H+
     log K=   6.3700    dlogK/dT=   0.0000


>m-FeOH2+
     charge=  1.0       mole wt.=   73.8622
     2 species in reaction
       1.000 >m-FeOH        1.000 H+
     log K=  -6.7200    dlogK/dT=   0.0000


>FeO-UO2OH
     charge=  0.0       mole wt.=   358.8815
     4 species in reaction
       1.000 >m-FeOH        1.000 UO2++       -2.000 H+
       1.000 H2O
     log K=  4.69    dlogK/dT=   0.0000


-end-

Data Template

>_____
     charge= __._       mole wt.=_____.____
     4 species in reaction
     ___.___ (species)     ___.___ (species)     ___.___ (species)
     ___.___ (species)
     log K=_____.____    dlogK/dT= _____.____
```

U(VI) on Goethite

U(VI) Sorption (continued) 4-6-00

GWB Input file for U(VI) sorption & benchmark results are attached below. (for Goethite)

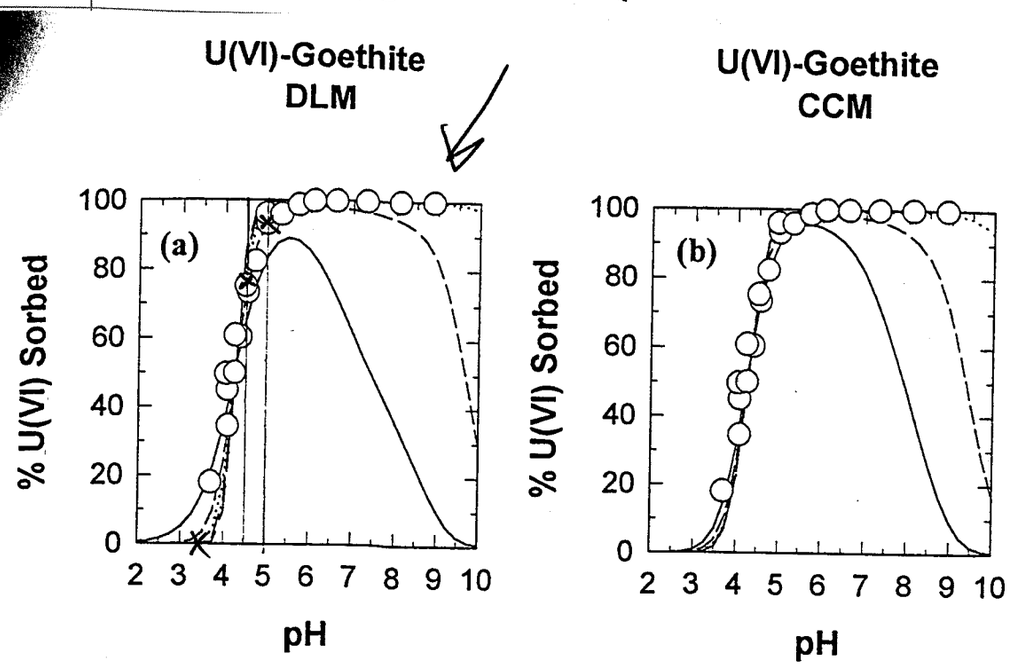
DaveU
GWB input File (configured for Goethite): DaveU

```
# React script, saved Thu Jun 10 1999 by lbrowning
data = thermo.dat verify
surface_data = "C:\program files\gwb\gtdata\FEOHU.dat"
work_dir  =  D:\
temperature = 25
swap O2(g) for O2(aq)
swap UO2++ for U++++
swap Goethite for Fe++
1 kg free H2O
fugacity O2(g) = .2
total molality UO2++ = 1e-5
free gram Goethite = 1
pH = 3.5
total molality NO3- = .1
balance on Na+
total molality Na+ = .1

suppress ALL
unsuppress  Goethite
```

LB
4-6-00

Goethite-U(VI) sorption (continued) 4-6-00



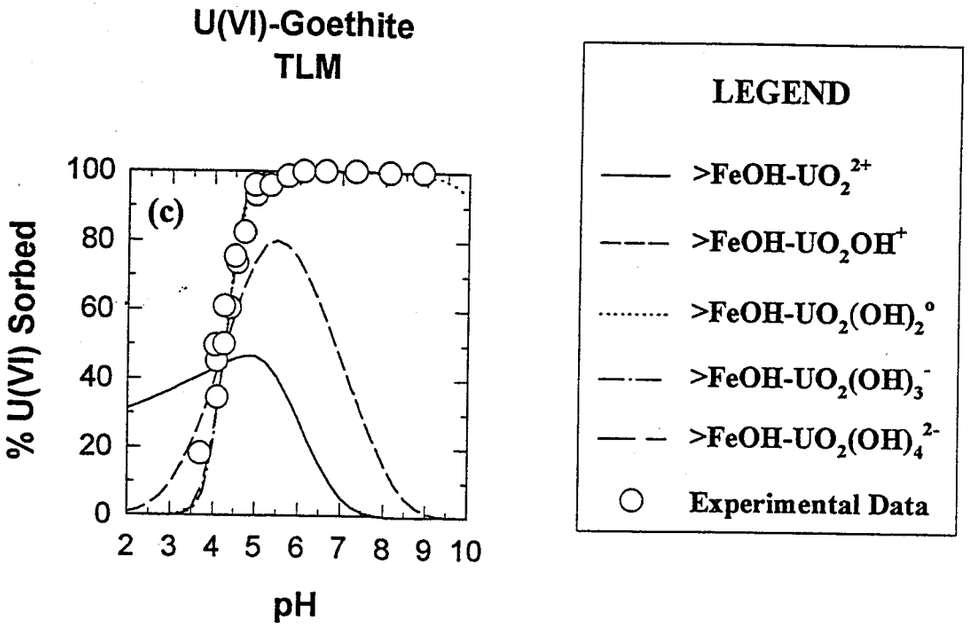


Figure 4-19. U(VI) sorption on goethite. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $U(VI)_T = 1 \times 10^{-5}$ M, 0.1 M $NaNO_3$, M/V=1 g/L. Model parameters from Tables 3-1 and B-19. Data from Hsi and Langmuir (1985).

LB 4-6-00

U(VI) on Ferrihydrite

U(VI) Sorption (continued) 4-6-00

GWB input file for U(VI) sorption on ferrihydrite, & benchmark curves are shown below.

```
                                                    UFerri
# React script, saved Tue Apr 04 2000 by lbrowning
data = thermo.dat verify
surface_data = "C:\program files\gwb\gtdata\FEOHU.dat"
work_dir  =  D:\
temperature = 25
swap O2(g) for O2(aq)
swap UO2++ for U++++
swap Fe(OH)3(ppd) for Fe++
1 kg free H2O
fugacity O2(g) = .2
total molality UO2++ = 1e-5
pH = 5
total molality NO3- = .1
balance on Na+
total molality Na+ = .1
free gram Fe(OH)3(ppd) = 1


suppress ALL
unsuppress  Fe(OH)3(ppd)
```

LB 4-6-00

U(VI) Sorption on Ferrihydrite (cont.)

4-6-00

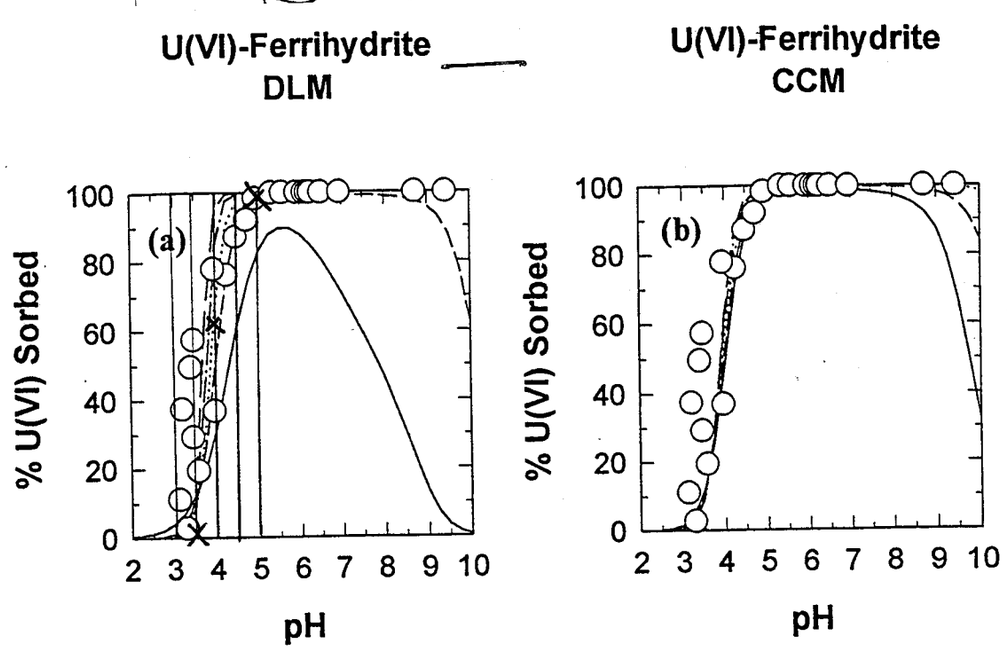


Figure 4-18. U(VI) sorption on ferrihydrite. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $U(VI)_T = 1 \times 10^{-5}$ M, 0.1 M $NaNO_3$, M/V=1 g/L. Model parameters from Tables 3-1 and B-18. Data from Hsi and Langmuir (1985).

LB 4-6-00

U(VI) Sorption on Magnetite

GWB input file & corresponding benchmark results are attached below.

UMt2

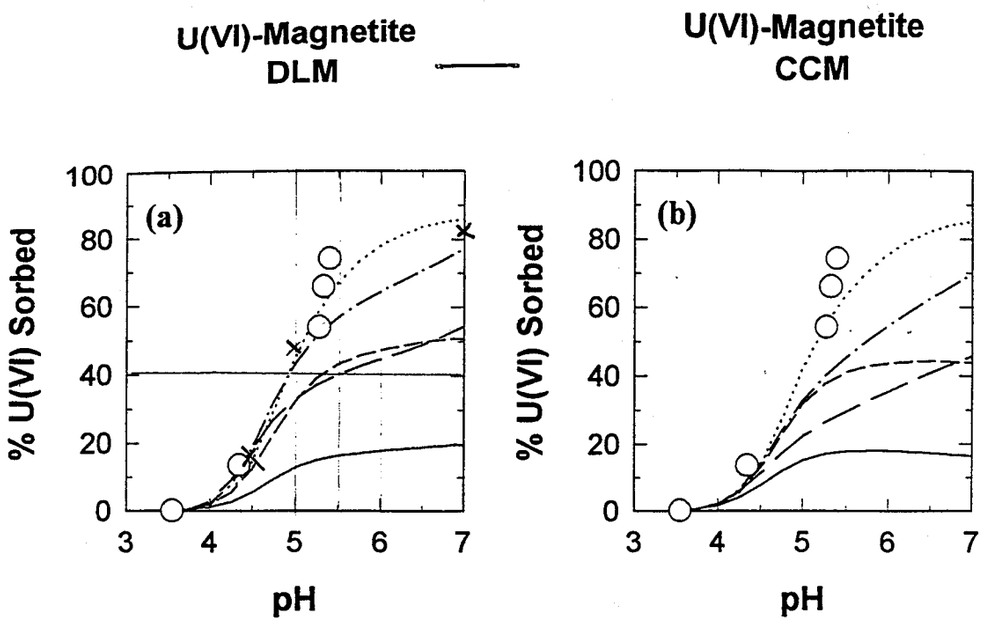
```
# React script, saved Thu Apr 06 2000 by lbrowning
data = thermo.dat verify
surface_data = D:\Radio.Transport\FeO-UO2-Ferri_Goethite\FEOHU3.dat
work_dir  =  D:\
temperature = 25
swap O2(g) for O2(aq)
swap UO2++ for U++++
swap Magnetite for Fe++
1 kg free H2O
fugacity O2(g) = .199572179
pH = 7
balance on NO3-
total molality NO3- = .1
total molality Na+ = .1
total molality UO2++ = 1e-4
free gram Magnetite = 8


suppress ALL
unsuppress  Magnetite
sorbate include
```

LB 4-6-00

4-6-00

U(h) sorption on Magnetite continued



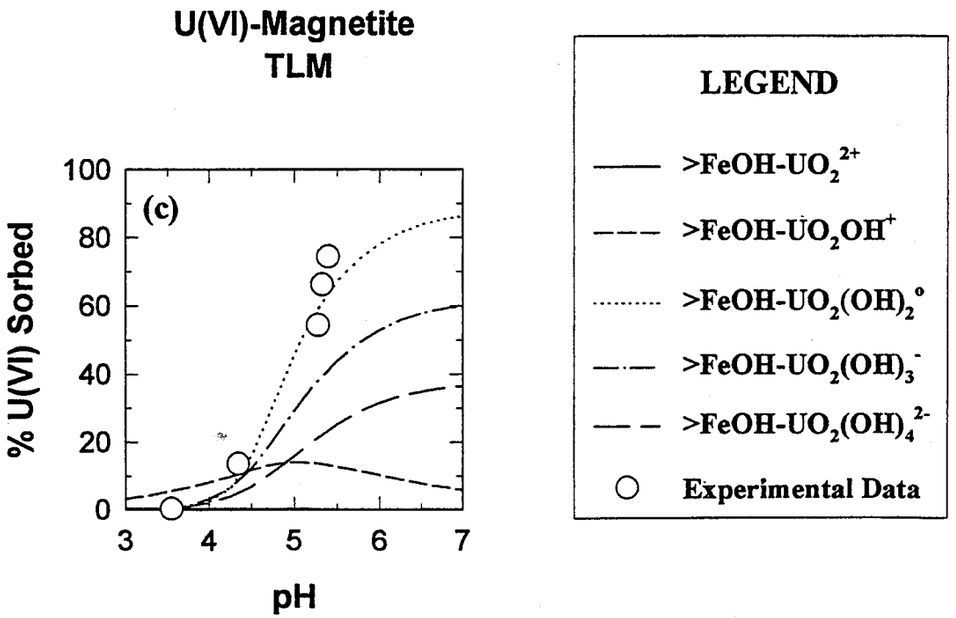


Figure 4-17. U(VI) sorption on magnetite. SCM results are calculated using parameters derived from the experimental data shown in the figure, and assuming a single adsorbed species (see text). (a) DLM; (b) CCM; and (c) TLM results. $U(VI)_T = 1 \times 10^{-4}$ M, 0.1 M NaCl, M/V=8 g/L. Model parameters from Tables 3-1 and B-17. Data from Venkataramani and Gupta (1991).

LBL 4-6-00

I have reviewed this scientific notebook and find it in agreement with QAP-001. There is sufficient information regarding methods used for conducting tests, acquiring and analyzing data so that another qualified individual could repeat the activity.

E.C. Pearcy
5/25/2004

ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK NO. 331

Document Date:	06/01/1999
Availability:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, Texas 78228
Contact:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, TX 78228-5166 Attn.: Director of Administration 210.522.5054
Data Sensitivity:	■"Non-Sensitive" □ Sensitive □"Non-Sensitive - Copyright" □ Sensitive - Copyright
Date Generated:	05/25/2004
Operating System: (including version number)	Windows NT OS
Application Used: (including version number)	Geochemists Workbench, Version 3.0
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	1- CD
File Types: (.exe, .bat, .zip, etc.)	Various
Remarks: (computer runs, etc.)	Media contains: Input/output files for EQ3/6 for referenced software; individual files referenced in the scientific notebook.